Abstract Booklet

of

Conference on Electrochemistry in Industry, Health and Environment – 2023 (EIHE-2023)

> February 7 – 11, 2023 DAE Convention Centre, Bhabha Atomic Research Centre, Mumbai

DAE-BRNS Sponsored Conference Organized by Indian Society for ElctroAnalytical Chemistry Mumbai, India



www.iseac.org.in











Editors:

A. K. Satpati M. K. Dey P. K. Mishra S. Sahoo

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EIHE – 2023

DAE-BRNS

Sponsored International Conference

on

Electrochemistry in Industry, Health and Environment

February 7-11, 2023 DAE Convention Centre, Anushaktinagar, BARC, Mumbai

> Editors A. K. Satpati M. K. Dey P. K. Mishra S. Sahoo

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EIHE 2023

Indian Society for Electro Analytical Chemistry (ISEAC) Welcomes you to the International Conference on Electrochemistry in Industry, Health & Environment - 2023

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डॉ. अजित कुमार मोहान्ती Dr. Ajit Kumar Mohanty भारत सरकार Government of India निदेशक, भाभा परमाणु अनुसंधान केंद्र Director, Bhabha Atomic Research Centre सदस्य, परमाणु ऊर्जा आयोग Member, Atomic Energy Commission



MESSAGE

Electrochemistry is one of the frontier areas of research in chemistry, which has provided microscopic understanding of the mechanism and strategies in solving several recent societal challenges, especially in relation with the energy, environment and health care. Over the years, these subject areas are gradually becoming interdisciplinary in nature with applications in many industrial challenges like, Li-ion battery, redox flow battery, supercapacitors, solar energy harvesting devices, biomedical sensors, electrochemical synthesis, electrochemical deposition of materials and fabrication of devices. Electrochemical techniques have also been utilized in the preparation and characterization of some of the advanced radiopharmaceuticals. I am glad that our Research Centre has the finest state-of-the-art facilities for this kind of frontline research and are actively pursuing this discipline, covering almost all of its dimensions, from laboratory scale studies to the industrial scale applications.

I am delighted to know that the 2nd DAE-BRNS international conference on, "Electrochemistry in Industry, Health and environment (EIHE 2023)" is jointly organized by Analytical Chemistry Division, Chemistry Group, Bhabha Atomic Research Centre, with the Indian Society for Electroanalytical Chemistry (ISEAC) during February 7 to 11, 2023 at DAE Convention Centre, Anushaktinagar, Mumbai. This conference has attracted participation of scientists from all over the world whose interaction with young researchers will pave the way into cutting-edge research in the coming days.

I am sure that the deliberations of the conference will be very exciting and will offer a common platform for the intense scientific discussions and exchange of ideas amongst the budding researchers in this field. It will bring out new ideas and understandings to carry forward quest for collaborative and interdisciplinary research.

I wish EIHE-2023 a grand success.

Ajit Kumar Mohenty

(Dr Ajit Kumar Mohanty)





Date : 02.02.2023



आसा परसाणु अनुसंधान केंद्र कातानत ताठलट प्राप्तताटन ट्रामा

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Government of India Bhabha Atomic Research Centre Chemistry Group Dr. A.K. Tyagi FNASc, FASc, FNAE Distinguished Scientist, DAE & Director, Chemistry Group, BARC



Message

The International conference under the thematic title of "Electrochemistry in Industry, Health and Environment, EIHE-2023" is being organised by Analytical Chemistry Division, Chemistry Group, Bhabha Atomic Research Centre along with Indian Society for Electroanalytical Chemistry (ISEAC) at DAE Convention Centre, Anushaktinagar, Mumbai 400094 during February 7-11, 2023. Under the scope of this conference the expediency of electrochemistry will be discussed in the context of important scientific and technological issues related to the recent societal problems. The topics of the conference includes; Catalytic electrochemistry, Photoelectrochemical water splitting for hydrogen generation using solar energy, Electrochemical instrumentations and devices, Energy storage systems like, Battery and Supercapacitor, Electrochemistry at nanoscale, Electrochemistry in Nuclear Energy/molten salt processes, Electrochemical Sensors and Biosensors for Health, Medical and Environmental Sciences.

I welcome all the invited speakers from India and overseas for accepting our invitation, I am sure that your presence in the conference will encourage the young researchers and students to take up challenging activity in this exciting field. I request all the students to remain attentive during the scientific deliberation and interact with the experts to enhance your scientific horizon in electrochemistry.

As chairman organising committee of **EIHE 2023**, I express my heartiest welcome to all the delegates of **EIHE 2023** once again and my best wishes to all of you in your future endeavours.

AATCAC

(A.K. Tyagi)

Dated : 02.02.2023



होमी भाभा राष्ट्रीय संस्थान

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Prof. P. D. Naik Vice Chancellor (Officiating) & Dean



Message from President, Indian Society for Electroanalytical Chemistry (ISEAC)

Wish you a very happy and productive new year 2023. As the President, Indian Society for Electroanalytical Chemistry (ISEAC), I welcome you to this International Conference "Conference on Electrochemistry in Industry, Health and Environment (EIHE 2023)".

Electrochemistry and its applications aspects are immensely useful in solving various societal problems. ISEAC has broadened the scope of the Society to include activities from all branches of Electrochemical Sciences and Technologies. The main aim of ISEAC is to promote electrochemistry in India, to disseminate scientific and technological knowledge within the country and to strengthen national and international cooperation in the area of Electrochemistry. ISEAC with support from DAE units organises one discussion meeting and one international conference every alternate year to provide a platform for discussion on the recent development in electrochemistry and allied fields.

ISEAC appeal to all electrochemist and allied field researchers to be a part of the ISEAC family. To encourage the researchers to join ISEAC as a member, we have kept a life membership fee nominal, Rs. 4000/- and the student membership fee is Rs. 1000/- (for 5-year validity).

It is encouraging to see a large number of participants registered for this international event, EIHE 2023, which indicates the popularity of the symposium among researchers and the importance and interest in the field. I take this opportunity to thank the authorities of Bhabha Atomic Research Centre for the kind support rendered in the organisation of this event at the beautiful campus of Anushaktinagar and BRNS for sponsoring the conference.

As president of ISEAC, I welcome you all to this international event and wish you all a fruitful interaction and the best for your future research endeavours.

(P. D. Naik)

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Bhabha Atomic Research Centre

Analytical Chemistry Division



Chandra N. Patra Head, Analytical Chemistry Division Tel: 2559 0295 ; Fax: 2550 5151 Email: <u>chandra@barc.gov.in</u>

3-237-S Modular Labs. Trombay, Mumbai 400 085



Greetings and a Happy New Year 2023 from the Organising Committee of EIHE 2023.

Electrochemistry and the allied subjects have provided a break-through in many industrial challenges due to its inherent association with the modern technologies and devices. Research in the field of molten salt electrochemistry, electrochemical metal processing, investigation of corrosion, and nuclear batteries are some of the important projects in recent years on which many scientific institutes including are working on. A number of devices, fabricated using electrochemical principles are at various stages of their operations and functioning.

On behalf of the Organising Committee, it gives me great pleasure in welcoming you all to the DAE-BRNS 2nd International Conference on, "Electrochemistry in Industry, Health and Environment (EIHE 2023)". The conference has been planned for five (5) days to provide ample opportunities to the students and young researchers to present their scientific findings and discuss, along with the international peers. The scope of oral presentations also provides students an excellent enthusiasm to enhance their presentation skills through comments and suggestions. The topic of the conference has been shortlisted considering the recent societal programs in scientific and technological challenges of the Department in Electrochemical Sensors and Biosensors for Health, Medical and Environmental Sciences.

This series of international conferences have been lauded by the national and international scientists as envisaged from the received responses from over 350 participants of eminent scientists and industry partners from India and overseas. The quest for scientific knowledge through the national and international experts is surely going to widen the scope of scientific collaborations.

I sincerely welcome all the invited speakers from India and abroad for accepting our invitation. A number of awards are instituted for the best poster and oral presentation from ACS, RSC, Elsevier and ISEAC, which should encourage the students to deliver the best, during poster and oral presentations.

With great hopes in mid, let's wish the conference a grand success!

Chandra N. Patra





Indian Society for ElectroAnalytical Chemistry (Reg. No. MAH/MUM/1173/2006 GBBSD) Bhabha Atomic Research Centre, Mumbai - 400085





Dr. Ashis Kumar Satpati Secretary, ISEAC and Convener, EIHE-2023 Head, Electrochemical Methods Section, Analytical Chemistry Division Bhabha Atomic Research Centre, Trombay, Mumbai 400085, Phone: 022-25590744 (O) Email: aksatpati@gmail.com

Dear Delegates

Greetings from ISEAC

On behalf of ISEAC and the organising team EIHE 2023, I welcome you all in this international event "Electrochemistry in Industry, Health and Environment, EIHE-2023" at Anushaktinagar, Mumbai. I thank all of you for coming here to attend this conference.

We have tried our best to organise this international event, and thank you for your cooperation and enthusiasm. Since its inception, scope of the society has been broadened to cover the entire spectrum of the scientific activities in the field, this has resulted the increased number of life members from the scientific fraternity across various institutes. I take this forum to request all of you to enhance the activities of the society and promote your colleagues and students to become the life member of this organisation.

In addition to the abstract booklet we are coming out with a Souvenir cum Bulletin of ISEAC during this conference containing articles on different aspects of electrochemical science and technology are being published in this volume, I thank all the authors for their contribution in the bulletin. I encourage all of you to participate in writing short articles for this series of Bulletin.

Being stationed at Bhabha Atomic Research Centre, we enjoy the fame of this institute and excellent logistics support, we thank our authorities for the same. I thank Heavy Water Board (HWB), Atomic Energy Regulatory Board (AERB), Nuclear Power Corporation of India Limited (NPCIL), American Chemical Society (ACS), Royal Chemical Society (RSC), Elsevier, for supporting this event. I sincerely thank all the industrial partners for their support.

From this very conference let us collectively make an effort to take the activities of the society forward and a make our presence at higher level. I wish all of you for excellent outcome from your research, ISEAC will provide all possible platform to promote your research activities. Let us join together and bring the fascinating science in the field of *ELECTROCHEMISTRY* to its fullest potential for the benefit of the society.

On behalf of the team of organising committee EIHE 2023 and the Secretary, ISEAC, I express my sincere appreciations once again to DAE-BRNS, the ISEAC life members, all sponsors and the delegates of EIHE 2023 to make this event possible.

(A K Satpati)

February 02, 2023

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Indian Society for ElectroAnalytical Chemistry

Reg. No. MAH/MUM/1173/2006 GBBSD (Website: www.iseac.org.in; Email: electrochembarc@gmail.com)

Since foundation, the Society has evolved magnificently to represent a truly National Organization and at present, it comprises more than 325 life-members from different parts of India and Overseas. The Executive committee of ISEAC, which manages the activities of ISEAC, is being elected triennially by all the members of ISEAC.

International Events organized by ISEAC:

ISEAC organizes International Conferences, Discussion Meets and Workshop cum Symposium on Electrochemistry and allied topics in association with the Departments of Government of India, International Society of Electrochemistry and other Scientific Organizations and Industries. ISEAC has organized thirteen International Events in India:

1. International Conference on Electrochemistry in Industry Health and Environments (EIHE 2020) at DEA Convention Centre, Anushaktinagar, Mumbai during January 21-25, 2020.

2. Discussion meeting on Spectro electrochemistry (DM-ISEAC-2022) at Multipurpose hall, Training School Hostel, Anushaktinagar, Mumbai 400094 on 16-07-2022

3. International Conference on Electrochemistry in Advanced Materials, Corrosion and Radiopharmaceuticals (CEAMCR-2018) at DEA Convention Centre, Anushaktinagar, Mumbai during February 15-17, 2018.

4. Twelfth ISEAC Discussion Meet in Electrochemistry (12th ISEAC-DM-2016) held at The Acres Club, Chembur, Mumbai during December 7-8, 2016.

5. Eleventh ISEAC International Discussion Meet on Electrochemistry and its Applications (ISEAC-DM-2014) held at Hotel Radisson Blu, Amritsar during February 20-25, 2014.

6. Fifth ISEAC Triennial International Conference on Advances and Recent Trends in Electrochemistry (ELAC-2013) held at Sitara Hotel, Ramoji Film City, Hyderabad during January 16-20, 2013.

7. ISEAC International Symposium cum Workshop on Electrochemistry (ISEAC-WS-2011) at Cidade de Goa, Dona Paula, Goa during December 7-10, 2011.

8. Fourth ISEAC International Discussion Meet on Electrochemistry and its Applications (DM-ISEAC-2011) at Mascot Hotel, Thiruvananthapuram, Kerala during February 7-10, 2011.

9. Fourth International Conference on ElectroAnalytical Chemistry and Allied Topics (ELAC-2013) at Toshali Sands, Puri, Orissa during March 16-18, 2010.

10. Discussion Meet on ElectroAnalytical Techniques and Their Applications (DM-ELANTE-2008) held at Tea County, Munnar, Kerala during February 25-28, 2008.

11. Third International Conference on ElectroAnalytical Chemistry and Allied Topics (ELAC-2007) at Toshali Royal View Resort, Shilon Bagh, Shimla during March 10-15, 2007.

12. Discussion Meet on Role of Electrochemistry in Biosensors, Nanomaterials, Fuel Cells and Ionic Liquids (DM-BNFL-2006) held at Bhabha Atomic Research Centre, Mumbai during September 24-25, 2006.

13. Discussion Meet on Coulometry (DM-COUL-2005) at Bhabha Atomic Research Centre, Mumbai on May 5, 2005.

14. Second International Conference on ElectroAnalytical Chemistry and Allied Topics (ELAC-2004) held at The International Centre, Dona Paula, Goa during January 18-23, 2004.

15. Workshop cum Seminar on ElectroAnalytical Chemistry and Allied Topics (ELAC-2000) held at Bhabha Atomic Research Centre, Mumbai during November 27 – December 1, 2000.

Objectives of ISEAC:

> Promote the growth of Electrochemistry in India.

> Provide a common world-wide platform to the experts, scientists and scholars working in the area of Electrochemistry and its Allied Sciences.

> Disseminate scientific and technological knowledge in the area of Electrochemistry to advance both national and international collaborations.

Share the information on Electrochemistry with other International Societies viz. European Society for Electroanalytical Chemistry (ESEAC), Society for Electroanalytical Chemistry (SEAC) and International Society of Electrochemistry (ISE), Bioelectrochemical Society (BES).

Work in harmony with other Indian Electrochemical Societies viz. Society for the Advancement of Electrochemical Science and Technology (SAEST) based at CECRI, Karaikudi and Electrochemical Society of India (ECSI) based at Indian Institute of Science, Bengaluru.

> Provide incentive by way of awards to researchers for the best thesis, the best paper published in the journal and the best paper presented in National and International Conferences/Symposia.

Encourage young as well as experienced Indian researchers for participation in International Electrochemistry Conferences by providing partial funds, if possible.

Procedure to join ISEAC:

ISEAC has the provision for individual to join as Life-members and for company to join as Corporate Member. The Life-membership fee w.e.f. April 1, 2011 is Rs. 4000/- (Rs. Four thousands only) for Indians

and \notin 300/- (Euro three hundred only) for others. The Fee has to be transferred electronically (NEFT or wire transfer) to ISEAC Bank Account and then you have to sign-up through "Join ISEAC as Life-Member" icon available on www.iseac.org.in with the fund transfer details.

Name of Bank: State Bank of India, BARC Branch, Mumbai-400 085, India Branch code: 1268 Beneficiary name: Indian Society for ElectroAnalytical Chemistry (ISEAC) Account number: 34209997299 BIC (Swift Code): SBININBB508 IFSC code (for within India): SBIN0001268

Please contact us for any further information:

The Secretary, Indian Society for ElectroAnalytical Chemistry (ISEAC) Analytical Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400 085, India Email: <u>electrochembarc@gmail.com</u>; web.: www.iseac.org.in Phone: +91-22-2559 0744 (office hours only); 8369268926 (after office hours)

You are Welcome to Join

ISEAC

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CP-21	Nitrogen-doped porous carbon coated on MnCo ₂ O ₄ nanospheres as electrode materials for high-performance asymmetric supercapacitors <i>S. Silambarasan^a</i> , <i>T. Maiyalagan^a</i>
CP-22	Synthesis of LaW/Ag/GnRbs nanocomposite: Application as transducer material for the simultaneous nano molar detection of synthetic dyes and as anode material for Li ion batteries. Santhosh A S ^a ; Gagan Kumar S K ^b ; Sumana S ^a ; Trishul A M ^b ; Sandeep S ^b ; karthik C S ^b
CP-23	One pot synthesis of FeNi alloy nanoparticles decorated on N-doped Carbon nanosheets for Oxygen Evolution Reaction in Alkaline media <i>K. Ram Kumar^a</i> , <i>T. Maiyalagan^a</i> *
CP-24	Highly Crystalline Ordered Macroporous Metal Organic Framework for Aqueous Aluminum Ion Battery: Effect of Redox Additive Electrolyte in Charge Storage <i>Puja De, Joyanti Halder, Debabrata Mandal, and Amreesh Chandra</i> *
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CP-26	Uranium Electrorefining in Engineering Scale Sourabh Agarwal, A.S Vipin, S. P. Ruhela, D. Sujish, B. Muralidharan,
CP-27	In-situ NADH Regeneration via Lactate Dehydrogenase-Catalyzed Electron Transfer Mechanism: A Spectroelectrochemical Study S. Michelraj ^{1,2} , S. Bagya ³ , Kore Arun Kumar ³ and V. Ganesh ^{1,2,3} ,*
CP-28	Multi-Scale Modeling of Metal Release Pathways of Blood Serum Iron-Transferrin Swarna P. Mantry ¹ and Mahesh Sundararajan ²
СР-29	Electrochemical Analysis of Cobalt Oxide Nanoparticles Synthesized by Hydrothermal Method. <i>R. B. Chrisma, E I Anila</i>
CP-30	Optimization of Praseodymium based Perovskite as Electrocatalyst for Oxygen Reduction Reaction. <i>Bibhuti Bhushan Nayak, Purnendu Parhi*</i>

CP-31	Electrochemical detection and decomposition of nitrate and polyphenolic compounds using reduced graphene oxide supported Ferrite based composite modified electrode <i>S. Sahoo and A. K. Satpati</i>
CP-32	MnMoO ₄ nanorods anchored on P-doped-g-C ₃ N ₄ nanosheets as an electrocatalyst for voltametric determination of antihistamine drug Promethazine <i>Sandeep S^a*, Karthik C S^a, Mallu P^a</i>
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CP-35	Covalently functionalized Graphene Oxide-NiMOF Hybrid as Electrocatalyst for Hydrogen Production Christy Ann Biji*, Jith C J*, Honey John* [#]
CP-36	Magnetic Field Dependent electrocatalytic HER and OER of CoFe ₂ O ₄ Debabrata Mandal ¹ , Lalit Bharti ¹ , Shyamal Shegokar ² , and Amreesh Chandra ^{1,2} *
CP-37	Hydrothermal Synthesized Sm ₂ O ₃ Nanoparticles as a Highly Efficient Photo catalysts for Degradation of Anthraquinonic dyes <i>Lipika Nayak, Purnendu Parhi</i> *
CP-38	Electrical and sensing properties of PANI/ MgO nanocomposites Sharanabasava V. Ganachari
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CP-41	Highly Stabilised Reduced Graphene Oxide/ Indole Composite as Efficient Electrode for High Performance Rechargeable Lithium-Ion Batteries <i>Vijeth Rajshekar Shetty^a</i> * <i>Vidyagayathri M^a</i> , <i>Shamala D^a and Lohit Naik^b</i> *
CP-42	MoS2 Wrapped N-doped Carbon for Sodium and Potassium Ion Batteries Surbhi Priya ¹ , Puja De ² , Debabrata Mandal ³ and Amreesh Chandra ^{1,2} *
CP-43	Repurposing the Graphite Recovered from Spent Lithium-ion Batteries for Second-life Application Shuvajit Ghosh ¹ , Dr. Surendra K. Martha ¹ *

CP-44	Tetrabutylammonium Tetrachloroferrate(III) Complex Derived urchin like Fe ₃ C/Fe Decorated N doped Carbon as promising bifunctional electrocatalysts for ORR, OER and Zn-Air Batteries in alkaline medium <i>Debojit Ghosh, Samarpita Das, Papu Biswas</i> *
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CP-46	Two-dimensional porous carbon nanostructure developed from tea waste for water purification <i>Amrutha Thomas</i> ¹ , <i>Pramod Gopinath</i> ^{1,3} , <i>Honey John</i> ^{1,2}
CP-47	Effect of dysprosium doping on oxygen reduction reaction activity of NiFe ₂ O ₄ Amulya Ratna Panda, Purnendu Parhi*
CP-48	Evalution of Oxygen Reduction Reaction of Transition Metal Doped Rare Earth Metal Oxides Supported on Vulcan Carbon <i>Tusharkanta Hati, Purnendu Parhi</i> *
CP-49	Facile low-temperature synthesis of nanosized highly entropic spinel-type oxide (FeCoNiMnCu) ₃ O ₄ for electrocatalytic application <i>Arpeeta Hota^{1,2}, Prasanna Kumar Panda^{1,2}, Rakesh Kumar Sahoo³, Bankim Chandra Tripathy*¹</i> ,
CP-50	Designing of an Effective Electrocatalyst with Optimized d-Band Center for Water Oxidation Reaction: a Sabatier Principle Approach Ankit Das, ^{#a} Althaf K, ^{#a} Arun Karmakar ^a , and Subrata Kundu *a
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CP-53	RuO ₂ /MoS ₂ heterostructures for supercapacitor applications Manuraj M ^a , Nagaraj P. Shetti*, Tejraj M. Aminabhavi*
CP-54	Functionalized porous covalent organic framework as promising electrode materials for aqueous supercapacitor Sanjay N. Bariya, Saurabh S. Soni*
CP-55	Enhancement of Electrochemical Supercapacitor Performance with Functionalization in Silica based Mesoporous Materials. <i>Yash G. Kapdi, Ashita Sharma, Saurabh S. Soni</i> *

CP-56	Fast electrochromic switching and high optical contrast of poly (2,5-dimethoxy aniline) film on flexible PET substrate and its spectral characterizations <i>B. Santhosh, S.Arun, K. Giribabu and C. Sivakumar</i>
CP-57	Electrodeposition of PEDOT Film on flexible PET and its fast electrochromic properties toward display applications <i>S. Arun, B. Santhosh, K. Giribabu, and C. Sivakumar</i>
CP-58	Hybrid PANI@Fe ₂ O ₃ -MXene Nanocomposite for Supercapacitor Applications Hemalatha K ^a , Apurva Nandagudi ^a , Basavanakote M. Basavaraja ^a *
CP-59	Preparation of GdW/S-GCN composite and its application as electrode material for the sensitive detection of antibiotic in water and food samples. <i>Trishul A M^a</i> , <i>Sandeep S^b*</i> , <i>Karthik C S^b</i> , <i>Manoj Kumar B^a*</i>
CP-60	Cationic surfactant mediated detaction of mefenamic acid at glucose modified carbon paste sensor in urine and pharmaceutical samples <i>Vidya D., Mahesh M. Shanbhag, Nagaraj P. Shetti</i> *
CP-61	Graphene oxide/cholesterol nanohybrids for the voltammetric analysis of cetirizine B. Kishore, Mahesh M. Shanbhag, Nagaraj P. Shetti*
CP-62	2D graphene oxide nano sheets-based sensor for electrochemical detection of carbendazim <i>Ranjan Shetti, Mahesh M. Shanbhag, Nagaraj P. Shetti</i> *
CP-63	Hafnium doped tungsten oxide nanorods for electroanalytical detection of perfluorooctanoic acid (PFOA) Madasu Sreenivasulu, Mahesh M. Shanbhag, Nagaraj P. Shetti*
СР-64	Electrochemical detection of diclofenac in urine and commercial tablets samples using XAD-4 sensor <i>Apoorva M. Pai, Mahesh M. Shanbhag, Nagaraj P. Shetti</i> *
CP-65	Electrochemical biosensor based on PPO enzyme immobilized on Ag doped Cu nanoparticles and PPy nanotubes for the detection of dopamine. <i>Chethana M H^a, Sandeep S^a*, Karthik C S^a, Mallu P^a</i>
CP-66	Novel triple layered hydroxides of Mg-Ag-Al (LTH) Nano-catalyst for Electroanalysis of Promethazine Sahana K M ^a , B. A. Thippeswamy ^a , S. Sandeep ^{a*} , Mounesh ^b , Bhari Mallanna Nagaraja ^b ,*
CP-67	Dibutyl Thiourea: Cathodic or anodic inhibitor? Venkata Muralidhar K, Vinay Jain and Beena Rai
CP-68	Rapid and Label-free Electrochemical-based Sensing of SARS-CoV-2 Spike Proteins <i>T. H. Vignesh Kumar¹</i> , #, Vinoth Krishnan ^{1, 2} , Kannadasan Anand Babu ³ , Sudhakar Natarajan ⁴ , Murugan Veerapandian ^{1, 2} , *

CP-69	Electrodeposition and Electrocatalytic study of Co-P alloy coatings Harshini Sai G. and A. Chitharanjan Hegde*
CP-70	Fresh leachate valorisation through microbial fuel cells (MFCs) for bioelectricity generation Mohammad Shaik Rafi, Gunda Mohanakrishna1*
CP-71	Modeling a flow cell for electrochemical reduction of CO ₂ Vedha Vaishnavi R, Hariharan RK, Himanshu Goyal*
CP-72	Redox regulation of anolyte with pretreated bagasse hydrolysate for sustainable bioelectricity generation <i>Naik P. Sneha, Gunda Mohanakrishna</i> *
СР-73	Development and characterization of composition modulated multilayer (Sn-Ni) alloy coatings for improved corrosion protection <i>Yathish Rai T. and A. Chitharanjan Hegde</i> *
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CP-75	Rapid and direct electrochemical detection of pramipexole using graphitic carbon nitride (gCN) sensor Yogesh M. Shanbhag, Nagaraj P. Shetti*
CP-76	Safety and Electrochemical Performance of Single crystal Lithium-rich Layered oxide Cathode for Li-ion Battery Using for Electric Vehicle Applications <i>M.Jayachandran</i>
CP-77	Augmenting the surface-active sites of Co-Fe LDH by doping of the Fe ²⁺ ions towards effective hydroxide adsorption for the water oxidation reaction: A high-performance OER Electrocatalyst in alkaline medium <i>Aditi De</i> ^{<i>a</i>} , <i>Arun Karmakar</i> ^{<i>a</i>} , <i>and Subrata Kundu</i> ^{*a}
CP-78	Electro-polymerization of synthesised BCN for voltammetric determination of Tryptophan in real samples Shubham Garga, ^b , Abhay Singh ^a , Avanish Singh Parmar ^b *, Rosy ^a *
CP-79	Room temperature synthesis of Bismuth Sillenite (Bi ₃₆ Fe ₂ O ₅₇) for electrochemical oxygen evolution reaction <i>Arushi Arora, Ritika Wadhwa and Menaka Jha</i> *
CP-80	Facile hydrothermal synthesis of NdCoO ₃ @NdO-rGO nanocomposite for energy storage and sensing of an antioxidant drug, alpha lipoic acid <i>Karuna Korgaonkar and J. Seetharamappa</i> *
CP-81	Solar light driven photoelectrocatalytic hydrogen evolution and pollutant degradation by carbon doped Zno nanostructures Jesna Louisa, ^b , M. K. Jayaraj ^c , Honey Johna, ^b

CP-82	TiO ₂ /g-C ₃ N ₄ hybrid photoanodes for PEC water splitting Christeena Sabin ¹ , Nisha T. Padmanabhan ¹ , M.K jayaraj ² , Honey John ^{1,3} *
CP-83	Synthesis and application of a 0D/2D nanocomposite for the nanomolar level detection of an antiandrogen drug <i>S. Santhosh</i> , * ^a <i>K. M. Sahana</i> , ^b <i>S. Sandeep</i> , * ^b <i>P. N. Prashanth Kumar</i> , ^c <i>Norah Salem</i> <i>Alsaiari</i> , ^d <i>Khadijah Mohammedsaleh Katubi</i> , ^d <i>Khamael M. Abualnaja</i> ^e and <i>J. R.</i> <i>Rajabathar</i>
CP-84	Hf-doped tungsten oxide as sensing materials for electrochemical detection of paracetamol and salbutamol <i>Mahesh M. Shanbhag, Nagaraj P. Shetti</i> *
CP-85	Green synthesis of Zn ₂ V ₂ O ₇ nanoparticles using Lawsonia inermis for supercapacitor application <i>Swathi T.P., Nishchith B.S., Ashoka S., Nagaraju G., J. Seetharamappa</i> *
CP-86	Tailoring the structure of NiTiO ₃ with TiO ₂ to enhance its activity for Oxygen Evolution Reaction <i>Ritika Wadhwa^a</i> , <i>Menaka Jha</i> *
CP-87	Sensitive Electrochemical Detection of Folic Acid Using Co ₃ O ₄ Modified Carbon Paste Electrode Aneena Kumar P P, Nygil Thomas
CP-88	An Efficient Electrochemical Sensor for Nitrite Based on a Mesoporous Nickel Cobaltite-Reduced Graphene Oxide (NiCo-RGO) Nanocomposite Shridevi Salagare ^a *, Prashanth S. Adarakatti ^b , Venkataramanappa Yarradoddappaa
CP-89	Novel Mn-Ni Based Selenide Heterostructure for High-Performance All-Solid-State Hybrid Supercapacitors Siddhant Srivastav ¹ and Sumanta Kumar Meher* ¹
CP-90	Fabrication of $Bi_2O_3 RuCo_2O_4$ for Flexible supercapatteries Nivedha $K^{a,b}$ and B.subramanian ^{a,b}
CP-91	Ni and Mo-Based Chalcogenide Heterostructure as Highly Efficient Electrocatalyst for Oxygen Evolution Reaction Neeraj Lamba ¹ and Sumanta Kumar Meher ^{*1}
CP-92	Bismuth oxide nanoflowers decorate with polyaniline nanowire arrays Bi ₂ O ₃ -PANI core–shell electrodes for energy storage device ^a Pritamkumar V. Shinde, ^a Dimple P. Dutta
CP-93	Interaction of catalase enzyme with Tetraalkyl ammonium cations at electrified liquid- liquid interface Sanjeev Kumar ^{1,2} , A. Esokkiya ^{1,2} , S. Sudalaimani ^{1,2} , K. Giribabu ^{1,2} ,*.

CP-94	Methodical designing of Pt _{3-x} Co _{0.5+y} Ni _{0.5+y} /C (x=0, 1, 2; y=0, 0.5, 1) particles using a single-step solid state chemistry method as efficient cathode catalyst in H ₂ -O ₂ fuel cells <i>Prateekshita Mukherjee</i> ^{<i>a</i>} , <i>Indrajit Patil</i> ^{<i>a</i>} , <i>Bhalchandra Kakade</i> ^{<i>a</i>} , <i>Sumanta Kumar Das^b</i> , <i>Akhila Kumar Sahu^b and Anita Swami^a</i>
CP-95	Optical sensing of acrylamide based on the fluorescence quenching of rhodamine B <i>Esokkiya^{a,b}</i> , <i>S. Sanjee vkumar^{a,b}</i> , <i>S. Sudalaimani^{a,b}</i> , <i>K. Giribabu^{a,b}*</i>
CP-96	Artificial Interphase Formation on Nickel-Rich Layered Oxides to Facilitate High Voltage Cycling of Lithium-ion Batteries Jyotirekha Dutta, Dr. Surendra Kumar Martha
CP-97	Enhanced electrochemical properties in partially Vanadium substituted NVPF cathode material in sodium ion batteries <i>S. Mahato^a</i> , *, <i>S. Das^b</i> , <i>K. Biswas^a</i> , <i>D. Gupta^c</i>
CP-98	Proton Exchange Membrane Fuel Cell (PEMFC) Electrocatalyst Adarsh Ajith Naik, Khantesh Agrawal, and Venugopal Santhanam
СР-99	Microwave Assisted Recycling of Spent Li-ion battery electrode material into Efficient Oxygen Evolution Reaction Catalyst <i>Ajinkya Kotkar¹</i> , Souvagya Dash ² , Piyali Bhanja ² , Satyaswini Sahu ² , Anil Verma ¹ , Ayan Mukherjee ^{2*} , Mamata Mohapatra ^{2,3*} , Suddhasatwa Basu ^{1,2*}
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CP-101	Rationalizing the Effect of Cobalt and Nickel substitution in Layered manganese Oxide towards Oxygen Reduction Reaction Rajesh Kumar Behera, Alaka Priyadarsini Sahoo, Swarna Prava Mantry, Kumar S. K. Varadwaj*
CP-102	Pulse Electrodeposited Copper on Copper for Electrochemical Reduction of CO ₂ to Hydrocarbon <i>Abinaya Stalinraja, Keerthiga Gopalaram</i> *
CP-103	Self-enhanced solid state ECL sensing platform of SiO ₂ PEI NPs and its application in detection of spermine <i>M. Sornambigai, A. Roselin Pavithra, K. Giribabu, and S. Senthil Kumar*</i>
CP-104	Development of Battery-Supercapacitor hybrid device using LiMn _{1.5} Ni _{0.5} O ₄ -high surface area carbon composite as cathode and carbon coated Li ₄ Ti ₅ O ₁₂ as anode <i>Subhajit Bhowmik¹</i> , <i>Sourav Ghosh¹</i> , <i>Udita Bhattacharjee¹</i> , <i>Surendra Kumar Martha^{1*}</i>
CP-105	Fe Doped NiCo ₂ Se ₄ Nanorod Array: Efficient Electrocatalyst for Overall Electrochemical Water-Splitting <i>Divya Rathore, and Surojit Pande</i> *

CP-106	Development and Feasibility of High-Performance Sodium ion Battery through Doping and Surface coating onto electrochemical active material <i>Rupan Das Chakraborty, Shuvajit Ghosh, Surendra kumar Martha</i> *
CP-107	Optical Immunosensor for the detection of clinical biomarker related to renal disease <i>Divya, Pranjal Chandra</i>
CP-108	Development of a Chemo-Nano Sensor Surface for Ultra-sensitive Detection of Lead in Surface Water Supratim Mahapatra and Pranjal Chandra*
CP-109	Electrochemical analysis of theophylline at cholesterol modified graphene oxide sensor <i>Prakashagouda L. Timmanagoudar¹</i> , <i>Mahesh M. Shanbhag²</i> , <i>Nagaraj P. Shetti²</i>
CP-110	Utility Scale Battery Energy Storage System–Techno-economic Perspective Biswajit Shown, Soumi Chatterjee
CP-111	Ni Nanoparticle Decoration on PANI (Ni@PANI) for Enhanced Ammonia and water Oxidation Reactions. <i>Pratiksha D. Tanwadea, Bhaskar R. Sathea</i> *
CP-112	Polymer sensing system over laser-induced graphene for creatinine detection Mrunali D Wagh, Subhendu Kumar Sahoo, Sanket Goel
CP-113	Enhanced Photoelectrochemical Water Oxidation Behavior of Mo-doped BiVO ₄ semiconductor <i>Paramita Hajra^a</i> , <i>Chinmoy Bhattacharya^b*</i>
CP-114	Outstanding performance of commercial-level mass-loading 2D WS ₂ for symmetric supercapacitors <i>Visakh V Mohan¹</i> , and R. B. Rakhi ²
CP-115	Highly Sensitive Electrochemical Detection of Biomolecules Nygil Thomas ¹ , Tony Thomas ² , Jasmine Thomas ³
CP-116	Optimization of Zn-Modified Bismuth Molybdate Semiconductor for Highly Efficient Photoelectrochemical Water Splitting Swarnendu Baduri ¹ , Surojit Pande ² , Chinmoy Bhattacharya* ¹
CP-117	Investigations on Ni based Alloys for Hydrogen Evolution Reaction in Alkaline Media Archana. P. Gaikwad*, Atindra Mohan Banerjee, M. R. Pai, A. K. Tripathi
CP-118	An Unsteady-state, One-dimensional Model for Predicting the Performance of Lithium-ion Batteries Sanjib D. Sharma, Biswajit Shown
CP-119	Facets-Directed Epitaxially Grown Lead Halide Perovskite-Sulfobromide Nanocrystals Heterostructures and Their Improved Photocatalytic Activity Sanjib Shyamal, Narayan Pradhan*

CP-120	Morphology Driven Activity of Layered Manganese Oxide towards Oxygen Reduction Reaction <i>Alaka Priyadarsini Sahoo¹</i> , <i>Rajesh Kumar Behera¹</i> , <i>Swarna Prava Mantry²</i> , <i>Kumar S</i> .
	K. Varadwaj ¹
CP-121	Performance of polymer electrolyte membrane water electrolysis using dendrimer protected platinum catalyst <i>Balamurugan Devadas, *, Martin Prokop, Karel Bouzek</i>
CP-122	Electrodeposited Molarity Dependent Bismuth Oxide Binder Free Flexible Electrode and ASSD (Bi ₂ CuO ₄ //AC) Supercapacitor Device <i>R.C. Ambare</i> ^{<i>a</i>*} , <i>R.G. Bobade</i> ^{<i>a</i>} , <i>B. J. Lokhande</i> ^{<i>b</i>*}
CP-123	Sensing of caffeine in real samples using Cu-MOF derived CuO nanoparticle decorated amorphous carbon as an electrochemical platform <i>Veeramuthu Saravanakumar</i> ^{<i>a,b</i>*} , <i>Venkatachalam Rajagopal</i> ^{<i>a,b</i>} , <i>Vembu</i> <i>Suryanarayanan</i> ^{<i>a,b</i>**} and Sambandam Anandan ^{<i>c</i>} ,
CP-124	One pot synthesis and characterization of binary and ternary metal organic frameworks (MOFs) as tri-modal catalysts for thiophene electrooxidation, water splitting and 4- nitrophenol reduction Mahendran Manivannan [*] , ^{a,b} Venkatachalam Rajagopal, ^{a,b,d} , Lalithambigai Krishnamoorthy, ^c Dhanasurya Selvame, Vembu Suryanarayanan ^{**} , ^{a,b} *, Thasan Raju, ^{a,b}
CP-125	Effect of Ni Doping on the Oxygen Evolution Reaction Performance of Co ₃ O ₄ Ashalatha Vazhayi ^l , Nygil Thomas ¹ *
CP-126	Metal oxide and Chalcogenides incorporated Graphene Sponge for enhanced water splitting <i>S. Manna and, A. K. Satpati</i>
CP-127	Electro oxidation of methylorange on the surface of poly(ribo-flavin) by using carbon paste electrode <i>Boppana R Krithi¹, Nikhil J Lakkad¹, Asha M¹, G J Manjunath², Sandeep S¹.</i>
CP-128	Investigation of Carbon Quantum Dots as an Aqueous Electrolyte for Energy Storage Devices Satendra Kumar, * N. Sathish, and Surender Kumar
CP-129	Effect of Morphology Variations in CuS electrode material for Na-ion capacitor <i>Manoj Goswami</i> , ^a * <i>N. Sathish</i> , ^a and Surender Kumar ^a ,
CP-130	Synthesis and characterization of Si:MoSe ₂ nanostructures for hydrogen Evolution reaction G Gautham kumar ¹ , Mathew K Francis ¹ , Nafis Ahmed ¹ and P Balaji Bhargav ¹
CP-131	One-Step Electrodeposited Cobalt Doped Bismuth Nanoparticles on Flexible Copper Substrate: Influence of Bismuth and Cobalt ratio variation for ASSD Device <i>R.G. Bobade</i> ^{<i>a</i>} , <i>V.B. Suryawanshi</i> ^{<i>a</i>} , <i>R.C. Ambare</i> ^{<i>a</i>*} , <i>B. J. Lokhande</i> ^{<i>b</i>*}

CP-132	A hybrid machine learning model for prediction of cobalt metal-organic framework- based ZIF-67 as corrosion inhibitor for X65 pipeline steel in CO ₂ -saturated brine <i>Valentine Chikaodili Anadebe</i> ^{*a} and Rakesh Chandra Barik ^a
CP-133	Alternative approach for highly sensitive and free-interference electrochemical dopamine sensing <i>A.G. Kamaha Tchekep^{1, 2}, V. Suryanarayanan^{2, 3}, Deepak K. Pattanayak^{1, 2*}</i>
CP-134	Design and development of electrodeposited Pd-thin film electrodes for acetaminophen detection <i>K. Ranjithkumar^{1,2}, S. Narmatha^{1,2}, R. Sekar³, P. Sathiya⁴, R. Thangamuthu^{1,2}, S M. Senthil Kumar^{1,2}</i>
CP-135	Co ₃ O ₄ -CuO Supported AgNPs Nanocomposite as a Potential Material for Supercapacitor Application Samarjeet S. Patil, Suresh S. Shendage, Jagdish C. Bhangoji, Ashok G. Awale
CP-136	Layered Porous Graphitic Carbon Nitride Stabilized Effective Inverse Spinels, Spinels and Perovskites as Bifunctional Electrocatalyst <i>S. Sathiya Bama and T. Selvaraju</i> *
CP-137	Meniscus-confined electrochemical additive manufacturing (MC-ECAM) technique for metallic nanostructures <i>Hafsa Siddiqui</i> ^{<i>a</i>} *, <i>N. Sathish</i> ^{<i>a</i>} , <i>and Surender Kumar</i> ^{<i>a</i>} ,
CP-138	Aqueous Alkaline hybrid Zinc/TEMPO Flow Battery: A High Voltage Green Energy Storage Device Swapnil Deshmukh, M. Ulaganathan, M. Kathiresan, P. Ragupathy,
CP-139	Binder free Aluminium doped MoS ₂ @CC electrode for supercapacitor Mathew K Francis ¹ , P. Balaji Bhargav ^{*1} , Balaji C ¹
CP-140	Electrochemically Generated Cu(I) Catalyzed Click Chemistry: Triazole Synthesis and Insights into their Photophysical Properties <i>M. Krishnan,</i> * <i>M. Kathiresan and C. Praveen</i>
CP-141	Cerium-based metal organic framework as corrosion inhibitor for Cu alloy in chloride environment Mahalakshmi Durai * ^a , Sabari Elango ^a , Chandra Sekar ^b , Valentine Chikaodili Anadebe ^b Rakesh Chandra Barik ^b
CP-142	The effect of Benzotriazole, 8-Hydroxyqunoline and €-2-(2,3,4 trihydroxybenzylidene)hydrazinecarbothioamide on the corrosion of AA 7075 in 3.5 % NaCl environment <i>B G Prakashaiah, R C Saxena, T Senthilkumar, Sudip K Ganguly</i>

CP-143	Co- doped Cubic NiO Nanoflakes: Facile, one-step synthesis, effective doping and
	excellent supercapacitor performance Shyamli Ashok C Ashalatha Vazhavil Jasmine Thomas Nyoil Thomas*
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CP-144	Development of selective and sensitive electrochemical sensor for the determination of
	antihistamine drug
	D. A. Imppeswamy , S. Sanaeep , , Mounesh , Dhari Mananna Nagaraja , .
CP-145	Fluorine-free synthesis of Tantalum carbide: Enhanced HER activity and Nitro
	compound reduction 4 Vijavaprabhakaran a, b* and M Kathirasana b
	A. rijuyuprubnukurun, unu m. Kumresunu,
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CP-147	Enhanced Energy Storage by Ternary Composite of Metalloid Induced Porous
	Polyacrylonitrile / polyvinylpyrrolidone Carbon Nanofiber, NiCo-MOF and Conducting polymer for Free-standing Symmetric Supercapacitor
	Karingula Sampath, Shekher Kummari, B. Thirupathi, K. Vengatajalabathy Gobi*
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	Bindhu S ^a , Nagashree S ^{*b} , Sandeep S ^b , Karthik C S ^b ,
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CP-149	Facile Synthesis of Pd(@Ag-Zn-rGO Nanocomposite and it's Selective Electro- Catalytic Application in Ethanol Oxidation
	Nagesh D. Pawar, Jagdish C. Bhangoji, Suresh S. Shendage*
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	Pradakshina Sharma, Mohd. Rahil Hasan and Jagriti Narang*
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	Mohd. Rahil Hasan, Pradakshina Sharma, Chhaya Rawat, Saumitra Singh, and Jagriti
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	Sravani Potham, and Kothandaraman Ramanujam*

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CP-163	Arsenic remediation from contaminated drinking water via sacrificial metal-based reactor column <i>Athira Prakash, E. Praveenraj and Dr. R. Malini</i> *
CP-164	One pot fabrication of CuO-CuFe ₂ O ₄ @rGO nanostructure for electrochemical sensing application of paracetamol <i>Jagdish C. Bhangoji* Suresh S. Shendage</i>
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CP-190	Development of g-C ₃ N ₄ modified electrode for the determination of aclonifen and its environmental application Hrishikesh S. Kolli ¹ , Mahesh M. Shanbhag ² , Raviraj M. Kulkarni ³ , Nagaraj P. Shetti ² *
CP-191	Environmental analysis of fungicide carbendazim using TiO ₂ nanoparticle modified carbon paste electrode J Mohan ¹ , Mahesh M. Shanbhag ² , Raviraj M. Kulkarni ³ , Nagaraj P. Shetti ² *
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CP-199	Nickel-Ferrous Derived Spherical Nanoalloy as an Efficient and Stable Electrocatalyst for Urea Oxidation Reactions Somnath C. Dhawale, ¹ Ajay V. Munde ^{1,2} and Bhaskar R. Sathe ¹ *
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CP-210	Defect engineering of BaSnO ₃ photoanodes for efficient photoelectrochemical water splitting Soniya Gahlawat, Ibbi Y. Ahmet, * Patrick Schnell, Igal Levine, Siyuan Zhang, Pravin. P. Ingole, * Fatwa F. Abdi*
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CP-213	Electrochemical and Spectroscopic Investigation of HER2-Targeting Peptide Amit Kumar Sharma ^{1,8} , Preeti Dwivedi ^{3,8} , Sudipa Manna ² , Suresh S. Shendage ³ , Drishty Satpati ¹ and Ashis Kumar Satpati ²
CP-214	rGO, CNT and Carbon nano sphere inclusion PEDOT for the Sensitive Determination of Dopamine and Uric Acid and ascorbic acid <i>Preeti Dwivedi</i> ² Sudipa Manna ¹ , Srikant Sahoo ¹ , P.K.Mishra ¹ , Suresh S Shendage ² and A.K. Satpati [*] , ¹
CP-215	Electrical Characterization of Doped/Co-doped LaScO ₃ S. Phapale ¹ , Akshada Gawade [#] , D. Tyagi ¹ , A.N. Shirsat ¹ , S. Varma ¹
CP-216	Electrochemical degradation of Poly-methylmethacrylate (PMMA) microplastic by photochemical route <u>Pankaj Kumar¹</u> , Manisha Meena ¹ , S Manna ² , A. K Satpati ² Raghava Varma ²

Abstract Presented as Plenary, Invited and Short Lectures

IT-01-EIHE 2023



Modified electrodes with electroactive redox polymers and nanomaterials for sensor and biosensor platforms



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Abstract:

Electroactive redox polymer films with nanomaterial films have been used for constructing novel modified electrodes. Inclusion of nanomaterials such as of carbon, metal or metal oxide nanoparticles, can promote synergistic effects [1]. Deep eutectic solvents (DES), greener alternatives to ionic liquids and to non-aqueous solvents, can be the medium for improved polymer film formation. DES are made by direct mixing of the usually solid components, occurring strong hydrogen bond interactions between a hydrogen bond acceptor, such as choline chloride, and a hydrogen bond donor such as ethylene glycol, in this case the resulting DES being designated as ethaline [2].

Nanostructured phenazine and triarylmethane redox conducting polymer films have been obtained by electropolymerisation, mainly in acid-doped ethaline e.g. [3] or in ternary DES [4]. Polymers include poly(methylene blue), poly(neutral red), poly(brilliant cresyl blue), poly(thionine) and poly(brilliant green). Sensor and biosensor platforms to be described include carbon nanotubes or nanoparticles of gold, iron oxide or copper oxide e.g. [5,6]. The enhanced performance of sensors for analytes such as ascorbate and acetaminophen and of enzyme biosensors, are superior to those of the same architectures containing polymer films formed in aqueous solution, and their application to commercial samples will be shown.

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Electrochemical reaction mechanism identification from potentiodynamic polarization data



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Abstract:

With the advent of clean-energy based vehicles, interest in hydrogen economy, and batteries, has picked up recently. Electrochemical energy storage plays a key role in this emerging field, and a variety of electrochemical techniques are used to characterize the relevant electrochemical reactions. While electrochemical impedance spectroscopy can be used to identify the reactions, the analyses tend to be very complex¹. In this talk, we demonstrate the application of reaction mechanism analysis to obtain useful information on the physico-chemical processes from polarization data². The method is illustrated using



polarization studies of hydrogen evolution reaction (HER) on noble metals such as Pt and Au. The results show that diffusion is rate limiting for HER in acidic solutions, whereas in alkaline solutions, the reaction is independent of alkali concentration. Detailed analysis and interpretation of the polarization data and modelling results are described. This methodology can be extended to identify the mechanism of HER on other catalysts, as well as to characterize other electrochemical reactions.

Fig. 1. Potentiodynamic polarization data of hydrogen evolution reaction on Pt in acidic medium, at a few electrode-

rotational speeds.

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Solid State Chemistry Approach Towards Green Hydrogen



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Abstract:

The design and development of catalyst systems for electrochemical reactions is vital for engineering the next-generation energy conversion and storage devices such as fuel cell, electrolyzer and battery. The recent literature is abundant with earth-abundant electrocatalysts that have shown the ability to replace the noble metal benchmark systems for reactions such as water splitting for green hydrogen generation, carbon dioxide reduction to value added fuels and nitrogen reduction to ammonia. A successful architecture of these multi-metallic electrocatalysts relies on the overall electronic structure, optimization of the active centers, elemental ratio, heterogeneous localization of the elements, coordination environment, shape and size of the nanostructures, and the atomic scale defects. Therefore, an effective catalyst design needs a substantial all-round knowledge of chemistry, especially the branches of basic inorganic chemistry, solid state chemistry and electrochemistry. This lecture will highlight a part of our efforts in making the electrocatalysts for water oxidation and reduction, towards the production of green hydrogen. A particular emphasis will be on the multi-metallic alloy nanostructures where the impact of electronic structure on the overall catalytic activity will be demonstrated. The methods to implement them at the industrial scale will be also discussed.

IT-04-EIHE 2023



Electrochemically Shape-controlled and Confined Micro and Nanostructured Materials for Methanol Electrooxidation



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Abstract:

Tailoring of surface structure of electrocatalyst is an effective way of improving the catalyst's activity and stability for a specific reaction process. A simple, cost-effective and scalable approach is essential to synthesize shape- and morphology controlled micro- and nanostructured materials for practical applications especially for commercialization of fuel cells. We have developed electrochemical surface

engineered approach for the rational design of efficient catalysts (i.e., a paradigm shift from precious like AgPd^{1,} Au-WO₃² to non-precious materials³ like brass, graphene-Cu-Cu₂O, graphene-CuNi based electrocatalytic systems) for methanol electrooxidation reaction. The role of structuredirecting, morphology-controlling agent and synthesis approaches like ultrasonic wave-assisted electrodeposition, pulse electrodeposition and anodization process will be highlighted to



understand electrochemical control of the shape of materials and confined directly on substrates with various structures and dimensions. Further, to mitigate sluggish reaction kinetics, high overpotential, and poisoning issues of methanol electrooxidation reaction, we have made structural optimization and performance of the constructed catalysts to enhance the reaction process.

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IT-05-EIHE 2023



In-Situ Activation of Pencil Graphite Electrode Surface and Its Active Site Mapping Using Scanning Electrochemical Microscopy and Electrocatalysis



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Abstract:

Using a low-cost carbon material like pencil graphite (PGE) as an electrode is a continued research interest in electrochemistry. Indeed, activation of the electrode is an essential factor for the extension to electrochemistry application. There are few chemical and electrochemical activation procedures wherein the conversion of graphitic structure to Carbon-Oxygen type functional group have been reported. Beside, the details of the electronic conductivity and surface structure details are known. In this work, we would like to investigate the electronic and surface properties of electrochemically activated PGE (PGE*, *=activated) using scanning electrochemical microscope (SECM) and electrocatalytic oxidation of dopamine as tools. An ultralow-cost micro-tip pencil graphite has been used as a test system. Activation of PGE was performed by electrochemical preanodization procedure. Initial experiments with Fe(CN)₆³⁻ redox probe showed a marked reduction in the peak-to-peak potential ($\Delta E_p = E_{pa}$ - E_{pc} , wherein E_{pa} and E_{pc} are anodic and cathodic peak potentials) of PGE* over the PGE. Chronocoloumetric experiments were performed to calculate the surface charge on the modified electrode. Electrocatalytic oxidation of dopamine has been found to be effective on PGE*. As an independent system, using the PGE*, sensitive and selective electrochemical sesing of dopamine has been demonstrated. In the end part of this work, SECM (specially designed cell) and AFM techniques have been adopted to reveal the intricking surface feature of the PGE*



Figure 1. (A) Schematic representation of SECM operation under feedback mode at $E_{sub}=0.3V$ vs Ag/AgCl, $E_{tip}=0.5V$ vs Ag/AgCl. (B) SECM and (C) AFM images of (B) PGE*.

IT-06-EIHE 2023



Nanoparticles functionalized theranostic liposome for antibiotic resistant bacteria and electrochemical sensing



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Abstract:

Nanoparticle functionalized liposomes are attracting high interest in bioimaging, drug delivary and biosening. However, theranostic applications of metal functionalized liposomes are not applied for bacterial sensing and treatment. Here α -Fe₂O₃-Au –streptavidine nanoparticles (STV-Mag) loaded cationic carbomate cholesterol is used as a carrier to release antibacterial thymol drug for Staphylococcus aureus (S. aureus) infected Caenorhabditis elegans (C. elegans). The thymol drug release and selective sensing of



S. areus in in-vitro was studied using cyclic voltammetry and square wave voltmmerty. Since S.areus growth requires high concentration of biotin, label free streptavidin-biotin electrochemical sensing was made using α -Fe₂O₃-Au –streptavidine – biotine sensing was made. The biotin sensing showed linear range from 10⁻¹⁵ to 10⁻³ M, which was not obtained by conventional methods, Selective release of thymol drug from STV-Mag-carbomate cholesterol (STV-

is confirmed electrochemically using other pathogens, E. coli, Proteus and Enterococcus bacterium through antimicrobial studies along with S. aureus.

Figure: Effects of thymol drug delivery on CV behaviour in presence different bacteria and C. elegans with S. auerus infection for 24 h

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Electrochemical Neutralization: Concepts to Devices



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Abstract:

Electrochemical energy storage and conversion devices such as H_2-O_2 fuel cells, supercapacitors, and batteries are propelled by their potentiality to construct zero emission energy technologies. Although H_2-O_2 or proton exchange membrane fuel cell (PEMFC) technology is a promising zero emission technology, issues with safety, storage, and transport of molecular hydrogen impede its realization. Alcohols as liquid H_2 carriers could be enablers, but state-of-the-art alcohol reforming is difficult, requiring high temperatures >200 °C and pressures >25 bar, and the resulting H_2 is carbonized beyond tolerance levels for direct use in fuel cells. We show that the modification of the cathodic interface of direct alcohol fuel cells with a pH dependent redox couple can introduce additional functionality to a fuel cell wherein electricity generation is accompanied by hydrogen fuel production at room temperature and pressure which eventually lead to the development of an alcohol reforming fuel cell (ARFC).Thermodynamics of ARFC suggest it is propelled by energy of neutralization and attempts to harvest the free energy of neutralization directly as electrical driving force without a net redox lead to the development of an electrochemical neutralization cell. Direct harvesting of neutralization energy without a net redox allowed the spontaneous desalination of saline water without contaminating the desalination pathway with an efficiency close to the state-of-the-art RO processes.

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And A transformer

Sensors for *in vivo* biochemical monitoring: A Membranes and materials adaptation



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Abstract

Changes in metabolite intermediates and oxygen can be quite rapid where the patient is metabolically stressed, eg in diabetes, shock and hypoxia¹. We have developed a range of enzyme based electrochemical sensors for subcutaneous tissue designed for continuous monitoring. *In vivo* use imposes a severe test on biosensor chemistry due mainly to issues of sterilisation, linearisation and stabilisation, the latter in the face of host tissue reactions. We designed miniature, semi-implantable, first generation devices protected by permselective membrane barriers to aid biocompatibility and allow intervention-free tissue operation. Tissue as an independent body compartment showed dynamic changes that did not reflect changes in blood. For glucose responses are found to show a lag, for lactate there is a highly blunted response², and oxygen showed intrinsic fluctuations³ that were likely to reflect blood flow variation due to changes in local capillary/arteriolar beds. Additional monitoring of lactate in sweat showed a lack of consistent exercise related variation whilst salivary lactate was able to track blood lactate during exercise. The possibility of biocompatibility improvement was explore recently using thermally addressable N-isopropylacrylamide/N-vinyl pyrrolidone copolymer, and the potential for degradable sensor design through use of protein only fabrication.

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IT-09-EIHE 2023



Investigative Research on the Critical Electrochemical Corrosion Driven by Combined Cathodic and Anodic Interference on a Pipeline



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Abstract:

Petroleum Pipeline Integrity is now a major focus. The reason for this renewed interest may be attributed to a couple of factors, which include new legislation, technical advancements, strict penalties for accidental leakages, environmental concerns and ageing of pipelines. Electrochemical corrosion driven by Interference can impact the ability to protect a pipeline from corrosion. Common sources are cathodic protection on other lines and DC transit systems. This paper describes outcomes of brain storming session, why-how analysis on the critical parameters impacting pipelines in common corridor and subjected to combined Cathodic and Anodic Interferences which is rare and critical. This work provides an overview and brief discussion on critical analysis and clear interpretation based on field study trials to monitor the pipe to soil potential over an extended time period. In this paper, exhaustive analysis of data has been discussed with reference to the critical Combined Cathodic and Anodic Interference phenomena observed on pipelines. The analyzed phenomena are representing the over potential along the foreign pipe under interference when it is at a distance of 3.5 m from the ground-bed. Current enters the pipe close to the ground bed with negative current density and locally protects the pipe. At distant areas, this gathered current leaks away, with corrosion danger as a logic consequence. The research work has given an indepth insight to the industry for the interference phenomena driven electrochemical corrosion and its impact.

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Theranostic Applications of Carbon Nanomaterial Modified Sensors: A Promising Future



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Abstract:

The last few years have witnessed a substantial technological renaissance that boosted the development of nanomaterials which have a great impact on biosensing. The unprecedented properties of carbon nanotubes, fullerenes and graphene have catapulted carbon materials in the hotspot of biomedical research. Of particular interest is the integration of these materials into analytical systems that impact key research areas, in particular: medical diagnostics, multi-modal drug delivery, bio-imaging, environmental monitoring and biocatalytic sensing. The interface of electrochemistry and nanotechnology is a captivating playground for the elemental research and has eventually emerged as a futuristic and sustainable platform. Efforts have been made in our group to develop new-fangled approaches for the electrochemical detection of non-steroidal anti-inflammatory drug; antihypertensive agent, antiviral drug and natural alkaloid related to hepatocellular carcinoma. The proposed nanomaterial-based sensors exhibited pronounced analytical performance and provided a new and powerful paradigm in terms of novel and augmented functionality that encompasses a wide variety of applications in clinical diagnostics and biological research. The developed electrochemical sensors had great potential for enhancing and superseding the capabilities of current molecular diagnostics by allowing rapid and highly accurate diagnoses, the integration of diagnostic and the realization of personalized medicine.

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IT-11-EIHE 2023



Pseudo-2D Nanostructure based High Performance Hybrid Supercapacitors: Correlating Theoretical and Experimental Studies



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Abstract:

Supercapacitors have been extensively investigated for decades as a promising high-power energy storage system with longer cycle life. However, the practical performance of the supercapacitor depends on the choice of the electrode materials [1-3]. Recently, high-performance supercapacitors based on hollow nanostructures are being reported. The enhanced behaviour is directly attributed to the higher specific surface area of hollow particles. This is an oversimplified assumption. If only the surface area was driving the enhancement then other solid morphologies, with higher specific area, should show better performance. Careful modelling and simulation studies by LAMMPS software show that hollow structures can actually be viewed as pseudo 2-dimensional (2-D) materials. This leads to performance similar to that reported in 2-dimensional materials ranging from metal oxides to MXenes. Further, the theoretically predicted behaviour is proven experimentally by fabricating hollow and solid nanostructure-based Li-, Al-, Na- and K-ion supercapacitors. The hollow nanostructures-based electrodes exhibit ~50-80 % increment in the specific capacitance, along with greater energy density, higher rate capabilities and excellent cycling stability. Their use in e-cycle and other areas are also shown.

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IT-12-EIHE 2023

Bioelectrochemical Sensing of Biomolecules Oxidative Damage



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Abstract:

Electrochemical methods can provide insight into the redox mechanisms and the electron-transfer reactions of a variety of fundamental biological processes. Oxidative damage to peptides, proteins, and DNA is considered to be one of the major causes of cancer- and age-related diseases. The interaction of biomolecules, nucleic acids, peptides, proteins and pharmaceuticals, with solid electrode surfaces is not only a fundamental phenomenon but is also a key to important and novel analytical sensing applications in biosensors, biotechnology, medical devices and drug-delivery schemes.

Peptides and proteins are essential components of organisms and are involved in a wide range of biological functions. The direct electrochemical oxidation behaviour of proteins without prosthetic groups on a solid electrode surface is complex, due to the protein three-dimensional morphological structure. Electrochemical studies in qualitative and quantitative analysis of proteins, not containing a centre with fast-reversible redox reactions, are still very few.

DNA nanostructures provide a methodology for nanoscale electrode construction of patterned structures that self-assemble into periodic and aperiodic lattices and have been characterised by atomic force microscopy. Detection of *in vitro* oxidative damage to DNA can be very useful for screening and evaluating the effect caused to DNA by carcinogens and oxidising substances, for which voltammetric methods are a miniaturisable, inexpensive and faster detection procedure, with very low detection limits.

Many compounds bind and interact with DNA causing changes in the structure of DNA and in the base sequence, leading to perturbations in DNA replication. The need for the analysis of gene sequences, the detection of oxidative damage to DNA, and the understanding of DNA interactions with molecules or ions led to the development of DNA-nanoscale electrochemical biosensors.

Tumour cells, like most normal cells, have a high diversity of receptors on their surfaces. Molecules on the outside of the cell can attach to these receptors, causing changes within the cells. Immunotherapeutic drugs, monoclonal antibodies (mAbs), have been recently used in clinical oncology, as they recognise and lock on to specific antigen proteins on the surface of cancer cells, helping the body's immune system recognise the cancer cells and destroy them.

The direct electrochemical oxidation mechanisms, of amyloid beta peptides involved in Alzheimer's disease, of important signaling proteins, chemotherapeutic and less toxic immunotherapeutic pharmaceutical drugs redox mechanisms and their interaction with DNA, have the potential for providing valuable insights into the understanding of oxidative damage.

Knowledge concerning the oxidative damage of important cancer- and age-related biomolecules relevant in human health, will trigger the development of early detection electrochemical sensing methods and better and more effective therapies.

IT-13-EIHE 2023



Molecular thin films for electrochemical supercapacitors: Are we heading toward the molecular power banks?



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Abstract:

Nanoscale molecular thin films can be attractive electronic components for next-generation highperforming energy storage devices. we present a simple, controllable, scalable, low-cost, and versatile electrochemical grafting approach to modulate chemical and electronic properties of graphite rods (GRs) that are extracted from low-cost EVEREADY cells (1.5 US \$ for 10 cells of 1.5 V). On the ANT-modified GR (ANT/GR, **Scheme 1**), the total capacitance unveils 100-fold enhancement as compared to an unmodified GR tested with 0.1 M H₂SO₄ electrolyte ensured by both potentiostatic and galvanostatic measurements. The ultra-low-loading nanofilms expose high surface area leading to extremely high energy density. The molecular films show exceptional galvanostatic charge-discharge cycling stability (10,000 cycles) that operates at low potential. The polyaromatic-based molecular nano-films serve as a remarkable benchmark that holds the potential not only to replace the traditional inorganic metal oxide-based electrodes but also towards the building up of molecular power banks.



Scheme 1. Schematic representation of electrochemically modified molecular nanofilms used for supercapacitor studies.

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IT-14-EIHE 2023

Tuneable synthesis of graphene oxide by electrochemical exfoliation of graphite



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Abstract:

Top-down approach of making graphene and its derivatives has become attractive among the researchers due to its ease of operation and low temperature of synthesis. However, control of microstructure and defect and scale-up of the process have always been a challenge. We have designed a novel electrochemical cell in order to enhance the productivity of electrochemical exfoliation of graphite to form graphene oxide (GO). The effect of different process parameters on the microstructure of GO has been studied. A kinetic model for the synthesis of GO has been developed. The mechanism of exfoliation in acidic and basic media has been proposed. The surface reaction of anions during intercalation and de-intercalation in the interstices of graphite has been found to be the rate-controlling step. Synthesized GO was characterized with transmission electron microscopy (TEM), Raman spectroscopy, X-ray diffraction (XRD), and Xray photoelectron spectroscopy (XPS).



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Characterisation of Semiconductor Photoelectrode Interfaces using Electrochemical/Spectroelectrochemical Investigations



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Substrates are generated through the improvised techniques of electrochemical deposition, atomic layer deposition and hydrothermal synthesis protocols. The transition metal oxides and sulphides synthesized using these synthetic routes were further subjected to the post synthesis treatments for enhancement in the electrochemical performance. The photoelectrode and water interfaces are complex and the investigations of such complex processes are important in developing catalysts substrates for energy harvesting and storage, development of sensors and gas storing devices and investigating the interactions of drugs and biomolecules. The interfacial processes have been investigated for noble metal doped 3D-grapehe, metal organic framework derived Ni-Co oxide, MoS2 MoS2/C-dots composite for their electrocatalytic and supercapacitor properties. Photoelectrochemical (PEC) investigations are carried out for splitting of water using solar radiation on BiVO4 and its modifications through doping and hetero junction formation. Modification of the interface has generated interesting properties. Electrochemical and photochemical techniques are utilised to probe the charge transfer processes of the modified interfaces. Scanning electrochemical microscope has been utilised to obtain the hole transfer kinetics for the PEC water splitting and to image the interfacial processes, some such investigations are shown in Figure 1.[1-3]



Figure 1: The set up used for the interfacial kinetics in PEC investigation (A) Chopped light voltammetry of the Co-Bi modified BiVO4 and its photo charging

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IT-16-EIHE 2023



Electrochemically mediated multi-modal detection strategy-driven sensor platform to detect and quantify pesticides



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Abstract:

With the emergence of modern agronomy practices and the use of multiple synthetic pesticide agents to keep control over crop and field throughput, there lies a broad requirement for smart, accessible technologies to track pesticide contaminants in food, water, and other environmental matrices. In this work, we report at a proof of feasibility level, a sensor system to perform pesticide detection in aqueous buffers for two pesticides at the opposite ends of polarity (Atrazine and Glyphosate) in a serially combinatorial manner. The sensor construct employs a universal FR-4 substrate gold interdigitated electrodes with active sensing elements based on selective antibodies (proteins) and polymeric network structures – poly(3,4-ethylenedioxythiophene). Further, to determine metrics of sensor deployment in real-case scenarios: multimodal (electrochemical impedance spectroscopy and chronoamperometry) and multi-approach strategies (affinity-binding and receptor-free) were used to obtain sensing measurements. Higher specificity repeatable outputs were obtained with the affinity-based method while greater sensitivity by means of dynamic range (0.5 ng/ml–10 μ g/ml for Glyphosate and 10 fg/ml–1 ng/ml for Atrazine) and limit of detection (0.5 ng/ml for Glyphosate and 1 fg/ml for Atrazine) was determined via receptor-free direct approach for both pesticides. This serves as a first-step study to perform potential combinatorial assessment and subsequently multiplexed analysis of pesticide antigens.

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Layered' transition metal oxides as cathode materials for Na-ion batteries



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Abstract:

Transition metal (T_M) oxides are a fascinating class of materials, whose properties can be suitably tuned in a variety of ways; such as by selecting T_M-ions/dopants having preferred electronic configurations, engineering the crystallographic site occupancy by dopants, controlling/modifying the degree of covalence of T_M-O bonds, modifying lattice spacing(s), tuning phase assemblage etc. Such modifications done from the fundamental perspectives influence the performances of T_M-oxides for a variety of applications. In the context of the upcoming Na-ion battery system, O3-type 'layered' Na-T_M-oxides are promising as cathodeactive materials due to their inherently high initial Na-content (as compared to the P2 counterparts); but suffer from instabilities caused due to multiple phase transformations during Na-removal/insertion and sensitivity to air/moisture. Against this backdrop, with the help of a dopant, having d^0 electronic configuration (viz., again no OSPE), we have been able to tune the composition and structural features to suppress the phase transitions upon Na-removal/insertion and also improve the air/water-stability in significant terms; so much so that long-term cyclic stability has been achieved with health/environmentfriendly 'aqueous processed' electrodes (sans, usage of toxic/expensive chemicals like NMP and PVDF) [J. Mater. Chem. A 8 (2020) 18064]. The changes in structural features, which have led to such outstanding water-stability, include differential contraction/dilation of the Na-'inter-slab'/T_M-'slab' spacing and partial occupancy of the dopant at tetrahedral sites of the structure. Furthermore, in the context of the more 'ratecapable' P2-type 'layered' Na-T_M-oxide based cathode materials, but which lacks in terms of having a lower starting Na-content (typically, 0.67-0.7 Na-ions *p.f.u.*), a newly evolved universal strategy towards designing high Na-containing P2-structured 'layered' Na- transition metal oxides will be discussed. In a nut-shell, increases in the average 'charge:size' ratio of the cation-combination in the T_M-layer and concomitant T_M-O bond covalency result in lower effective negative charge on O-ions; which renders the prismatic coordination of O-ions around Na-ions more favourable even at higher Na-content. Accordingly, by careful selection of the combination of non-T_M-/T_M-ions in the T_M-layer, a high Na-containing (viz., ~ 0.84 p.f.u.) P2-type Na-T_M-oxide has been successfully developed, which, as a cathode material for Naion batteries, exhibits a high desodiation capacity of ~178 mAh/g (@ C/5; within 2-4 V vs. Na/Na⁺), exceptional cyclic stability pertaining to $\sim 98\%$ capacity retention after 500 galvanostatic desodiation/sodiation @ 2.5C and also stability upon exposure to air/water [Chem. Mater. (2022); https://doi.org/10.1021/acs.chemmater.2c02478)].



IT-18-EIHE 2023

Electrochemical impedance of porous electrodes for battery applications



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Abstract:

Electrochemical Impedance Spectroscopy (EIS) is one of the important characterization methods to quantify various transport and kinetic resistances present in any electrochemical device. It is also a useful tool to decouple various processes at different time constants. EIS is used extensively to study electrodeelectrolyte interface in flat or near flat electrode setups, however, practical battery electrodes are porous electrodes with significant thickness (50-250 µm) which cannot be approximated by flat electrodes. Significant effort in the literature is being devoted to understand the porous electrodes EIS.¹ Thick electrodes require additional understanding of the ionic transport resistance in the pores and electronic transport resistance in the solid phase viz-a-viz the kinetic resistances at the interface of solid and the electrolyte phase.^{2, 3} The ratio of transport to kinetic resistance becomes extremely important to figure out the workings of such electrodes and determine the bottleneck in the battery performance.

This talk will focus on the better understanding of the porous electrode impedance spectra in the context of ionic resistance, electronic resistance and the charge transfer resistances.

Acknowledgement: My colleagues Robert Morasch and Johannes Landesfeind and Prof. Hubert Gasteiger at Technical University of Munich.

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Development of composite electrolyte and electrode materials for IT-SOFC



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Abstract:

One of the greatest challenges in the field of solid oxide fuel cell (SOFC) technology is to reduce the operating temperature of the system in the intermediate temperature range (500–700 °C). To achieve this target, there has been a continued worldwide interest in the development of novel electrolyte materials. For electrolyte application in the intermediate temperature range, doubly doped ceria based composite electrolyte materials have been developed, which are essentially nano-composite materials comprising of doped ceria-based oxygen ion conductor and secondary perovskite-based proton conducting phase. The effect of co-doping on the microstructure of sintered electrolyte specimens was studied through scanning electron microscopy (SEM) coupled with energy dispersive spectroscopy (EDS). The electrical properties of the composite electrolytes were characterized by electrochemical impedance spectroscopy (EIS) under air in the temperature range of 300 - 800 °C. The effect of secondary conducting phases on the electrical conductivity of the composite electrolyte was studied. The effect of second phase in the composite on the total conductivity and activation energy for conduction has been compared with that of doped ceria-based oxygen ion conductor of similar compositions. The talk will also focus on development of composite electrode material based on LSCF-GDC system produced through a novel solution combustion technique. The effects of processing route on the functional properties of composite electrodes shall be discussed.



Designing artificial H₂ producing cobalt catalysts with neurotransmitter and vitamin



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Abstract:

Hydrogen (H₂) production from the water via electro or photocatalytic pathway has been reckoned as a vital step in our renewable energy-based future energy landscape. The bio-inspired synthetic catalyst design has emerged as one of the leading methodologies in this pursuit of developing efficient all-weatherready molecular catalysts for promoting green H₂ production. The appropriate inclusion of outer coordination sphere (OCS) features, a hallmark of enzyme architecture, around a synthetic core, has resulted in new genres of active H₂ production catalysts. However, we have rarely explored this OCS feature beyond natural amino acids or amino acid-derived peptide and protein motifs. Here, we have rationally incorporated neurotransmitter dopamine and vitamin B₆ molecules around a cobaloxime center to generate the first-ofits-kind synthetic catalyst containing non-amino acid-based biomolecules as OCS. The resultant complexes displayed significant H₂ production from water under elevated temperatures, oxygen exposure, and under natural solar irradiation while displaying the best energy efficiency observed for a cobaloxime core to date.



Solar Water Splitting Using Earth Abundant Conjugated Photocatalysts



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Abstract:

Photocatalytic and photoelectrochemical hydrogen generation are two simple approaches for solar water splitting. In both approaches, the photocatalyst is a prime requirement, determining the light absorption and overall hydrogen generation efficiency of the process [1]. Since, past four decades, oxide semiconductors have dominated the research area but due to large band gap, their inability to utilize the visible light photons to the extent of yielding required solar to hydrogen (STH) efficiencies as per DOE (Department of Energy) targets was uncertain [2]. Chalcogenides, are narrow band gap materials, suffers from high recombination rate and poor photostability. Relatively, nitrides are medium band gap materials sandwiched between oxides and chalcogenides. Among nitrides, graphitic carbon nitride, g-C₃N₄ is a stable, metal free polymeric, n-type conjugated organic semiconductor with favourable electronic, optical,

structural and physicochemical properties as compared to metal oxides [3]. Present talk will deliberate modifications, in the parent carbon nitride by various strategies such as exfoliation, by dispersion of carbon nanodots and metal nps, composite formation with calcium ferrites, etc. so as to impart improved photocatalytic properties and facilitate the charge carrier separation.



Investigations on metal-support interactions, band gap alignment and charge carrier kinetics in metal dispersed carbon nitrides will be revealed. The difference in behaviour of plasmonic and non-plasmonic metal dispersed carbon nitrides will also be discussed (Fig.1).

Figure: A Schematic depicting the sequence of most probable events occurring due to Schottky or surface plasmon resonance (SPR) effect to drive a photocatalytic reaction under given conditions for different M/CN photocatalysts.

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BiVO₄ - a futuristic Semiconductor for Photoelectrochemical Applications



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Abstract:

क्त सेवा में पुरु

Solar to hydrogen generation via photo-assisted water splitting has attracted extensive attention due to its great potential for low-cost and clean hydrogen production. This technology will require developing a stable and inexpensive photo-electrode that can absorb optical energy, particularly in the visible region, separate charge carriers, and promote water oxidation and reduction reactions. The water oxidation reaction is particularly challenging because many potentially attractive photoanode materials suffer from the need for large over-potentials to drive this reaction, resulting in poor solar conversion efficiencies. The present topic gives a comprehensive study of efficient photoanodes BiVO₄, which have been synthesized, particularly, from an aqueous medium, through cost-effective routes. The material has been demonstrated to precede the water oxidation reaction under visible light irradiation. Optimizations of the growth conditions, the role of surfactant, additive components and co-catalysts on the performance of the n-type BiVO₄ will be highlighted. Electrochemical and physicochemical properties of the semiconductor have been explored to support the efficacy of BiVO₄ towards future solar energy harvesting devices. The primary target for the present study is the tailoring of the band positions, growth of uniform surface with better crystallinity, and lowering of charge transfer resistance of the material for higher photoelectrochemical performance.

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Electrochemical sensors for the detection and degradation of toxic molecules



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Abstract:

In the current scenario, pollution is the biggest problem that is difficult to deal with as many new pollutants are introduced into the environment continuously. This necessitates the need for developing more sensitive, reliable, simple and selective analytical tool. In many countries, pesticides have been widely used in crop promoter to protect crops from pests, but when it is assorted with non-target regions of water and soil, it tends to pollute the environment. Of all the techniques used in electro-analytical research, cyclic voltammetry (CV) and square wave voltammetry (SWV) find extensive applications. Carbon-based and metal-based nanomaterials and their composites sensor assembly could be used to detect toxic molecules. Developed materials were characterized by different techniques (XRD, SEM, AFM and TEM). Under optimal conditions, the effect of pH, immersion time, modifier amount, scan rate, temperature and concentration were studied. Some vital electrokinetic parameters were determined, such as the heterogeneous rate constant, transfer coefficient, activation energy, and the number of protons and electrons involved in the electrode process. The agricultural and environmental relevance of the developed method was successfully used for monitoring toxic molecules in water and soil samples. Selectivity, stability, and reproducibility of the fabricated sensor were investigated.

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The Effect of Low Dose Radiation on Neurotransmission



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Abstract:

There has been high interest in addressing the health risk of low dose radiation from environmental and medical origin. Low-dose effects are being continually investigated, and there is now documentation of detrimental effects on early brain development. Specialised areas of the brain required for cognition and information processing associated with the hippocampus are reported to suffer from functional impairment resulting in mental retardation and cephalic disorders. The DoReMi consortium, a European research platform, has been concerned with low dose exposure effects, focusing on questions of more subtle low-dose risks and will be covered in this presentation. Investigation of low level irradiation between 0.1 Gy and 1 Gy has focussed on brain activity in *in vivo* animal models with the hope of understanding the biological consequence of radiation exposure at this level. The project investigates ionising radiation effects on neurotransmission *in vivo*. Neurophysiological experiments coupled with imaging technologies and microarray data on mice hippocampal and cortex tissue hope to assemble information exploring changes to the neuronal network *via* synapse re-formation. TUNEL staining has also been used to qualitatively detect apoptotic (programmed cell death) status in neuronal cultures post-irradiation to determine DNA degradation.

IT-25-EIHE 2023



Bioelectrochemical systems (BES) as a sustainable approach for water and wastewater treatment along with renewable energy generation



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Abstract:

Bioelectrochemical systems (BES) designated as renewable energy generating processes which simultaneously treats wastewater having diverse types of pollutants. Standard BES contain anode and cathode chambers which separated by a membrane (proton exchange membrane, PEM/cation exchange membrane, CEM). Membrane is crucial which helps to build the potential across two different half cells. Desalination is a BES application that helps in the removal of ions/salts from wastewater. Microbial desalination cells (MDCs) are three chambered systems, in which anion exchange membrane (AEM) and CEM were employed to facilitate the mobility of ions. The middle chamber acts as barrier for transfer of ions to anode to cathode. The efficiency of MDCs is high as 95% and bring down TDS from 30 g/L to potable range. Bioelectrochemical treatment systems (BETS) is another approach in which the complex electrochemical and biological processes deals for the extended treatment of wastewater and desalination. BETS is highly suitable for complex and recalcitrant industrial wastewaters. Integrated biorefinery approach extend the treatment of BETS that needed for polishing step. Overall, the desalination process does not demand any external energy. In this direction, both MDCs and BETS are found effective bioelectrochemical processes for energy generation and desalination.

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Electrochemistry beyond Redox Processes: from Collective to Single Molecule Switching



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Abstract:

We typically think of electrochemistry as comprising chemical reactions where the redox state of the participating atoms changes, such as metal electrodeposition or water electrolysis. While this is also true, the remit of electrochemistry is much wider. In my talk, I shall discuss mechanisms for controlled switching of the structure and properties of 2D materials at solid–liquid interfaces, from the collective scale down to single-molecule manipulation, at ambient temperatures and pressures. The 2D materials include self-assembled structures of tailored organic molecules but also hexagonal boron nitride, an atomically thin insulator. The switching events invariably depend on tipping the balance between intermolecular and adsorbate–substrate interactions [1,2], and may be controlled by external stimuli: the interfacial potential at electrochemical solid–liquid interfaces [3,4], the chemical potential of ionic species in solution [5], intercalation of atomic species [6], or the electric field between an STM tip and the substrate [7].



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Electrochemiluminescence based imaging for visualizing sebaceous fingerprint



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Abstract:

ECL microscopy/imaging is an emerging analytical technique not only possesses low background, high- throughput and -spatiotemporal resolution, but also visualize the distribution of electrochemical active sites and its interaction of particular analyte during electrochemical reaction. Particularly it has been used for detection of a wide range of analytes including small molecules, DNA, proteins, and cells at the level



of single molecule. Recently, researchers are using a simple smartphone camera to collect the ECL imaging which could be used as cost effective and portable clinical diagnostic for the bio-sensing application. Our group demonstrated a novel and non-decaying visual ECL emission from the $[Ru(bpy)_3]^{2+}$ /dicyclohexylamine (DCHA) system for the simple and rapid smartphone-based ECL mapping of a sebaceous fingerprint via a non-

destructive mode at physiological pH conditions, with a quantum efficiency (\Box ECL) of 95.5 %. The obtained ECL image could clearly detect the fingerprint ridges with the first-stage details (cores) that represent the overall shapes of the papillary ridges; and (ii) the second-stage details such as (bifurcations, crossovers, and lakes) represents the ridge pathway deviations

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Electrocatalysis of reduced graphene oxide-supported nanocomposites for fuel cell reactions



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Abstract:

Development of high performance electrocatalysts capable of electrooxidizing small organic molecules like CH₃OH, C₂H₅OH, HCOOH etc., are extremely important in realizing fuel cells as energy conversion devices.^[1] Herein, some important electrocatalyst configurations developed in our research group comprising of metallic/metal oxide nanoparticles dispersed on reduced graphene oxide (RGO) support for methanol oxidation, formic acid oxidation, ethanol electrooxidation will be discussed. Electrocatalysts such as Pd-CeO₂/RGO,^[2] Pt-Pd/RGO, Pt-Ru/RGO-TiO₂ etc were prepared by a simple solution-phase chemical reduction method. In most of the cases, oxygen functionalities present on graphene oxide acted as better anchoring sites to enhance the interaction of metal ions and subsequent reduction allows better dispersion of metal particles on to RGO support. Electrocatalytic activities and durabilities of the developed electrocatalysts for methanol oxidation reaction (MOR), ethanol oxidation reaction (EOR) and formic acid oxidation reaction (FAOR) were evaluated through cyclic voltammetry and chronoamperometry. Due to synergistic effects offered RGO support and metal/metal oxides resulting electrocatalysts.

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Metal-Ligand Equilibria: A Unified Theory and Protocol for Voltammetry and Potentiometry



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Abstract:

A single mathematical expression that is applicable to non-equilibrium polarographic and equilibrium potentiometric studies of $M_pL_qH_r$ complexes investigated by acid-base and ligand titrations will be discussed in details. For the first time in polarographic studies, this new expression requires making use of mass-balance equations to compute the free metal ion and free ligand concentrations needed to compute formation constants. The same theory is equally applicable to a wide range of $M_pL_qH_r$ complexes that can be seen on the polarographic time-scale as fully labile, inert, non-labile and mixed metal-ligand systems containing labile and non-labile/inert complexes in a solution sample. The general protocol applicable to the study of metal-ligand equilibria will be discussed and this includes:

- (1) Designing best experimental conditions,
- (2) Maximising analytical signals,
- (3) Predicting major species in a multicomponent solution,

(4) Single-point calculations of excellent guesses of formation constants needed for rigorous refinement operations,

- (5) Validation of the proposed metal-ligand system,
- (6) A concept and usefulness of the experimental and computed complex formation curves.

This is the new school of speciation representing a united multi-analytical approach that provides a complete and unique platform suitable to metal complexes in wide ranges of the total ligand and metal ion concentrations.



Effect of Cation Doping on Ni-based System for Overall Water-Splitting Reaction



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Abstract:

Electrocatalytic water-splitting reaction, which generates hydrogen and oxygen is extensively considered a prominent approach for the production of clean, secure, and sustainable forms of energy.¹ Water-splitting involves hydrogen and oxygen evolution (HER and OER) at the cathode and anode, respectively, with a requirement of 1.23 V potential difference to split water.² Due to the very high

overpotential of OER and HER, in practical, a voltage of 1.8-2.0 V pertains commercially during the water-splitting reaction. The wide application of water-splitting is still limited due to the use of noble catalysts such as Pt, and RuO₂, IrO₂ for HER and OER, respectively.³ The major limitations of these electrocatalysts are efficiency and durability in alkaline and acidic medium for HER and OER, respectively. So, to overcome these issues we need an alternative electrocatalyst with high efficiency and



stability in a wide pH. Consequently, investigation for the substitution of these noble catalysts with doped transition metal-based electrocatalysts having low overpotential and higher stability is being considered.^{4,5} The incorporation of the second metal as a dopant generally improves the electrocatalytic activity by increasing charge transportation. Moreover, doping with heteroatom makes the catalyst more metallic and influences the chemical environment of the catalytic surface.

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Porous Organic Polymer and its Composites for Electrocatalysis



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Abstract:

क्त सेवा में पर्

Porous organic polymers (POPs) can be conveniently engineered and produced at the molecular level, known for their high surface area and ample porosity. The POPs have confined molecular spaces for photons, excitons, electrons and holes to interact, thereby providing great catalysis ability. Among various types, triazine based porous organic polymers exhibit excellent chemical and thermal stability due to which they find numerous applications in chemical catalysis and electrocatalysis. Electrocatalysis highly relies on the ionic/electrical conductivity of a material and in this regard, bare POP sometimes lacks such essential characteristics. There are numerous strategies followed to improve the conductivity of POPs and they include composite formation, metal doping, carbonization, etc. Although these methods are very convenient, carbonization is usually adopted over composite formation. Latest studies have further shown that carbonization of doped porous organic polymers (POPs) with heteroatoms is an effective strategy to develop highly efficient 'N' and other heteroatom doped electrocatalysts.



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IT-32-EIHE 2023



Carbon-based Dots as Efficient Sensitizer in Photoelectrochemical Water Splitting Reactions



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Abstract:

High energy density of Hydrogen (H₂) drives to replace all the available non-renewable energy sources in near future and can function as efficient fuel.¹ H₂ generation via water splitting thorough photoelectrochemical (PEC) approach is a greener, renewable, and promising pathway.² So, to attain adequate quantity of H₂ stable and efficient photoelectrodes should be developed for the PEC water splitting. The overall efficiency of photoelectrode depends on the light absorption, charge separation and transportation, and finally charge collection and reaction efficiency of the semiconductor photoelectrode.



On the way of developing efficient photoelectrodes, initially morphology of the photoelectrodes is tuned in such a way that the optical activity of the material has been enhanced to a greater extent and result of which PEC activity of the electrode enhances. Further, the surface the photoelectrode is sensitized with carbon

based dots to increase the charge carrier mobility of the photoelectrode. In this regard, a visible light active and an UV light active photoelectrodes are targeted as the model semiconductors.^{3,4} Vertically grown 2D nanosheets of the semiconductors are developed first thorough wet-chemical method which shows enhanced efficiency of H₂ generation. Further, the surfaces of the semiconductors are decorated with carbon based dots. It is observed that the efficient sensitization leads to enhanced photoconversion efficiency of both the semiconductor materials. The carbon based dots functioned played an important role. It functions as optical antenna as well as suitable charge transportation channel to generate high photoelectrochemical activity due to increase in light absorbance, an increase in charge carrier density, and transportation ability.

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Mass transfer kinetics of copper in erosion-corrosion environment



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Abstract:

Mass transfer in a corrosion phenomenon is the transport of species to and from the working electrode surface. This is significant during the flow-induced or accelerated corrosion where the dissolved oxygen or the dissolved metal-ions must diffuse from the solution to the metal or from the metal to the



solution, respectively. In the present study, a rotating cylinder electrode (RCE) is used to investigate the mass transfer kinetics of copper in 3.5 wt% NaCl solution with and without the sand particles (erodent). The limiting current (Figure 1) of the cathodic reactant i.e. dissolved oxygen reduction on copper surface is measured with respect to different velocity (7.0 cm/s to 15.0 cm/s) under flow corrosion and erosion-corrosion condition. Mass transfer kinetics is compared for the oxygen reduction with and without erodent. The mass transfer coefficient (k_m) for copper in 3.5% NaCl solution with and without sand particles was calculated to be 4.3 x 10⁻⁴ and 6.08 x 10⁻⁴ m/s respectively.

Figure 1: Cathodic polarisation curves for oxygen reduction using RCE at the copper in 3.5 wt.% NaCl solution (a) with and (b) without sand at room temperature at different velocities.

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A critcal issue of piping failure: Flow accelerated corosion and erosion corrosion



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Abstract

Pipeline corrosion occurs due to several reasons which consist of physical, chemical, and environmental factors. The physical factors are structural (material properties, crevices, inclusions, etc.) and products (temperature, pressure, flow rate, flow pattern, etc.) properties. However, chemical factors are controlled by pH, dissolved solids, gases (H₂S and CO₂), and microorganisms. Environmental factors are the most essential factors which consist of oilfield composition, soil composition, and moisture level, and nature of the working area. Flow accelerated corrosion (FAC) is crucial internal corrosion problems in many industries by the turbulent fluid flow over a surface, which promotes mass transfer and enhances the dissolution and thinning of protective films in metallic pipes. FAC is the major reason for steel pipeline failure in the oil and gas industry. Pipe fittings such as elbow, tee, and reducer often undergo failure when they are subjected to corrosive environments under turbulent flow conditions. The present work focuses on the FAC of API grade steel in a synthetic solution of oilfield water under a turbulent flow condition. The FAC experiments were performed at the elbow test section using potentiodynamic polarization tests and electrochemical impedance spectroscopy (EIS) tests. The formation of the protective film and its chemistry were characterized using XPS and Raman spectroscopy. FAC of API steel depends on hydrodynamic parameters of the fluid flow such as wall shear stress and flow velocity. Corrosion current density for all the located specimens at the intrados and the extrados of the elbow are found to be increased however, charge transfer resistances were significantly decreased along the fluid flow path.

Keywords: Internal corrosion, Flow accelerated corrosion, hydrodynamic conditions, Corrosion rate, Film resistances



Membrane based potentiometric sensors for lanthanides and actinides



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Abstract:

Determination of lanthanides and actinide ions in different types of samples is required at several occasions. Potentiometric technique possesses a simple, low-cost, easy sample preparation, relatively fast, with desired precision and accuracy. However, determination of lanthanides and actinides using potentiometric technique has several challenges, such as poor sensitivity, poor selectivity among different lanthanides and hydrolysis of the metal ions at higher pH. Here we use different diglycolamide (DGA) or tripodal amides based ionophores in the polyvinyl chloride (PVC) matrix for the preparation of membrane based sensors for the detection of lanthanides (Eu^{3+} , Gd^{3+}) and actinide (Th^{4+}) ion. The membranes were casted by blending the polymer, plasticizer, ionic additive and the ionophore together in tetrahydrofuran (THF) on a flat bottom petri dish. The sensor membranes were characterized using different techniques, such as thermogravimetric (TG), atomic force microscopy (AFM), Fourier transform infrared (FTIR) spectroscopy and photoluminescence (PL) spectroscopy. The membrane sensor showed good sensitivity towards analyte ions with wide linear dynamic range and low detection limit. The membrane sensor also exhibited fast response time and stability over more than two months. The effect of different monovalent, divalent, trivalent and tetravalent interfering metal ions on the potentiometric response was also tested in the presence of analyte ions. Finally, the membrane sensors were employed for direct potentiometric determination of analyte ions in various samples.





Hexagonal Boron Nitride for Na- Ion/Metal Batteries



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Abstract:

Sodium-ion/metal batteries (SIBs) have gained enormous attention as an alternative electrochemical energy storage system. A significant challenge for its practical viability is finding an anode material that can provide high specific capacity along with good cycling stability. Recently, numerous theoretical works have proposed hexagonal boron nitride (hBN) as a promising anode material for SIBs.¹⁻⁴ Nevertheless, there has been no reported experimental verification for the said theoretical claims. To fill the knowledge gap, this presentation will talk about the experimentally investigated electrochemical performance of hBN under the capacity of a potential anode for SIBs. In addition, the preferable adsorption affinity of hBN for Na⁺ will be discussed to explain the observed effect of hBN coated separators for mitigating the dendritic growth of Na during repeated striping and plating.

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IT-37-EIHE 2023

Two's Company or Crowd? The Importance of Being Single for Energy Delivery



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Abstract:

Continuous addition of renewable energy, such as solar photovoltaic and wind, to the grid requires an energy storage platform to maintain the resilience of the electric grid. A continuous decline in installation cost and a friendly policy allows rapid expansion of renewable energy installations. Complications associated with the seasonal and diurnal fluctuations of energy production can be handled effectively having an energy storage option attached to the grid. One of the promising approaches to manage energy efficiently is storing the energy in redox flow batteries. Although matured technologies such as vanadium redox flow batteries are available, their entry into commercial space is prohibited by the cost of vanadium. This situation calls for cheaper local content in place of redox active material. Our group explores various organic redox active molecules/scaffolds for aqueous and non-aqueous redox flow battery chemistries. Besides, our interest is in exploring various degradation pathways contributing to the capacity decay of the redox flow battery. Once the degradation pathways were identified either by molecular engineering or suitable means, we could stabilize the capacity of the battery.

In this talk, besides organic redox flow battery I will share an account on our laboratory's developments in the vanadium/lead redox flow batteries.



Electron Transfer in Nano-Structured and Atomically Stepped Electrodes: Theoretical Aspects



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Abstract

We develop theory for the outer sphere heterogeneous electron transfer (OS-HET) rate constant at atomically stepped nanocorrugated metal surface. Theory accounts for the contributions from the nature of metal, local curvature of nanocorrugated atomic step, the density of atomic steps and kinks, dipolar solvents, and the frontier molecular orbital of electroactive molecules. Our theoretical approach models the free energy of activation obtained using the alignment of Fermi energy level in metal with one of the frontier molecular orbital of electroactive species. The activation free energy is a function of local curvature of nanocorrugated atomic steps obtained as a product of modified work function (WF) and the fractional electronic charge for the alignment of levels. Theory shows that the increase in step density lowers the WF of metal compared to the basal plane. The theoretical results highlight the step density-dependent nonmonotonic variation in fractional electronic charge as well as activation free energy. With an increase in step density, the Fermi energy level shift closer to LUMO and away from HOMO energy levels of electroactive species. This causes the reduced (for LUMO) and enhanced (for HOMO) activation free energy for ET kinetics compared to the basal plane. The LUMO and HOMO dichotomy results in anomalous enhancement and suppression in the OS-HET kinetics at atomically stepped metal, respectively. Finally, the strong influence of kinks along the step edge on the HET rate constant is predicted to change up to 6 decades (compared to the basal surface of Pt metal). Talk will also highlight some anomalies in experimental results and their theoretical understanding based on our fundamental equations.

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Nanoengineered Electrochemical Sensors for Tracking Biomarkers In Miniaturized Settings



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Abstract:

Robust, reliable and quantitative detection of biomarkers at ultra-low concentration is of great importance in clinical settings. Sensor, an analytical device used for sensitive and selective detection of biomarkers offers various advantages over the conventional clinical diagnosis, which is both time consuming and not suitable for point of care/onsite diagnosis. A revolution in the understanding and synthesis of nanomaterials in the last couple of decades contributed significantly to the development of the electrochemical biosensors in terms of sensitivity, catalytic activity, biocompatibility, and robustness.



Additionally, nanomaterial engineering helped in miniaturization of the sensing platform eventually helping in the commercial success of portable biosensing devices. Such platforms have tremendous promise in detecting various analytes including disease biomarkers, microbes, chemical compounds. This presentation is focused on the engineering design of electrochemical sensor systems and analytical parameters having key role in the development and success of point-of-care biosensors. Recently developed nanoscale materials based transduction system will be discussed with standard biomarkers that can be further directed towards the detection of various biomarkers in clinical research. Recently reported signal transductions strategies, promising personalized smart phone assisted electrochemical sensing platform for disease diagnosis will also be discussed.

Keywords: Nanobioengineering; Disease; Biosensors; Human Heath, Material Engineering

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Electrochemcial Investigation of Uranyl Species in Ethaline-DES and Possibility of UO₂ Deposition



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Abstract:

Deep eutectic solvents (DESs) have emerged as an interesting type of neoteric solvents in the 21st century that are now garnering attention in variety of fields such as hydrometallurgy, solvent extraction, non-aqueous electrodeposition etc ^[1]. As solvent, DESs have many advantages such as low volatility, low melting points, low/non-flammability, a large electrochemical window and the potential to be classed as

probe redox speciation of uranyl ion at



green solvents with low toxicities ^[1-2]. In the present study, the Ethaline DES (Choline Chloride and Ethylene glycol) was synthesized and was used to dissolve uranyl nitrate for subsequent electrochemical investigations. Cyclic voltammetry, chrono amperometry, chrono potentiometry and differential pulse voltammetry were performed to

different temperatures. The results indicated that the reduction of uranyl species was diffusion controlled both at Pt and GC electrode. The diffusion coefficients measured were in the range $\sim 10^{-7}$ cm².s⁻¹ which is lower than aqueous medium. As an extension of this work, electrodeposition of dissolved uranyl species from ethaline medium was explored on Cu-plate at constant current mode. The deposited uranium



species were characterized by XPS and GIXRD, which indicate the major species as UO, UO_2 and UO_3 . The present studies have potential application in reprocessing of spent nuclear fuel and associated waste management in nuclear fuel cycle.

Figure: (a) CV comparison plot of blank Ethaline and uranyl nitrate dissolved in Ethaline (b) CV plots with varying scan rates from 10 mV/sec to 150 mV/sec

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Electrowinning of light rare earth metals and alloys using molten salt electrolysis route



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Abstract:

Rare Earth metals find extensive applications in the field of renewable energy, automobiles, smart electronic & optical devices, aerospace, atomic energy and defence technologies. The production of rare earth metals by molten salt electrolysis has an important role because large scale production of rare earth metals by this route is considered more economic compared to other existing methods. The present talk will focus on the extraction light rare earth metals i.e. La, Ce, Pr and some of their alloys i.e. La-Mg and NdFe by molten salt electrolysis of chloride salt. Studies related to determine electro-kinetic parameters such as electron transfer rate constant, diffusion co-efficient in the electrolodeposition of these metals in molten salts will be presented. The design of electrochemical set-up used and studies related to optimization of process parameters like temperature of operation, electrolytic composition and cathode current densities to get maximum current efficiency and yield in the bulk deposition of metals and alloys will be covered in the talk.

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Technology demonstration for Hydrogen production by Iodine Sulfur thermochemical process



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Abstract:

The energy demand is ever increasing. Presently used fossil fuel has a problem of limited supply & greenhouse gas emissions. Alternately H₂ is seen as, one of the attractive energy carriers. Out of many thermochemical processes; globally, R&D on Iodine-Sulfur process (I-S), is in advanced stage, as it has high efficiency & all fluid process. The process consists of 3 reaction steps,

 $2H_2O + I_2 + SO_2 \longrightarrow H_2SO_4 + 2HI \quad (1)$

2HI \longrightarrow I₂ + H₂ (2)

 $H_2SO_4 \longrightarrow H_2O + SO_2 + \frac{1}{2}O = (3)$

Reaction (1), called Bunsen reaction, produces two acids viz. HI & H_2SO_4 . The produced acids are separated. Reaction (2) is HI section where, initially HI along with I_2 is distilled to separate I_2 , and HI is decomposed to produce H_2 and I_2 . Reaction (3) is H_2SO_4 section where, H_2SO_4 is concentrated &

decomposed to produce SO₂, O₂ & H₂O. I-S process needs to be demonstrated in closed loop using industrial material of construction. To achieve this objective, a bench scale facility is setup in BARC, Mumbai in industrial material of construction. Flow sheeting, P&ID development, Process equipment design work is carried out. All equipment, components, systems are installed & tested. The process



is commissioned. H_2 is produced at 150 Nlph. The process is being scaled up. The talk will cover developmental activities of Iodine-Sulfur process in BARC.

Figure: Metallic Closed loop Iodine-Sulfur Process

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IT-43-EIHE 2023

Design of Electrode Materials for Advanced Sodium-Ion Batteries



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Abstract:

With growing demand and escalating price of lithium resources, sodium ion batteries (SIBs) are being considered as promising potential alternatives to lithium ion batteries, owing to their similar electrochemical properties, greater abundance and lower cost. However, SIBs have poor energy density and cyclability which impedes its practical application. Therefore, to improve the performance of SIBs, extensive research is being carried out globally to develop appropriate cathode and anode materials for SIBs. The cathode materials for SIB constitutes layered transition metal oxides, polyanionic compounds, and Prussian blue analogues. The anode materials for SIBs can be categorised based on the reaction mechanism during sodiation/desodiation processes:(1) the insertion reaction materials, which include carbonaceous materials and titanium-based oxides; (2) the conversion reaction materials, represented by transition metal oxides or sulfides; and (3) the alloying reaction materials, including Na–metal alloying compounds containing elements from groups 14 or 15. However, in-depth material understanding is required to mitigate the existing loopholes and explore the commercial aspects of the respective materials. Rationally designed nanostructures endow the electrodes with high reversible capacity, superior rate capability, and long-term cyclability. This talk will emphasize on the work done by our group on these various types of SIB cathode/anode materials.



Multifunctional Prussian Blue Analogues Molecular Magnets for Energy Storage Applications



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Abstract:

The research and development work on Prussian blue analogues (PBAs) molecular magnets have generated great interest recently because of their energy storage applications in terms of batteries and electrochemical supercapacitors [1-2]. In addition, PBAs based molecular magnets show wide range of interesting properties such as magneto-optical switching, photoinduced charge transfer, electro-photo catalysis, ion sensing, and gas adsorption [3-5]. The porous network of PBAs is ideal for in-or -out insertion of alkali metal ions for battery electrode and gas storage. In this presentation, I will explain how one can optimize number of vacancies, porous network structure, and transition metal ion derivatives to discover the wide range of capabilities (multifunctional properties) of such compounds, along with electrochemical capacitance and gas adsorption [1-2].

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IT-45-EIHE 2023



Electrodeposition of Radioruthenium: Process Development and its Applications for the Treatment of Eye Cancers



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Abstract:

Amongst the radioisotopes produced in nuclear fission, Ru-106 is the most preferred choice by doctors for ocular brachytherapy. The high beta radiation (3.54 MeV) emanating from the decay of its daughter is utilized for selective dose delivery to the tumor while minimizing collateral damage to the healthy parts of the eye. The fact sheet has evolved over the three decades of use of Ru-106 based plaque sources supplied by M/s Eckert & Ziegler BEBIG all over the world. Recently, a team at Bhabha Atomic Research Centre (BARC), Mumbai, has developed Ru-106 plaques of three different configurations (**Figure-1**) and successfully deployed them for the treatment of eye cancers. More than 150 patients have been treated with all excellent post-treatment results. The present indigenous development allows



greater penetration of eye cancer treatment and positively impact more lives including patients from underprivileged society. Ru-106 plaque is fabricated through the multistep process under stringent quality control measures. The major steps of Ru-106 plaque

fabrication include (i) separation of the radioelement in radiochemically pure form, (ii) electrodeposition of Ru on a silver substrate and (iii) sealing of the source. The sealed source is then subjected to extensive quality control tests before being despatch to hospitals through BRIT. Electrodeposition of Ru on the silver substrate is one of the important process steps in the plaque fabrication process. The challenges faced during the electrodeposition of the rare transition metal ions and the processes evolved to meet the requirements are unique in comparison to the processes discussed in the open literature. Under the optimized conditions, a mirror-finished silvery shiny deposit of the radioelement is obtained with >95% of homogeneity level. This electrodeposition process development was an important milestone towards the successful development of the Ru-106 plaques at par with international standards.

Figure: BARC developed Ru Plaques configurations deployed for eye cancer treatments

Acknowledgments

The work presented in this paper is the result of the dedicated work of many scientists and engineers of BARC. Authors wholeheartedly thank each of them for their contributions. Authors also gratefully acknowledge the contribution of Doctors and Radiation Physicists who were involved at different stages of plaque development and performance evaluation process.



IT-46-EIHE 2023

New Modifications of Graphene for Water Splitting and Fuel Cell Reactions



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Abstract:

The energy security and supplies of energy are the key components for progressing countries. Developing efficient viable alternate renewable energy sources in the context of the ever growing demand for energy is the need of the hour. Renewable energy resources are rapidly being recognized as clean sources of energy to withstand damages to environment and to avoid future crisis. Many materials related challenge exist in electrochemistry covering the entire span of electrode materials as an active component of fuel cells and next generation energy conversion devices. With this motivation, surface engineering at nanoscale



plays an important role in energy generation, conversion and utilization applications. Our current research is systematically

examining and

developing the efficient and cost-effective electro-catalysts for hydrogen generation reactions from hydrogen rich species, water splitting and fuel cell reactions, wherein metal nanostructures anchored on carbon based materials (enhancing surface area/activity) and substitutional doping of non-metal demonstrate extraordinary electro-catalytic performance in water splitting and other hydrogen generation reactions. The observed efficient electrocatalytic activity of the as-synthesized electrode is attributed to the co-operative response and associated structural defects due to their oxidative functionalization along with their cooperative functioning at nanodimensions. We expect that these findings will stimulate future research on synthesis of other innovative and sustainable metal-free nanomaterials and investigation of the fundamental structure-property relationships for renewable energy and other applications.

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IT-47-EIHE 2023



Non-Precious Electrocatalysts for Electrochemical Water Splitting; Current status and future prospects



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Abstract:

Electrochemical water splitting is a promising approach for large-scale and sustainable hydrogen production with no carbon emission. However, its kinetics is slow and requires precious metal catalysts to efficiently operate. Therefore, great efforts are being undertaken to design and prepare low-cost and highly efficient catalysts to boost the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Currently, we developed different noble metal free materials as efficient catalysts for HER, OER, and full water splitting. Efficient electrocatalysts requires (1) highly active intrinsic sites, (2) abundant accessible active sites, (3) effective electron and mass transfer, (4) high chemical and structural durability, and (5) low-cost and scalable synthesis. It should be noted that all these requirements should be fulfilled together for a practicable electrocatalyst. Much effort has been devoted to addressing one or a few aspects, especially improving the electrocatalytic activity by electronic modulation of active sites for electrochemical water splitting. In this presentation, I will summarize current advances in the synthesis of low-cost earth-abundant electrocatalysts for overall water splitting. In addition to the currently used precious metal-based electrocatalysts, emerging non-precious metal-based electrocatalysts such as, Iron and Vanadium co-doped Ni₃S₂ Nanosheets, MoVN nanoflakes on MoNi₄/MoO₂ nanorods and Lollipop-shaped interconnected MnO₂ nanotube/Co₃O₄ polyhedron composite derived from zeolitic-imidazolate framework-67 have been developed for cost-competitive water electrolysis.





Real time monitoring system for aflatoxins in real samples



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Abstract:

There is an exponential rise in the popularity of biosensors as powerful analytical tools. Electrochemical biosensors are the preferred over other transducers because of their cost-effectiveness, reproducibility and excellent detection limits. Fabrication of biosensors particularly the immobilisation of the bioreceptor plays a key role in assigning selectivity, sensitivity, stability and self life of sensing device. Retaining of the conformation and biological activity of the biomolecule, accessibility of its active site to the target analyte and the proximity of the biological component to the transducer are some of issues which an immobilisation procedure ought to guarantee. Among the different immobilisation protocols, the commonly used are adsorption, cross-linking with functional reagents, covalent/non-covalent coupling via electrostatic or affinity interactions and entrapment using scaffold or copolymerisation within a polymeric matrix. Disposable homemade screen printed electrodes with choice of sensing surfaces offers innumerable options for functionalization to provide a stable matrix of specific ionophore/ protein/ antibody/aptamer etc. A facile fabrication of polymer modified screen printed electrodes as model label-free immunosensors is demonstrated for monitoring aflatoxins, a common fungal toxin infecting the food chain. The biosensor exhibited a low detection limit, good sensitivity, reproducibility, selectivity and storage stability, paving the way to its potential exploitation as disposable lab-on-chip device in the monitoring aflatoxins in real samples of cattle feed and milk.



Fig 1. Electrochemical Sensor as alternative tool to ELISA for aflatoxin monitoring





Electrochemical Synthesis of Sustainable Carbon-Free Fuels



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Abstract:

The increasing demand for energy and environmental concerns has induced global efforts to find and explore alternative energy sources for fossil fuels. Electrocatalysts have been played a key role in a wide range of electrochemical energy devices such as Polymer electrolyte fuel cells, and electrolyzers [1]. As an ideal candidate, hydrogen produced from water splitting is an attractive green approach for the nextgeneration energy conversion devices. Innovative design for highly efficient and durable catalysts has been considered. Replacing noble metal or metal oxides is a promising approach to overcome high-cost and elemental scarcity, greatly hindering their widespread applications. First, I will describe our recent research on developing low-cost, efficient, and robust electrocatalysts catalysts for water splitting to store sustainable energy resources. The Co@NC electrode shows the OER overpotential of 330 mV with an ultra-stability over the noble electrode. The long-term water electrolysis cell stability testing using alloy core-carbon shell catalysts shows over 760 h stable activity (voltage loss of 4%) and outperformed the commercial (noble) catalysts [2]. Electrochemical ammonia synthesis by N_2 fixation has proven to be a promising alternative to the energy-consuming, befouling Haber-Bosch process. Considering the low faradaic efficiency and sluggish kinetics of nitrogen reduction reaction (NRR), it is significant to design a robust and selective catalyst. A hybrid nanocatalyst fabricated by a single-step *in-situ* nitridation method is a potential costeffective electrocatalyst for NRR will be discussed [3]. For the stable electrochemical reduction of nitric oxide (NO) to value-added chemicals such as ammonia (NH_3) with high selectivity and efficiency, the catalyst design strategy is crucial to circumvent the electrocatalyst reconstruction during electroconversion. We developed a core-shell catalyst in which Ni nanoparticles are wrapped by a porous nitrogen-doped carbon shell (Ni@NC) for the stable electrosynthesis of NH₃[4].

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IT-50-EIHE 2023



Tackling complexity in electrocatalysis: A modeling framework to capture structure and complexity at the solid-liquid interface



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Abstract:

The solid-liquid interface can be incredibly complex. I will discuss some of our recent state-of-theart simulation studies that demonstrate the complexity during selective dealloying/corrosion in Au-Ag alloys [1] and during electrodissolution of copper [2]. Current continuum-level electrochemical models are inadequate as they cannot capture this complexity. A new modelling framework to capture structure and complexity at solid-liquid interfaces is introduced [3]. The short-range order (SRO) parameter is a useful mathematical quantity for the global structure in such cases. SRO refers to the likelihood of finding atoms/molecules of a particular type, in the vicinity of others atoms of same/another type. The SRO parameter is dictated by both micro- and macro-scopic parameters, such as interactions, thermodynamics and kinetics (reactions, diffusion, and other transport processes). I will discuss evolution equations for the SRO parameter. These equations can help provide an accurate picture of the thermodynamics and kinetic behavior in a variety of complex systems. Examples will be provided on how the formalism can bridge experiments and atomistic methods.

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Electrochemical fate of Actinides: Aqueous and Non aqueous routes



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Abstract:

Actinides are important in view of their use as fuel in nuclear industry [1]. The starting, intermediate, and final product of the fuel has to pass through a series of quality control check before putting it into the reactor core [2]. Another major concern among the inhabitants living in the surrounding of nuclear facilities like mining & ore-processing, fuel fabrication and nuclear reactors is the health hazards associated with the radiochemical and biological toxicity of the radioactive elements over their accidental release in environment. A large number of very reliable destructive and non-destructive analytical techniques are available in the arsenal of an analyst for sensitive, precise and accurate quantitative determination of actinides nuclear fuel and their separation in the back end cycle along with quantitative determination in environmental samples. Most of the techniques require expensive and complex instruments with high cost of operation and maintenance. Electrochemical techniques are fast, capable of detecting sub-ppb level of analyte, require very small volume of solution. The low cost portable instruments and simple experimental set up make the voltammetric techniques suitable for on-site environmental monitoring. Therefore, our group has developed voltammetric methods for the determination of actinides in sub-ppb to mM range employing electrodes modified with metal nanoparticles, conducting polymers, graphene, carbon nanotubes etc. Also we have developed electrochemical techniques based on different aqueous and non aqueous routes for the separation and purification of actinides in the back end of nuclear fuel cycle with minimum generation of radioactive waste via electrochemical techniques.

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IT-52-EIHE 2023



Electrodeposition of Rhodium and Platinum-Rhodium alloy on stainless steel substrate: a durable catalyst surface



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Abstract:

Rhodium is known to form a durable and adherent coating. Pulsed electrodeposition is evaluated for optimum deposition of Rh on stainless steel (AISI304) substrate. The process has been evaluated for



platinum deposition and Pt-Rh alloy deposition as well. The deposition parameters like pH, temperature of bath, current density and pulse profile were optimized. The mechanism of deposition has been determined by analysing the chronoamperometric graphs. The experimental curves were closer to the instantaneous nucleation mechanism which

indicates better size control of the deposits with the variation of the duty cycle of deposition. The depositions were characterized by SEM, EDX and XRD and also the electroactive surface area of the noble

metal deposited specimen was evaluated. The noble metal deposited substrates were evaluated for their catalytic activity for a host of applications ranging from electrocatalytic hydrogen evolution, photocatalytic dye degradation among others. The Pt-Rh alloy deposited substrates have shown better performance as compared to the individual metal deposited ones. The electrochemical corrosion potential (ECP) of the noble metal deposited substrates was also determined at 250 °C. The electrodeposited specimen have shown higher



variation in ECP as compared to the hydrothermally deposited ones.



Nanomaterials based Sensors for Healthcare Applications



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Abstract:

क्त सेवा में परु

Detection of cancer at an early stage is crucial in improving the survival rates of the patients. The current diagnostics are mostly lab-intensive, expensive, complex and sometimes invasive, thereby resulting into a resistance among the patients to take the tests in the early stages of the disease when there are no clear symptoms. Hence, development of the diagnosis methods that are easy-to-use, simple, and cost-effective becomes critical. This talk will discuss two different types of sensors – resistive and electronic sensors for the efficient detection of the biomarkers of lung cancer, that were developed by our research group. The resistive sensors were developed using CuO nanostructures for detecting the vapor biomarkers of the disease. Selectivity is a major concern with metal oxide-based sensors. An approach to resolve the problem will be discussed. Additionally, novel electronic sensors for two protein biomarkers that are overexpressed case of multiple cancer, including lung cancer were developed. The developed sensors were tested with clinical samples were found to have better limit of detection than enzyme linked immunoassay (ELISA) kits which are commercially used for quantifying different proteins. An overview of the developed method will be presented.

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IT-54-EIHE 2023

Applications of Electrochemical Sensors for Sodium Systems



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Abstract:

Electrochemical sensors for sodium systems are developed in the authors' laboratory and deployed in sodium-cooled fast reactors and large sodium circuits. A couple of applications of electrochemical sensors for sodium systems will be discussed in this talk. A comprehensive hydrogen detection system is developed to track steam leaks into sodium by monitoring hydrogen in liquid sodium and in argon cover gas simultaneously and its performance is demonstrated. Detectors for hydrogen in sodium and argon cover gas are deployed to track the hydrogen in liquid sodium and in cover gas to assess the extent of the steam leak. A cold trap is one of the crucial modules of the sodium coolant circuit, as it controls hydrogen, oxygen and other impurities in liquid sodium within the threshold levels in dynamic mode. In-situ regeneration of the CT during the reactor operation would be cost-effective while generating power. During the regeneration process, hydrogen release behaviour as a function of time with varying temperature and cover gas pressure was investigated by deploying in-house developed online hydrogen sensors. The quantity of total hydrogen that evolved and decomposed NaH was determined after the successful regeneration of the cold trap. Details of the experiments, results and analysis will be discussed during the presentation.

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Electrochemical Interactions at 'soft' liquid-liquid interfaces



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Abstract:

Biological interfaces are 'soft' and 'electrified'. An electrified liquid-liquid interface, (ITIES: Interface between Two Immiscible Electrolyte Solutions), can be used as a biomimetic interface to study both fundamental aspects and practical applications of drug- peptide interactions. In this presentation an overview of aspects of the following studies carried out at a liquid-liquid interface will be presented.

- 1. Drugs and Chiral Interactions.
- 2. Drug-Peptide aggregation Interactions
- 3. Lipid bi-layers and redox molecules
- 4. Interaction of nanoparticles with Lipid bi-layers.
- 5. Bacterial Biofilms and identification of metabolites.



Electrochemical Biosensors for Cancer Biomarker Detection



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Abstract

Cancer is one of the major health challenges worldwide. Its detection in the early stage is crucial for an effective treatment. One of the conventional technique for detection of cancer is based on estimation of cancer biomarkers¹, which are basically biological molecules found in blood, other body fluids, or tissues that is a sign of a normal or abnormal process, or of a condition or disease. Electrochemical biosensors offer a promising platform for development of diagnostic devices for detection of cancer biomarkers². With the ever-increasing demand for such devices, newer materials and sensor design strategies are urgently required for the development of reliable, user friendly biosensors. The various approach adopted for mediator and substrate-free amperometric biosensor for simultaneous detection of multiple cancer biomarkers will be discussed. The talk will present an overview of our efforts in designing polymer and nanomaterials based electrochemical biosensors³⁻⁵ for detection cancer biomarkers such as alphafetoprotein, carcinoembriyonic acid and prostate specific antigen.

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IT-57-EIHE 2023

Applications of Electrochemistry In Development of Radiopharmaceuticals



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Abstract:

Radiopharmaceuticals have remarkable contribution in healthcare which is highlighted by their involvement in precise identification of tumors and their metastatic spread through whole-body nuclear medicine imaging techniques and therapeutic applications thereof. Cancer targeting molecules like antibodies, peptides, small molecules mediate the transport of radionuclides (diagnostic/therapeutic) to the diseased site. Amongst the different vectors, peptides are the most promising molecules which can be rapidly and easily synthesized in the laboratory in high purity without involving any complex procedures. High affinity towards the target expressed on cancer cells and favourable in vivo clearance pattern make them attractive and competitive molecules for development of radiopharmaceuticals. Interaction of peptides with DNA, nanoparticles, lipid membranes can be easily studied through sensitive, simple and cost-effective electrochemical methods.¹ Voltammetric techniques are important analysis tools which aid in determining the conjugation of peptides/small molecules with nanoparticles. Another area where electrochemistry has an important contribution is during production of certain radionuclides (¹¹¹In, ⁶⁴Cu) in cyclotron that requires preparation of solid target assembly by electroplating.² Thus, electrochemistry has diverse applications in the field of healthcare starting from production of radionuclides to studying interaction of potent molecules with their target.

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Application of cavitation in graphite decontamination



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Graphite constitutes a major waste stream in the nuclear industry. Sourcing of high purity nuclear graphite is a challenge due to its import restrictions in many countries. With the surge in demand of graphite from conventional and new industries (battery and graphene based applications), the cost of graphite is projected to increase 5 times by the turn of this decade. Therefore, it is an imperative to develop a technology to clean and reuse the contaminated graphite from the nuclear industry. The porous nature of graphite prevents its complete decontamination using nitric acid.

Ultrasound based cavitation has been found to be an excellent intensification technique for cleaning activity from the pores [1-5]. A comparative study of decontamination kinetics of three different contaminants viz. uranium, ceria and yttria, has been made to comprehend the degree of intensification achieved. The degrees of intensification achieved on the application of ultrasound versus the silent reaction (without ultrasound) were found to be 60% for uranium, 85% for yttria and 90% for ceria. It was found that both uranium and yttria dissolution in leachant follows product layer diffusion control mechanism, while ceria dissolution follows surface reaction control mechanism. This is mainly attributed to the fact that dissolution rate of ceria is 10 times less than that of yttria and uranium in 4 M nitric acid. The influence of a few operating parameters like temperature and concentration of the acid, the frequency and intensity of the ultrasound were studied to arrive at the optimum conditions of operation.

This non-destructive decontamination facilitates the recycle of graphite. Therefore, properties like electrical conductivity, compressive strength and porosity, were measured over 15 cycles. While the change in electrical conductivity and compressive strength of graphite were not appreciable (<1%), the porosity increased by 9% after 15 cycles. The process is being scaled up to a 400 litre bath for industrial graphite decontamination.

IT-59-EIHE 2023



Electrochemical methods: Indispensable for the fabrication and characterization of organic solar cells



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Abstract:

Organic and inorganic-organic hybrid solar cells emerge as next-generation low-cost and efficient solar energy converters. Although these solar cells show promise, environmental and intrinsic instabilities in these devices limit their commercial applications. Understanding device physics and proper characterization of solar cell materials and devices, such as energy level matching, characterization charge transporting layers, charge generation, transport, charge accumulation, trap states, and so on, are prerequisites for improving device stability. Here, electrochemistry plays a crucial role in characterizing devices and elucidating charge transport in such devices. For example, electrochemical impedance spectroscopy (EIS) is an indispensable tool for gaining insight into charge transport in perovskite solar cells. Figure 1 shows the typical equivalent circuit used to fit perovskite solar cells. In addition, electrochemical methods are widely used for the characterization of photovoltaic materials, the design of electrodes, and device characterization. In the talk, how electrochemical methods are used to enhance the power conversion efficiency of solar cells will be presented.



Figure 1: The equivalent circuit model of typical perovskite solar cell consisting of the following elements: series resistor (Rs) arising from wires and external contacts, high-frequency resistance (RHF), constant phase element capacitance (QHF) and low-frequency resistance (RLF) and constant phase element capacitance (QLF).



IT-60-EIHE 2023

Lithium and sodium storage capacity of Mo₂C based composite



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Abstract:

Mo based compounds like Mo₂C, MoS₂ etc are found to be promising anode materials for lithium as well as sodium ion battery. The bulk Mo₂C shows relatively low capacity as the whole particle could not participate in electrochemical process. The nanosize Mo₂C shortens the Li⁺ diffusion path. When rGO is added to Mo₂C, it facilitates migration of electrons and cushions the developed stress due to lithiation and delithiation. The electrochemical performance improves drastically by the addition of just 1% carbon which further increases in the composite having rGO. The as developed Mo₂C/C/rGO composite exhibits a specific capacity as high as 630 mAh/g after 1600 cycles with nearly 100% efficiency. The high capacitive current in the composite contributes to superior electrochemical performance. A full cell with NMC 622 cathode could be fabricated which delivers around 114 mA h/g capacity at 50 mA/g. This material could be used as anode material for sodium ion battery also. This unique design of Mo₂C/C/rGO exhibited specific capacity of 498 mAh/g at 50 mA/g current density and it retained 96.4% of its initial capacity after 750 cycles. Theoretical calculations reveal that strong interaction of Mo₂C and graphene induces modification of the geometrical (widening of Li/Na movement channels) and electronic structures of Mo₂C, which in turn improves the overall performance of the composite electrode.



CNT aerogel electrochemical bio-sensor: A new era in ultra-sensitive biomedical technology



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Abstract:

Carbon nanotube-based electrochemical bio-sensors are a rapidly growing field in biomedical research due to their unique properties that allow for highly sensitive and selective detection of biomolecules. However, the conventional CNT-based electrochemical bio-sensors have limitations such as complex fabrication process, limited selectivity and sensitivity, high cost and limited life span. In our Lab, a new generation of CNT aerogel based electrochemical bio-sensors have been developed that overcomes these limitations. These sensors are fabricated using a floating catalyst CVD process and consist of freestanding CNT aerogel films that possess high porosity, electrical conductivity, tensile strength, and mechanical integrity. These properties make them ideal for use as ultra-sensitive biomolecule detectors, as they are able to detect even trace amounts of biomolecules with high sensitivity and selectivity. Furthermore, the CNT aerogel films retain their bio-sensing characteristics in different distorted conditions like bend, twist, stretch, and knot. This makes them suitable for use in wearable sensing devices. The use of CNT aerogel based electrochemical bio-sensors is expected to revolutionize field of biomedical sensing and diagnostics by providing a sustainable, reliable, and cost-effective solution for the detection of biomolecules in complex matrices.

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Abstract Presented as Oral and Poster

<u>CP-1-EIHE 2023</u>



Prussian blue derived metal oxide and sulphide based materials for high performance energy storage applications



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Abstract:

Electrochemical super capacitors have drawn great attention as advanced energy storage applications because of their decent energy storage capacity, high charge-discharge rate, long cycle life, outstanding power density than batteries. Composite metal oxides and sulphides are exhibited high performance electrode material for electrochemical storage devices, fuel cells, water splitting and Li ion batteries. Metal oxides and sulphides are providing high energy storage capacity due to the involvement of redox reactions in the energy storage process compared with carbonaceous materials. where electrochemical double layer is primarily responsible for energy storage. The metal compounds derived from Prussian blue and Prussian blue analogous (PB/PBAs) have a lot of advantages in catalytic as well as electrochemical storage applications due to their availability of multiple redox centres, good stability, electrical conductivity etc. The development of ecofriendly friendly and high-power energy resource is fetching exciting and more significant ¹⁻³. The PB/PBA derived metal oxide and sulfides materials were synthesized using both hydrothermal and wet chemical method. The electronic properties and stability of the material have been characterized by impedance measurements and cyclic voltammetry and the charge-discharge properties of the materials have been studied by Galvano static charge-discharge experiments. The cyclic voltammetry (CV) experiment was carried out in 1M KOH supporting electrolytes at scan rate 10mV/Sec. The PA/PBA derived oxides and sulphides based composite material exhibited pseudo capacitive in nature and the material shows highly stable up to the 2000cycle. The specific capacitance was obtained different composite materials in the range of 400 to 700 Fg^{-1.} The multiple galvanostatic charge discharge indicated that the material is stable up to the 500 cycle and the symmetrical to each other and highly linear.

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<u>CP-2-EIHE 2023</u>



Photoelectrochemical Splitting of Water Using FeOOH as cocatalyst over Tin Oxide/Hematite for Green Energy Production



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Abstract:

Hematite is a promising photoanode material for the photoelectrochemical (PEC) oxidation of water^{1,2} and production of green and renewable energy with the most important advantage for being the earth abundant in nature. However, the recombination of electron and hole after photoexcitation is the detrimental factor responsible for the decrease in the photocurrent efficiency in the PEC water splitting. Herein photoelectrochemical property of electrodeposited α -Fe₂O₃ on SnO₂ coated FTO (Fluorine doped tin oxide) has been investigated using three electrode systems under Sunlight source using Solar simulator having AM 1.5G illumination in 0.1M NaOH. The FeOOH cocatalyst has been photoelectrochemically deposited over Tin-oxide/hematite with an aim to retard the electron hole recombination process. Photo response of photoanode materials were performed by Chopped Light Voltammetry (CLV) technique. Significantly enhanced photoresponse has been observed. In order to understand the mechanism of the photoelectrocatalytic activity, incident photon to current efficiency (IPCE) was measured (vs Ag/AgCl) in 0.1M NaOH solution from 350 nm to 550 nm wavelength range and its values ranges between 25 to 30%. Further. the stability test of SnO₂/Fe₂O₃/FeOOH photoanode was performed bv chronoamperometry method for dynamic light illumination for 7200 s. The photoanode material is stable over appreciable period of time. The results from the CLV and the stability tests are shown in Figure.1.



Figure 1. (A) Chopped light Voltammetry plot for (a) SnO₂/Fe₂O₃ (black) (b) SnO₂/Fe₂O₃/FeOOH (red) and (B) Stability test for SnO₂/Fe₂O₃/FeOOH at 0.6V vs Ag/AgCl

CP-3-EIHE 2023



Microporous Polymer derived Porous Carbons and Au-Mn₃O₄//GO nanocomposites for Supercapacitors



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Abstract:

Porous carbon-based materials are extensively used for catalysis, adsorption, and energy storage devices. We will discuss the synthesis of N-doped porous carbons from microporous organic polymers via chemical activation and its applications in the electrochemical energy storage device (supercapacitors). By tuning the surface and porosity properties, we could able to achieve the highest specific capacitance of around 420 F g^{-1} at 1 A g^{-1} and 100% capacitance retention up to 10,000 cycles in 1 M H₂SO₄ electrolyte.



Figure: N-doped carbons from microporous polymers and Au-Mn₃O₄//GO composites

We will also discuss the synthesis and characterization of Au-Mn₃O₄ and graphene oxide nanocomposites by redox-mediated modified hydrothermal reaction. The optimized composite Au-Mn₃O₄/GO1 has a specific capacitance of 475 F g⁻¹ (1 A g⁻¹) in the H₂SO₄ electrolyte. The symmetric supercapacitor device retains 93% of its original capacitance after 10,000 charge-discharge cycles in a polymer gel electrolyte. We found that the graphene oxide framework and the addition of Au (2-3%) to the composite increases cycle stability compared to Mn₃O₄.

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<u>CP-4-EIHE 2023</u>



Electrocatalytic Barium-oxide decorated MWCNT Amperometric sensor for the quantification of local anesthetic drug Procaine



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Abstract:

Procaine hydrochloride (P.HCl) is one of the oldest local anesthetic drugs used by humankind for attaining clinical nerve blocks during medical procedures when administered in appropriate amounts. Concomitantly, if administered excessively, it results in adverse effects such as cardiological and neurological toxicities. Thus, developing a sensor for P.HCl is crucial to enable real-time monitoring of the drug and assist in quality control procedures during its industrial preparations. Therefore, through this work, we have fabricated a highly selective and sensitive amperometric sensor for P.HCl detection based on a Barium-oxide multiwall carbon nanotube-modified carbon paste electrode (BaO-MWCNT/CPE). Various characterizations techniques including X-ray photoelectron spectroscopy (XPS), Electron Impedance Spectroscopy (EIS), Powder X-ray diffraction analysis (pXRD), TEM and FESEM were examined for the modified electrode. Experimental conditions, including supporting electrolytes, pH, and scan rate, were



optimized to achieve a well- defined P.HCl anodic peak current at 631 mV. The developed sensor exhibited remarkable analytical performance over a wide linear dynamic range of 2.0 to 100.0 μ M with a detection limit of 0.14 μ M. The selectivity of the fabricated sensor towards P.HCl was noteworthy in the presence of various interferants such as

dopamine, epinephrine, starch, ascorbic acid, and uric acid. Finally, the utility of the sensor was validated by implementing it for the trace analysis of urine and blood serum real samples.

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<u>CP-5-EIHE 2023</u>





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Abstract:

सेवा में फ

The application of amitrole to control a wide range of perennial grasses and aquatic-weeds poses rising concerns regarding global water-borne contamination. For the reason that its toxicity leads to cancer, thyroid dysfunction and other illness, amitrole is considered an important analytical target. Although the environmental protection agencies worldwide have introduced several directives that set concentration limits for chemicals to impede water pollution, there is yet no facile and efficient analytical method to evaluate amitrole. Hence the development of an efficient real-time monitoring device is the key. Thus copper-oxide decorated multiwall carbon nanotubes (CuO-MWCNT) were prepared at various temperatures (150 °C, 200 °C, 300 °C, 400 °C) and under optimal conditions, amitrole oxidized efficaciously at CuO-MWCNT@400 modified carbon paste electrode. This is attributed to the distinguished synergistic



characteristics such as stability, porosity, and surface area of the carbon-hybrid that facilitated good amperometric quantification with selectivity and sensitivity. The sensor rendered quantification sensitivity of 16.5 nanoMolar and the proof-of-concept was determined by anti-interference and sensitive detection of amitrole from two different spiked water samples. We consider the fabricated amperometric sensor's

performance will protect our environment and enhance the awareness.



A Miniaturized Potentiostat for Electrochemical Enzymatic Glucose Detection



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Abstract:

The dependency of electrochemical sensors on bulkier potentiostat equipment is a major drawback for the real time application. Hence, though there are several electrochemical/ biosensors reported for various diagnosis, analysis and detection, yet, they cannot be commercialized as point-of-care (POC) device [1]. In order to resolve this, a miniaturized, portable, potentiostat with minimal hardware and their compatible electrochemical platforms are needed. The present work demonstrates the fabrication of a miniaturized portable field programmable gate array (FGPA) electrode meter[2] based potentiostat. As a prototype, a compatible miniaturized electrochemical sensor for enzymatic glucose detection was also realized. A flexible, laser-induced graphene (LIG) based three-electrode system compatible with the designed FGPA was fabricated. The sensor was chemically modified with glucoseoxidase (GOx) enzyme [3] and a Nafion polymer. The electrode showed an excellent selective electro-catalytic activity towards glucose in a linear range of 700 nM-10mM with a limit of detection (LoD) of 458 nM, and a limit of quantification (LoQ) of 15uM. Further, parameters like the effect of variable scan rate, solution pH, changing concentration and interference from other bio-chemicals was examined. To validate practicality, real blood serum sample was tested. Scheme I shows the stepwise electrode fabrication procedure and the real image of the miniaturized device.



Scheme I: Diagrammatic representation of (A) laser induced graphene-glucose oxidase (LIG-GOx) biosensor preparation (B) Real image of the miniaturized potentiostat (C) Chronoamperomatry studies of glucose detection in real blood serum

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<u>CP-7-EIHE 2023</u>



Designing binder free electrocatalyst to enhance electrocatalytic activity towards HER in wide pH range



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Abstract:

Owing to the increasing global population, the demand for energy and its sources is continuously increasing. As a result, there is an urgent need for clean and renewable energy source and the electrochemical water splitting can be to an efficient and green source of energy. Hydrogen gas has been found as clean energy source due to the largest energy density, eco-friendly nature, and earth abundance. However, the production of hydrogen by water splitting remains a great challenge and hence we need to develop electrocatalysts in order to enhance the production of hydrogen gas. In the recent times, transition metal dichalcogenides (TMDs) were regarded as active electrocatalysts for HER. Transition metal selenidebased catalysts have been introduced as a choice to replace noble metals in the production of hydrogen (H₂) energy via water electrolysis. Metal atom doping is an efficient method to enhance the electrocatalytic activity by increasing the active sites in the electrocatalyst. Meanwhile, the synthesis of nanomaterials on the conductive substrate can also enhance the catalytic activity of the electrocatalyst due to their large surface area and the synergistic effect between substrate and electrocatalyst. Hence, in this work, we report a one-pot synthesis of NiSe₂ electrocatalyst on Ni foam. NiSe₂/NF required a low overpotential of 126 mV and 158 mV to reach the current density of 10 mA/cm² for HER in 0.5 M H₂SO₄ and 1 M KOH, respectively. Moreover, the developed catalyst was stable in the acidic as well as in alkaline medium even after continuous electrolysis for 12 h.

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Enhanced studies on sensitivity of unique multilayer CuCo₂O₄ for non-enzymatic glucose sensing



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Abstract:

In our quest to improve the selectivity and sensitivity of novel structured multi-metal oxides for electrochemical non-enzymatic sensing of glucose, we report here the synthesis of highly porous layered CuCo₂O₄ under hydrothermal condition. The physicochemical characterization of the material was performed by PXRD, TGA, SEM and TEM. The cyclic voltammetry and chronoamperometry measurements showed good sensitivity of 364 μ A mM⁻¹ cm⁻², linear range within 2.2 mM, detection limit of 1.5 μ M and response time of 6 s under a wide dynamic concentration range of glucose during the sensing studies.¹⁻⁴ The novel CuCo₂O₄ showed good selectivity to glucose, even in the presence of high concentrations of other sugars as well as reducing species, good reproducibility and long term stability for non-enzymatic electrochemical sensing of glucose and is a promising and sensitive material for electrochemical detection of glucose.



Fig. 1 Layered CuCo₂O₄

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<u>CP-9-EIHE 2023</u>



Flexible Carbon Aerogel based Supercapacitor having Outstanding Energy density



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Abstract:

Supercapacitors (SC) are highly promising electrochemical energy storage (EES) device for pulse power energy applications, where it requires high power in a short interval of time. Since SC has high power density, fast charge-discharge rate, and long cycle life, it finds many versatile applications such as electric vehicles, power electronics, and pulsed power devices. The present work demonstrates a flexible supercapacitor based on free-standing carbon nanotube (CNT) aerogel showcasing higher energy and power density compared to the reported values. The CNT aerogel electrode showed a maximum specific capacitance of 168 F/g, high energy density of 45.97 Wh/Kg, and power density of 1.4 kW/Kg in 1M KOH electrolyte (vs. Ag/AgCl) at a current rate of 2 A/g. The CNT aerogel-based electrode exhibited high electrochemical stability after 10000 cycles with 95.5 % capacitance retention. Thus, our study can take the flexible supercapacitors to the commercial level with the advantage of scalable production of extremely lightweight CNT aerogel electrodes.



Fig.1 Cyclic voltammetry of CNT aerogel-based electrode in 1M KOH electrolyte

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Mineralization of Congo Red Dye by Electrochemical Method



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Abstract:

Pollution poses serious threats to both the environment and the organisms. Availability of potable water is a challenging problem faced all over the world¹. Many organic pollutants are toxic and proved to be carcinogenic² even if present at very low concentrations. Congo red dye is one of the non-biodegradable organic pollutants discharged from the textile industries. Hence it needs to be treated well to avoid its unfavourable impact on human beings and environment. In the present work, Congo red dye is treated using a platinum electrode in presence of oxidizer. A table top experimental set up is developed and is being utilized to carry out Congo red dye effluent treatment experiments for optimizing process parameters. Congo red dye is treated at optimized process parameters i.e. strong electrolyte (NaCl) of 0.5 M to 1 M, pH from 3 to 4, applied potential from 6 to 9 V and concentration of oxidizer from 10 to 20 mM. It has been observed that 50 ppm Congo red dye is successfully mineralized to a safe discharge limit of 1 ppm³, which is also recommended by United States Environmental Protection Agency (USEPA) for land water. The treated solution has been analyzed by High Performance Liquid Chromatography (HPLC) and Total Organic Carbon (TOC) analyzer.

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<u>CP-11-EIHE 2023</u>



Phase Dependent, Mesoporous Potassium Tantalate-Reduced Graphene Oxide Nano cube Architecture for High Performance Hybrid Supercapacitors



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Abstract:

Among advanced energy storage devices supercapacitors are noteworthy due their high power density. However, advancements have been noteworthy in the field of high-performance hybrid supercapacitors, which comprises of pseudo capacitance and EDLC combined. We have prepared Perovskite Potassium tantalate nano cubes (KT-NCs) and Potassium tantalate - Reduced graphene oxide composite nano cubes (KT-rGO NCs) using hydrothermal method. Detailed study of both KT-NCs and



KT-rGO NCs were done using characterization techniques like XRD, FTIR, BET, Raman, HRTEM for structural analysis. KT NCs showed Specific capacitance of 565 Fg⁻¹, thus we have synthesized rGO composite to bare tantalate to enhance its performance. Herein, we have fabricated a hybrid supercapacitor electrode material KT-NCs and KT-rGO NCs and tested their electrochemical performance. The materials showed high performances with specific

capacitance of KT NCs and KT-rGO NCs at 565 Fg⁻¹and 850 Fg⁻¹ at run rate of 1 mVs⁻¹. Energy densities of both were found to be 28.24 Wh/Kg and 29.50 Wh/kg with good retention capacities. Electrochemical measurements were used to analyse various parameters pertaining to its charge storage capacity.

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<u>CP-12-EIHE 2023</u>



Heterogenous Bimetallic Cobalt tantalumselenide as Electrode Material in High Performance Asymmetric Supercapacitor



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Abstract:

Energy storage devices like batteries and supercapacitors are of high interest in present day due to its varied uses. Further, growing demand for light and portable devices has led to discovery of thin and flexible supercapacitors. An effective tool in enhancing the cell voltage and performance is to fabricate a faradaic positive electrode and EDLC negative electrode to form an asymmetric device. Relative lower electronegativity of selenides leads to more flexible structures, preventing disintegration. Thus, selenides are more preferred than oxides and sulfides. Herein, we have synthesized a bimetallic selenide comprising



of cobalt and tantalum with high synergistic effect between the selenium ions and the valence electrons of metals. Due to this, CoTaSe has exhibited improved electrochemical performance when compared to a single metal selenide. Specific capacitance of CoTaSe was found to be 460 Fg⁻¹ and that of 370 Fg⁻¹ for tantalum selenide at constant run rate of 10 mVs⁻¹ with high retention capacity for bimetallic composite. The synthesized materials were characterized using XRD,

SEM, TEM and XPS. Electrochemical analysis like cyclic voltammetry, Electrochemical impedance spectra and Chronopotentiometry were done to measure its charge storage capacity.

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<u>CP-13-EIHE 2023</u>



Nanoscale 'all-organic' molecular electrochemical supercapacitors: A step closer to molecular power banks



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Abstract:

Modified graphite rods (GRs) are produced by covalently bonded anthracene (ANT) layers with azo groups as bridges to graphite rods (GRs) recovered from spent inexpensive EVEREADY cells (1.5 US \$ for 10 cells of 1.5 V) via a simple, controlled, scalable, inexpensive, and adaptable electrochemical grafting method.^[1] The potentiostatic and galvanostatic measurements show that the overall capacitance of the ANT-modified GR (ANT/GR) is 100 times greater than that of an unmodified GR tested with 0.1 M H₂SO₄ electrolyte. The presence of various types of nitrogen atoms in molecular layers plays a critical role in the increase of capacitance due to its higher hydrophilicity, host-guest interactions, and larger numbers of available electroactive sites.^[2] The molecular films exhibit outstanding galvanostatic charge-discharge (GCD) cycling stability (10,000) that works at low potential. Since DC measurements are restricted to the



capacitor's frequency response, electrochemical impedance spectroscopy (frequency ranges of $10^{-1} - 10^4$ Hz) was used to fully understand the charge storage capabilities. The "allorganic" films exhibit excellent electrical conductivity and capacitance balance, a high diffusion coefficient toward ferrocene, strong thermal stability (80 °C), and are simple to produce in good yield, even on flexible electrodes.

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<u>CP-14-EIHE 2023</u>



Design of Mn-N-C electrocatalyst for oxygen reduction reaction



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Abstract:

A Mn single-atom catalyst (SAC) was designed with high Mn content (7.34 wt%) using polypyrole hydrogel derived nitrogen doped porous carbon matrix. The catalyst with densely populated Mn-N-C active sites shows excellent activity towards electrochemical oxygen reduction reaction (ORR) both in acidic and alkaline medium. With an onset and half-wave potential of 0.907V and 0.818V vs RHE in alkaline medium the catalyst demonstrates ORR performance comparable to that of Pt/C. Oxygen reduction reaction (ORR) is of vital importance in energy conversion and storage devices such as fuel cell and metal air battery [1]. Owing to the high cost and scarecity of platinum group metals (PGMs), design of non-PGM electrocatalyst is essential, which is indeed a challenge. Among the PGM free catalysts, nitrogen-coordinated metal (M-N-C) based single-atom catalysts (SACs) have demonstrated comparable ORR activity to that of Pt/C. Among the M-N-Cs, the best performing Fe-N-C catalyst is often criticised for promoting Fenton's reaction leading to H₂O₂ formation, which is detrimental to fuel cell operation. As a PGM-free and Fe-free catalyst, we synthesised a Mn-N-C catalysts using a poly-pyrrole derived N-rich substrate. The XRD patterns of the catalysts show no peak due to crystalline phase, SEM and EDS mapping shows uniform morphology and elemental distribution and CV and LSV shows excellent ORR activity in alkaline medium. The catalyst demonstrates on E_{on} and E_{1/2} of 0.907V and 0.818V vs RHE in O₂-saturated 0.1M KOH and a limiting current density (J_{lim}) of -4.693 mA/cm² with just 400µg/cm² loading.



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Copper-Silver Ionization Electrochemical Cell for Disinfection in Drinking Water



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Abstract:

Water is a necessary resource for life and must present high microbiological quality for consumption purposes. Therefore, the disinfection of drinking water plays crucial role in controlling and preventing it from transmitting pathogens and spreading diseases [1]. Copper-silver ionization is a disinfection process, primarily used to control Legionella, the bacteria responsible for Legionnaires' disease [2,3]. In the present study, Cu-Ag ionization electrochemical cell is configured for disinfection of drinking water. The electrochemical cell is configured such that cathode (copper sheet) and dual anode consisting of silver rod impeded on copper sheet are separated by diaphragm (microfiber mesh) maintaining zero gap between the electrodes. This electrochemical cell of 1L (volume) removes >90% bacterial colony when operated for one hour at a current density of 2mA/cm². The schematic diagram of electrochemical cell and digital photograph of culture plates showing bacterial colonies in water before and after the electrochemical disinfection are



ppm of Ag [Drinking water specification of Cu (1.5)ppm) and Ag (0.1ppm)]. The negligible amount (in µg level) of Cu and Ag ions are released

from anode, hence these sacrificial anodes can be used for long duration (>1000 hrs) of time.

Figure: 1) Schematic diagram of electrochemical device of Cu-Ag Ionization and 2) Bacterial colonies in feed water (lake) (A) Treated water (B)

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<u>CP-16-EIHE 2023</u>



Understanding magnetic field assisted superior electrocatalytic activity of hard carbon supported metal oxides for hydrogen and oxygen evolution



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Abstract:

Considering the current need for world energy market, a cleaner, safer and eco-friendly energy technology such as fuel cell (specially hydrogen and oxygen), is much appreciated. Electrolysis of water can produce large scale H₂ and O₂ in a greener way without generating CO₂. In the past few decades, investigations are going on in this field to find an efficient electrode candidate to achieve high activity and acceptable stability for more effective water splitting. In this work we report an advanced strategy of improving electrocatalytic activity by introducing external magnetic field. Hard carbon [Nanocarbon Florets (NCF)] supported NiO nanoparticles achieved more than 10% and 40% decrement in the overpotential and Tafel slope value for both hydrogen and oxygen evolution under the influence of external magnetic field of 200 mT. The current density could be increased upto 5-fold at a constant overpotential of 450 mV by applying some desired magnetic fields. The time dependent LSV study further demonstrates the magnetic property and sustainability of magnetoresistance and the magnetic field-induced spin-polarized kinetics. This investigation provides a promising way for numerous energy conversion technologies leading to highly effective catalysis.



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<u>CP-17-EIHE 2023</u>



In-Situ EQCM Based Structural Elucidation of Etodolac-Anti-Inflammatory Drug-Metabolite and Its Electrochemical pH Sensor Application



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Abstract:

Etodolac (ETO) is an anti-inflammatory drug that has been widely used to treat osteoarthritis and rheumatoid arthritis. The drug undergoes bio-activation in the presence of enzyme, Cytochrome P450 leading to the formation of highly toxic phase-I metabolites. In this study, etodolac's biomimetic ex-situ pharmacokinetic investigation was explored by electro-analytical technique utilizing a glassy carbon electrode modified with multiwalled carbon nanotube (GCE/MWCNT) as a carbon network system that mimics biological functional. Under the electrochemical potential cycling condition of the modified electrode with drug, in a window, -0.4 V to 1.2 V vs Ag/AgCl led to formation of a well-defined surface-confined redox peak at apparent potential $E^0 = 0.25$ V in pH 7 phosphate buffer solution and calculated surface excess value is, $\Gamma = 49$ n mol cm⁻². The drug chemically modified electrode is designated as GCE/MWCNT@ETO-Redox. The modified electrode and its extract were subjected to several ex-situ physio-chemical characterizations including IR, NMR, HPLC, and HRMS to reveal the true active drug species. In further, in-situ characterization using electrochemical quartz crystal microbalance (EQCM) was also subjected to support the analysis (given below). The estimated gravimetric drug-redox species mass loaded on the electrode surface was 1.2µg, and its molecular weight was 319 g/mol. Obtained results



correlate with the pharmacokinetic of the ETO drug. As an independent study, the redox feature of the modified electrode system was explored for voltammetric pH sensor application. A plot of Epa/V vs pH showed a linear line with a slope value, -63.2 mV/pH in a pH window, 2 -11. Impedimetric analysis was also performed for the pH-related sensor application. As the pH was raised, the electrode displayed a linear increase in resistance (R_{ct}) and a reduction in double-layer capacitance (C_{dl}).

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<u>CP-18-EIHE 2023</u>



Design and Synthesis of Nano-sheet and Nano particle Embedded MOFs for Electro-catalytical Splitting of Water



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Abstract:

Porous coordination polymers (PCPs), which also known as metal-organic frameworks (MOFs) are emerged as potential materials of the decade, particularly for gas storage, separation, catalysts and sensors etc. However, MOF existing in the literature were mostly instability with respect to moisture and bulk water. Besides these traditional MOFs, we have been designed and synthesized an organic rich low density based ligands and converted them in to MOFs shown exceptional superhydrophobic properties¹⁻⁴. In the present study, we achieved few Nano-sheet based superhydrophobic MOFs and also Nano particle embedded superhydrophobic MOFs for the electro-catalytical applications for water splitting applications.⁵ We will be presenting in this study synthesis, characterization and electro-catalytical properties of few Nano-sheet/ Nano particle embedded superhydrophobic MOFs.



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<u>CP-19-EIHE 2023</u>



Investigation of Electrochemical CO₂ Reduction to Formate on Sn Foil and Mechanistic Analysis



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Abstract:

Electrochemical carbon dioxide reduction reaction (CO_2RR) provides an alternative pathway for producing value-added chemicals or fuels, transforming carbon dioxide into products such as formic acid, carbon monoxide, etc¹. This work emphasizes understanding the electrochemical CO_2 reduction to formate on the tin foil using an H-cell. polarization studies were conducted in 0.1 M KHCO₃ solution at different reduction potentials varying from -1.3 to -1.9 V. We achieved a faradaic efficiency of above 80 % towards formate at -1.8 V vs Ag/AgCl with a partial current density of above 8 mA/cm² using the Sn foil. The major mechanisms suggested in the literature are based on density functional theory (DFT) and most mechanism steps are described in acidic media². Here we are presenting a kinetic-based model to assess the mechanism of electrochemical CO_2 reduction to formate on the Sn surface in alkaline or neutral media.

Keywords: CO₂ reduction, H-cell, Formate, Mechanistic analysis.

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Chalcogenide/MXene Heterostructures as Electrocatalysts for Efficient Generation of Hydrogen Fuel



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Abstract:

To hasten the worldwide transition to renewable resources, developing environmentally sound and economically viable energy production methods is inevitable. Molecular Hydrogen has long been flaunted as the ideal fuel for the future due to its high gravimetric energy density. The widespread adoption of the hydrogen economy can be fulfilled by water electrolysis, where the creation of long-lasting, extremely effective catalysts is crucial.¹ MoS₂, a 2D layered chalcogenide, is a promising HER (Hydrogen Evolution Reactions) electrocatalyst due to its high specific activity surface area, durability, and cost-effectiveness, compared to noble metals. However, their HER efficiency is severely constrained by the problematic nanostructuring and/or phase engineering for exposing active edge sites.² Herein we report the facile fabrication of MoS₂/Mo₂CT_x heterostructures with a robust interfacial relationship established by the *insitu* growth of MoS₂ over functionalized-MXene. The strongly coupled MoS₂/Mo₂CT_x, while suppressing the catalyst oxidation at its surface during electrolysis, affords highly active HER sites delivering lower overpotentials and smaller Tafel slopes for HER compared to bare MoS₂ or 2D MXenes. Moreover, the robust interface established between the layered MoS₂ and Mo₂CT_x structures was advantageous for long-lasting operations at higher current densities, meeting the requirements of rigorous industrial-scale water splitting.

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CP-21-EIHE 2023



Nitrogen-doped porous carbon coated on MnCo₂O₄ nanospheres as electrode materials for high-performance asymmetric supercapacitors



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Abstract

Spinel-based nanostructured materials are commonly used as promising electrode materials for supercapacitor applications. The combination of Heteroatom doped carbon materials coated with spinel substantially improves the specific capacitance and cyclic stability. In this work, dopamine-derived Nitrogen-doped Carbon was coated on spinel phase MnCo₂O₄ nanospheres using simple solvothermal and calcination methods [1]. The electrochemical performance of MnCo₂O₄@nitrogen doped carbon electrode material was analyzed by cyclic voltammetry, Galvanostatic charge-discharge, and electrochemical impedance spectroscopy techniques. MnCo₂O₄@nitrogen doped carbon exhibits the highest specific capacitance of 1200 F/g at 1 A/g compared to MnCo₂O₄ spheres are 726 F/g and exhibits excellent cyclic stability (capacitance retention of 87 % at 7 A/g after 3000 cycles). The excellent cycling stability might benefit from the synergistic effect between a coating of conductive nitrogen-doped carbon on porous MnCo₂O₄ spheres. Furthermore, an asymmetric supercapacitor device was fabricated by using the optimized composition of MnCo₂O₄@nC-2 as a positive electrode and nitrogen, sulphur doped reduced graphene oxide (NS-rGO) as a negative electrode, respectively. This asymmetric supercapacitor device achieves a maximum energy density of 61.0 Wh kg⁻¹ at a power density of 2889 W kg⁻¹ and possesses excellent capacitance retention of 95 % after 5000 cycles at 7 A/g.

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CP-22-EIHE 2023



Synthesis of LaW/Ag/GnRbs nanocomposite: Application as transducer material for the simultaneous nano molar detection of synthetic dyes and as anode material for Li ion batteries.



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Abstract:

In this present research, We have synthesized the lanthanum tungstate/silver nanoparticle/graphene nanoribbons (LaW/Ag/GnRbs) nanocomposite as a novel system for the simultaneous electrochemical determination of two synthetic dyes sunset yellow (SY) and acid yellow (AY). The as-synthesized LaW/Ag/GnRbs nanocomposite was characterized by UV, XRD, FESEM, EDX, TEM and XPS analysis. The enhanced anodic peak currents represented the excellent analytical performance of simultaneous detection of SY and AY in the range of 20 nm to 450nM, with a low limit of detection (LOD) of 0.025nm for SY and 0.050 nM for AY.

The electrochemical performance of the LaW/Ag/GnRbs nanocomposite for lithium ion battery has shown considerable progress in terms of cyclic performance, better rate capability and high discharge capacity. The half-cell of lithiated LaW/Ag/GnRbs nanocomposite vs. SCE delivers a capacity of 227.86 mAhg⁻¹ up to 10 cycles at 0.08 mA. The full cell configuration LaW/AgNPs/GnRbs|aq. saturated Li₂SO₄|LiMn₂O₄ delivered a discharge capacity of 240.24 mA h g⁻¹ in the potential window of 1.0 V to 0.0 V. The battery performance of the cell has been increased significantly with 96.95% columbic efficiency.

<u>CP-23-EIHE 2023</u>



One pot synthesis of FeNi alloy nanoparticles decorated on N-doped Carbon nanosheets for Oxygen Evolution Reaction in Alkaline media



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Abstract:

The development of cost-effective, highly efficient and robust multi-functional electrode materials can dramatically reduce the overall cost of electrochemical devices. FeNi alloy catalysts have received increasing attention due to their low cost, easy availability, and excellent oxygen evolution reaction (OER) catalytic activity [1]. Although it is considered that the co-existence of Fe and Ni is essential for the high catalytic activity, the identification of active sites and the mechanism of OER in FeNi alloy catalysts have been discussed in recent literatures [2]. FeNi alloys and the related mechanism in the alkaline water oxidation process from the perspective of crystal structure, composition, modulation and structural design. Here we report FeNi alloy nanoparticles decorated on nitrogen doped carbon nanosheets shows the overpotential of 302 mV at a current density of 20 mA cm⁻² in 1 M KOH alkaline electrolyte.

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<u>CP-24-EIHE 2023</u>



Highly Crystalline Ordered Macroporous Metal Organic Framework for Aqueous Aluminum Ion Battery: Effect of Redox Additive Electrolyte in Charge Storage



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Abstract:

Rechargeable aqueous aluminum-ion batteries (RAIBs) are considered as a promising candidate due to aluminum's abundance and safety issues amongst all of the proposed nonlithium-based battery systems. To date, exploring compatible cathode materials and its coupling with a suitable aqueous electrolyte, to get the high performance, is a key issue for the industrialization of RAIBs. In this work, we present the excellent aluminium intake characteristics of ZIF 67 as a cathode in aqueous electrolyte. The ordered macroporous framework of ZIF 67, have regularly interconnected macroporous channels and large surface area. As a result, when evaluated as a cathode material for RAIBs, the ordered porous structure could effectively facilitate the diffusion of AI^{3+} and also increase the contact area with electrolyte, while ensuring higher exposed active sites. Thereby, the well-defined and extremely porous structure of ZIF 67 exhibit superior discharge capacity of 288 mAh g⁻¹ at 0.2 A g⁻¹ of current density. Furthermore, enhancement in the charge storage capability of ZIF 67 can be obtained by developing a novel redox additive based electrolyte. In redox modified electrolyte, the ZIF 67 cathode exhibits 51% increment of specific capacity, with improved rate capability and cycling stability via redox transformation and intercalation of redox species.

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High performance in-situ grown FeVO₄@PANI composite for low-cost aqueous Al-ion battery



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Abstract:

Aqueous Al ion battery has the potential to become a cost-effective, safe, and environmentally benign energy storage device. But, very few materials have been explored as a cathode for aqueous Al ion batteries. Hence, designing high performing cathode materials for aqueous Al ion batteries is drawing a lot of attention. Here, we will present a new cathode material by the in-situ growing of PANI nanorod on the nanocapsules of FeVO₄. The prepared nanocomposite provides a higher number of ion transport channels and delivers the highest specific capacitance of 473 mAh g⁻¹ (at 0.2 A g⁻¹). The value is almost 50% higher than the pristine FeVO₄ cathode (320 mAh g⁻¹ at 0.2 A g⁻¹). The reported value is amongst the best reported cathode materials for aqueous Al ion batteries. The FeVO₄@PANI composite shows improved cycling stability (~98% after 1000 cycles) at 3 A g⁻¹ in comparison to pristine FeVO₄. Additionally, we report the performance of FeVO₄ and FeVO₄@PANI composite at different electrolytes like KCl, NaCl, and KOH, to confirm the Al ion intercalation/de-intercalation into and from the host structure. XRD patterns of the as-fabricated cathode materials, after the cycling test, confirms the stability of the material.

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S. Nandi, S.K. Das; ACS Sustain. Chem. Eng., 2019 7 (24), 19839-19847.



Uranium Electrorefining in Engineering Scale



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Abstract:

PyroProcessing Research and Development Facility (PPRDF) is a facility being setup in IGCAR for Engineering scale development of pyrochemical reprocessing in India [1]. Metal fuelled Fast Breeders Reactors (FBRs) in combination with pyrochemical reprocessing is one of the most promising nuclear fuel cycle options from doubling time, proliferation resistance, minor actinide recycling, co-location and nuclear waste generation point of view [1]. In this regard execution of first U- Electrorefining in High Temperature ElectroRefiner (HTER) in PPRDF was successfully completed with 4.5kg Uranium deposit on solid cathode (Fig.1). The execution of first U-Electrorefining experiment was carried out in planned manner with several major intermediate activities, such as, achieving required leak tightness (0.1vol% per hr) and purity ($O_2 \& H_2 O < 50$ ppm each) of 500m³ containment box containing argon, transfer of 900kg of molten salt from salt storage vessel to HTER vessel & maintaining its temperature at 450°C, in-situ preparation of 2 wt% UCl₃ in molten salt by reacting it with CdCl₂, loading of 10Kg U metal into anode basket & remotely transferring it into HTER vessel, putting solid cathode into HTER vessel and finally commencement of Electrorefining operation.



Fig.1: Uranium deposit on solid cathode after Electrorefining operation

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CP-27-EIHE 2023



In-situ NADH Regeneration via Lactate Dehydrogenase-Catalyzed Electron Transfer Mechanism: A Spectroelectrochemical Study



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Abstract:

In this work, electrochemical regeneration of NADH on ITO electrode and concurrent monitoring using in-situ spectrophotometry is demonstrated (Scheme 1). NADH cofactor is typically used as a reducing agent in the Krebs cycle or TCA cycle to create lactate from pyruvate [1]. This study has demonstrated on the heterogeneous path which is effective and compactable than homogenous systems. Particularly in reagent-less biosensor applications, the regeneration of NADH on the heterogeneous surface is especially beneficial. In the same way, the conversion of NAD⁺ to NADH by electrochemical reduction is an advantageous in regenerative technique, as it enables the monitoring of entire biofuel production pathways by electrochemical methods. Here, the enzyme (lactate dehydrogenase-LDH) and coenzyme (NAD⁺) were coimmobilized with redox mediator (5,5-Dithiobis(2-nitrobenzoic acid) -DTNB) to acquire the bioelectrocatalytic NADH regeneration, followed by get the more effective conversion of lactate into pyruvate on the heterogeneous surface. In order to confirm NAD⁺ electrochemically converted into NADH, the cyclic voltammetry technique was carried out (the potential applied from -0.40 V to -0.86 V vs Ag/AgCl) which involved 2-electron and 1-proton reaction. As a result, the reduction of immobilized NAD⁺ produces four different variety of isomers, including (NAD-NAD) dimer, 1,2 NADH, 1,4 NADH (active form), and 1.6 NADH, which are studied on the modified ITO electrode. Even more important, the dimerization of cofactor which renders it to be enzymatically inactive. Therefore, it is crucial to figure out how to renew a higher percentage of active NADH on the heterogeneous interface, when surface-confined reagents are present [2]. This is evidenced by the spectrophotometric technique, it has been employed for

understanding the characteristics of charge transfer process associated with the surface-confined redox-active molecules. The absorbance peaks allow us to determine the type of molecules that are formulating NAD+ (260 nm), 1,2 NADH (395 nm), 1,4 NADH (340 nm) and 1,6 NADH (345 nm) respectively.



Scheme 1: Pictorial representation of the NAD⁺/ NADH regeneration on ITO electrode.

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<u>CP-28-EIHE 2023</u>



Multi-Scale Modeling of Metal Release Pathways of Blood Serum Iron-Transferrin



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Abstract:

Human serum transferrin (sTf) is a glycoprotein that regulates iron transport in the human body. Iron-loaded sTf binds with transferrin receptor (TfR) internalized into the cell at pH 5.5[1]. The acidic endosomal condition facilitates the release the iron by the endocytosis-mediated process. Different pathways have been reported regarding the release of iron into cell [2]. However, there is an ambiguity concerning the exact redox potential and the structural changes involved in the iron release process. Herein, we have employed density functional theory-based calculations on different synthetic models of sTf and the protein itself to unveil the metal release pathways. We find that the computed redox potential is too low



in agreement with the experimental data thus the reduction pathways are ruled out. The reduction can be modulated for the actual protein itself through the redox Bohr effect. The computed hardness parameters of Fe(III) and Fe(II) ions and the proton affinities of the amino acid ligands predict a protoncoupled electron (PCET) transfer pathway. The computed redox potential of PCET species is 0.43 V which is favorable at the physiological condition. Multi-scale model calculations are in progress in our laboratory to substantiate our quantum

chemical predictions.

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Electrochemical Analysis of Cobalt Oxide Nanoparticles Synthesized by Hydrothermal Method.



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Abstract:

Intensive research in the area of electrochemical devices found cobalt oxide nanoparticles as an effective material for tunable applications owing to their excellent electrode properties. The present work focuses on the spinel-type cobalt oxide nanoparticles (Co_3O_4), synthesized through a one-step hydrothermal method, using cobalt nitrate hexahydrate as a precursor. X-ray diffraction (XRD) and Raman spectroscopy were performed to study the structural behaviour of the sample. Williamson-Hall plot assured the microstrain effect from the XRD analysis. The Raman active modes of the sample were concordant with the standard modes identified. Due to the charge transfer between oxidation states, the absorption spectrum and Tauc plot ascertained the two direct bandgaps of Co_3O_4 . Brunauer-Emmett-Teller-specific surface area measurement was carried out for this sample. The electrochemical analysis of cobalt oxide nanoparticles



was explored using nickel foam as the substrate. Preliminary studies, including cyclic voltammetry (CV), galvanostatic charge-discharge and electrochemical impedance spectroscopy (EIS), were tested in 3 M KOH electrolyte. The Co_3O_4 electrode showed a specific capacitance of 416 Fg⁻¹ at a current density of 5 Ag⁻¹ and attained cyclic stability with a retention ratio of 92% after 500 cycles, proposing its possible application in electrochemical capacitors.

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<u>CP-30-EIHE 2023</u>



Optimization of Praseodymium based Perovskite as Electrocatalyst for Oxygen Reduction Reaction.



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Abstract:

ABO₃-type oxides with flexible and adjustable A- and B- site are ideal model catalysts to unravel the relationship between the electronic structure and electro catalytic activity e.g.-oxygen reduction reaction (ORR). It has been well understood in our recent work that the secondary metal dopant at A-site can regulate the electronic structure and improve the ORR activity. Praseodymium based perovskites Pr_{1-x}Sr_xMnO₃



(x=0.1, 0.2, 0.3, 0.4), denoted as PSM-0.9, PSM-0.8, PSM-0.7 and PSM-0.6 respectively were prepared by sol-gel technique. The structural properties and morphology of the prepared catalysts are

studied with the help of XRD, SEM and XPS. Oxygen reduction reaction (ORR) activities of the prepared catalysts are reported in alkaline medium. Among the prepared catalysts PSM-0.7 with onset potential - 0.02 V is found to be the most active ORR catalyst. The Koutechy-Levich plot obtained from rotating disk electrode shows a higher number of electron transfer "n" for PSM-0.7 catalyst. Further, lower tafel slope of PSM-0.7 catalyst justifies its higher catalytic activity. The higher catalytic activity is ascribed to the oxygen vacancies and Mn⁴⁺ concentration as confirmed by XPS analysis.

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<u>CP-31-EIHE 2023</u>



Electrochemical detection and decomposition of nitrate and polyphenolic compounds using reduced graphene oxide supported Ferrite based composite modified electrode



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Abstract:

Nitrate is one of the dreadful water contaminants worldwide. The sources of nitrate contamination in the surface and underground water are due to the excessive use in the fertiliser for agriculture. The detection and degradation is very much important due to their detrimental effect on the environment, industry, agriculture and biological systems. Again, phenols, polyphenols and their derivatives are the toxic organic pollutants that are generated from industrial processes. Ferrite based materials are exhibited good electrocatalyte for the detection and degradation of nitrate and phenolic compounds. The Nickel and cobalt ferrite nanocomposite materials exhibited good catalytic activity towards the reduction and degradation of nitrate and organic polyphenolic compounds due to their enhanced the charge transfer property. The ferrite nanocomposite modified electrode demonstrated wide linear dynamic range with micro to nano molar detection limit for nitrate as well as phenolic compounds. The degradation of the nitrate was carried out by imposing the cathodic potential of -1.2V to the working electrode. Nitrate is being reduced to nitrite followed by evolution of the N₂ in the alkaline condition. The percentage of degradation of nitrate has been accomplished up to 90% in the duration of electrolysis around 1500s containing 1mM concentration of KNO₃. Similarly, the degradation of polyphenolic compounds was achieved up to 88% in the duration of electrolysis around 1800s containing 10mM concentration of Phenolic compounds. Hence, the ferrite based composite material was found to be suitable for the detection and degradation of inorganic as well as organic pollutants.

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<u>CP-32-EIHE 2023</u>



MnMoO₄ nanorods anchored on P-doped-g-C₃N₄ nanosheets as an electrocatalyst for voltametric determination of antihistamine drug Promethazine



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Abstract:

The varied usage of antihistaminic drugs became an ecological contaminant which in turn needs to be potentially scrutinized. In this concern, the present work was aimed to develop an electrochemical sensing probe to monitor a Phenothiazine derivative drug, Promethazine hydrochloride (PMZH), by modifying a glassy carbon electrode (GCE) with manganese molybdate (MnMoO₄) unified with Phosphorus doped graphitic nitride nanosheets (P-g-C₃N₄). The electrochemical examination of the developed sensor was performed using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques. The as-prepared MnMoO₄/P-g-C₃N₄ nanocomposite was characterized and it was confirmed by diverse analytical techniques like XRD, FT-IR. In addition to that, the physical morphology of the MnMoO₄/P-g-C₃N₄ nanocomposite was scanned with HR-TEM. The MnMoO₄/P-g-C₃N₄ nanocomposite



modified GCE plays a crucial role in electrochemical detection of PMZH, which results in excellent antiinterference ability, a lower detection limit of 68.37 pM, wide linear ranges from 0.1 to 0.01 μ M, and good sensitivity of about 0.8169 μ A nM⁻¹ cm⁻². The MnMoO₄/P-g-C₃N₄/GCE are

proficiently employed in real-time sensing of PMZH in lake water and urine samples. These electrochemical studies show the integral new vision on the electrocatalytic functioning of the modified GCE and have also shown excellent reproducible results in nano-trace levels.

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<u>CP-33-EIHE 2023</u>



Electrochemical Performance of Na₃V_{1.96}Co_{0.02}(PO₄)₂F₃@C as Cathode Material in Sodium-ion Batteries



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Abstract:

Moulding a suitable cathode with optimum electrochemical performance is of utmost importance for an efficient Na-ion battery. The polyanionic compounds have emerged as a propitious cathode in light of its high operating voltage, superior ionic mobility and enhanced structural stability. However, the highly established, sodium super ion conductors (NASICON), Na3V2(PO4)2F3 suffers from low electronic conductivity [1]. In this work, we explore the effect of Co2+ substitution in vanadium site of carbon coated NVPF (NVPF@C) on its electrochemical performance as cathode material in SIB. Morphological studies indicate that Co2+ substitution in NVPF@C leads to a reduction in particle size which positively impacts its electrochemical performance. NVPFCo@C shows high reversible capacity of 142 mAh g-1 at 0.1C with better rate capability and enhanced cycle performance compared to pristine NVPF@C. EIS studies indicate decreased charge transfer resistance with Co2+ substitution in NVPF@C which improves Na+ ion diffusion in the electrode/electrolyte interface.

Experimental data obtained in this work indicates that Co2+ doping in NVPF@C improves the sodium ion diffusion and electronic conduction which results in enhancement in its electrochemical performance.



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Role of Polymer Electrolytes in Metal-Ion Batteries



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Abstract:

Intensive research effort is aimed worldwide to improve performance, cost, safety, and energy density of batteries as they play a vital role to reduce carbon footprint and achieve net zero 'C' target¹. Conventional batteries contain liquid electrolytes due to high ionic conductivity and energy density, good contact with electrodes, better wettability though they have several issues such as safety, harmful leakage, poor physical and chemical stability, use of separators². Therefore, there is a need to replace toxic liquid electrolyte by highly conductive solid electrolytes with advantages like lack of dendrite formation, high conductivity, lower costs, high safety, good chemical and physical stability³. Though solid ceramic electrolytes show high conductivity, they suffer from poor surface properties and high interfacial resistance. Therefore, several researches have been reported on solid polymer electrolytes for large scale metal-ion battery application because of their favourable mechanical properties, ease of fabrication, high safety, lower costs, chemical stabilities, light weight, handling in flexible and thin film batteries, lack of interfacial transport issues and high energy density^{4,5}.

Here we provide a summary on the recent developments, perspectives, current challenges of polymer electrolytes in metal-ion batteries and strategies to improve them for the successful commercialization in near future.

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<u>CP-35-EIHE 2023</u>



Covalently functionalized Graphene Oxide-NiMOF Hybrid as Electrocatalyst for Hydrogen Production



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Abstract:

In regard to the pursuit of clean hydrogen energy, exploration for advanced materials as electrocatalysts for water splitting reaction is a growing interest in renewable energy research.¹ 2D-nanomaterials with enormous effective surface area for hydrogen adsorption-desorption kinetics have proved their potential in hydrogen evolution reactions (HER) by water splitting. In this context, we have developed graphene oxide (GO)-NiMOF hybrids with well-defined morphology via covalent functionalization. Typically, the GO-NiMOF hybrid was synthesized via facile sonochemical technique utilizing 1:1 w/w of ester functionalized GO and Ni-MOF. The structural characterisation of the as developed GO-NiMOF hybrid is done using FTIR, Raman, XRD analysis and the morphology is analysed using FESEM and TEM analysis. The hybrid possess high specific contact surface area with exposed surface sites for intermediate adsorption-desorption^{2,3} while the covalent functionalization favours charge transfer and ensure microstructure stability while preserving the large surface area.⁴ The charge transfer between GO and NiMOF is expected to reduce the overpotential of HER. Owing to morphology dependent synergistic effect of both charge transfer and microstructure stability, GO-NiMOF hybrids exhibited excellent electrocatalytic activity under alkaline conditions.

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<u>CP-36-EIHE 2023</u>



Magnetic Field Dependent electrocatalytic HER and OER of CoFe₂O₄



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Abstract:

Till date, magnetic field dependent variations in specific capacitance have only been reported in simple binary oxides or alloys. Ternary spinels are often considered to be a composite of two or more monocationic entities, which allow them to deliver high electrocatalytic performance. Herein, spherical particle like electrode of $CoFe_2O_4$ was fabricated to serve as a bifunctional electrocatalyst for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) [1]. Such measurements are mostly performed under ambient condition. We will show that performance of ternary or higher oxides, having magnetic atoms, can be enhanced by varying the magnetic field. Kinetic Tafel slope analysis suggests that the HER follows the Volmer–Tafel mechanism (~25 mV dec⁻¹) under 75 gauss magnetic field, indicating that the recombination of the two adsorbed hydrogen atoms is the rate-determining step. During the OER under 75 Gauss, the $CoFe_2O_4$ acts as a chemical and electroconductive host to stabilize the key intermediate. It is indicated that the magnetoresistance (MR) effect caused by spin electron scattering is dominant in affecting the apparent electrocatalytic activity in the magnetic field-assisted OER process. All electrocatalysts also have a high probability of experiencing the magnetic field-assisted OER process.

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<u>CP-37-EIHE 2023</u>



Hydrothermal Synthesized Sm₂O₃ Nanoparticles as a Highly Efficient Photo catalysts for Degradation of Anthraquinonic *dyes*



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Abstract:

Catalyst or template-free synthesis of Samarium Oxide (Sm_2O_3) nanoparticles were synthesized by hydrothermal method using $Sm(NO_3)_3 \cdot 6H_2O$ starting materials under basic pH condition. The prepared sample was characterized by powder X-ray diffraction (XRD) transmission electron microscope (TEM), Fourier transform infrared spectroscopy (FTIR) and UV–Visible diffuse reflectance spectroscopy (DRS). The powder XRD pattern confirmed the formation of cubic phase Sm_2O_3 with particle size of 8.46nm. The photocatalytic activity of the synthesized nanoparticles was evaluated by studying the degradation of a model dye, Alizarin red S (ARS) under visible light irradiation. The degradation of different concentrations of ARS was studied with 30 mg Sm_2O_3 and a feasible mechanism was proposed. More than 95% of ARS (50 mg/L) was degraded within 30 min.



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Electrical and sensing properties of PANI/ MgO nanocomposites



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Abstract:

The in-situ oxidative polymerization method synthesised the fibrous structure of polyanilinemagnesia (PANI/MgO) composites. The conducting polymers (CP) are processed and characterised by Fourier transform infrared spectroscopy to know the bonding in the processed CPs, X-ray diffraction to determine the unit atom's crystalline structure, and scanning electron microscopy to study the topological features of the material. The obtained composites are used for the development of probes for the gas sensing of ammonia. The ammonia sensed by the sensors was inspected at room temperature. PANI/MgO nanocomposite nanofibers had good selectivity to adsorb the ammonia. It was also found that the content of MgO had a great impact on both the morphology and the sensing properties of PANI/MgO nanocomposites.

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<u>CP-39-EIHE 2023</u>



Boosting supercapacitance of hierarchically porous carbons by heteroatom doping and application in energy storage



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Abstract:

Heteroatom doped hierarchically porous carbon materials have shown their prominence as active materials for electrochemical energy generation and storage. In the present study, efficient B/P/N/O co-doped hierarchical porous carbon materials have been fabricated¹ by mixing nitrogen rich polymer precursor with different concentrations of dopants, followed by grinding and then pyrolysis at 900 °C. Here polymer spheres based on phloroglucinol-salicylaldehyde-melamine (PSM@silica)² act as the carbon precursor, ammonium phosphate ((NH₄)₃PO₄) as the doping agent for N and P and boric acid (H₃BO₃) for B and O. Another set of samples have been prepared by using both (NH₄)₃PO₄ and H₃BO₃ simultaneously. The role of B, P, N and O are to modify the surface properties with appreciable amount of heteroatoms to introduce surface polarity into the carbon framework. Detailed electrochemical studies have been carried out for the samples by cyclic voltammetry, galvanostatic charge/discharge and electrochemical impedance spectroscopy in 1 M H₂SO₄ electrolyte.³ The results suggest good capacitive behaviour for all the materials. Simultaneous doping by 1:1 (NH₄)₃PO₄ and H₃BO₃ shows the best results with specific capacitance of 1046 F·g⁻¹ at 0.6 A·g⁻¹ current density. It also shows high specific energy density and power density of 117.75 Wh·kg⁻¹ and 270 W·kg⁻¹, respectively, at a current density of 0.6 A·g⁻¹.

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<u>CP-40-EIHE 2023</u>



Simultaneous detection of Cd(II)and Hg(II) using Gold Nanoparticles Modified GCE by SWASV



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Abstract:

Cadmium (Cd(II)) and Mercury (Hg(II)) are heavy metal ions released into water bodies from various natural and industrial sources. At high concentrations, above the permissible limits set by W.H.O., they are highly toxic to all life forms. In this work, the simultaneous detection parameters of these three ions were optimized using Gold Nanoparticles (AuNPs) modified Glassy Carbon Electrode (GCE) by using Square Wave Anodic Stripping Voltammetry Technique (SWASV). Gold nanoparticles (AuNPs) were synthesized by phytosynthesis using the leaf extract of Hibiscus Rosasinesis and hydrogen chloroaurate. They were characterized using transmission electron microscopy (TEM), Fourier Transform Infrared (FTIR), UV-visible spectroscopy (UV-vis), and X-ray diffraction. Electrochemical sensing of heavy metal ions was carried out successfully using Hibiscus-synthesized gold nanoparticles (H-AuNPs) modified GCE. Electrochemically Active Surface Area was computed by Cyclic Voltammetry of unmodified and H-AuNPs modified GCE. Optimization of pH, deposition time, and deposition potential was carried out for individual and simultaneous detection of Cd(II) and Hg(II) by Square Wave Anodic Stripping Voltammetry (SWASV). A real water sample of the Mahanadi river was analyzed and both Cd(II) and Hg(II) were found to be present but below 0.2 ppb. Both were found to be within the W.H.O. limits.



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<u>CP-41-EIHE 2023</u>



Highly Stabilised Reduced Graphene Oxide/ Indole Composite as Efficient Electrode for High Performance Rechargeable Lithium-Ion Batteries



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Abstract:

The synthesis of N,N'-bis-Ind[-1H-indol-3-ylmethylidene]benzene-1,2-diamine (N,N'-bis-IBD) has been carried out by conventional wet-chemical method, followed by the lithiation using ball milling. The physical and spectrochemical characterizations of this as-prepared material in its lithiated and unlithiated forms are found to be significantly different. The activity of the electrode material Li-N,N'-bis-IBD towards battery application is evaluated using cyclic voltammetry and galvanostatic charge potential limitexperiments. The obtained electrochemical results rendered intense redox properties and anodic behaviour of the active electrode material in aqueous electrolyte. The battery performance by lithiated



moiety shows an appreciable discharge capacity of 277 mAhg⁻¹ at 100 cycles in aqueous medium. Interestingly, on addition of 20 wt. % reduced graphene oxide (rGO) to the Li-N,N'-bis-IBD sample, the battery performance is observed to be enhanced significantly; a high discharge capacity of 625 mAhg⁻¹ is obtained at 100 cycles. The obtained experimental results significantly based on the formation of aqueous solid-state-interphasedue to super-concentrated electrolytic medium leads to water in salt electrolyte condition.The enhanced

electrochemical performance suggests that the rGO-doped lithiated indole-based composites will be an effective anode material for lithium ion batteries.

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MoS₂ Wrapped N-doped Carbon for Sodium and Potassium Ion Batteries



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Abstract:

With the growing need for energy storage devices, the economics and geopolitical issues related to Li-ion has forced us to look for alternatives. The solutions could be Na⁻, K⁻, Al⁻ and Zn⁻ batteries, all because of its chemical properties and abundancy in nature. We will present the use of 2D MoS₂ material for Na and K batteries. MoS₂ wrapped MOF-derived N-doped carbon nanocomposite can be used as anode material. A facile hydrothermal method is used to fabricate the composite, followed by the carbonization treatment. Carbon materials are known materials with high capacity. But, due to its alloying effect, very high-volume change can occur after Na or K insertion resulting in formation of internal cracks, loss of electrical contact, and eventual failure of the electrode. To overcome this problem, electrodes with large interlayer spacings are needed. Here, we will show that, transition metal dichalcogenides have efficient intercalation-deintercalation properties. Therefore, a composite using nitrogen doped carbon, derived from MOF and exfoliated MoS₂ is synthesized for use in batteries. The fabricated Na and K batteries delivers a very high discharge capacity of ~1550 mAh g⁻¹ and ~537 mAh g⁻¹ respectively at C/10 scan rate. The performance under different C-rates will also be discussed to prove the industrial usefulness of these batteries.

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<u>CP-43-EIHE 2023</u>



Repurposing the Graphite Recovered from Spent Lithium-ion Batteries for Second-life Application



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Abstract

Recycling has become an absolute necessity. Spent Lithium-ion batteries (LIBs) are a hazardous waste but a potential source of purified minerals. Industrial focus on LIB recycling is mostly centered on costly and scarce cathode materials. Graphite is often overlooked as it fails to generate useful revenue. Herein, the waste LIBs are recycled following an all-components-recovery route that minimizes cross contamination. Solvent wash followed by thermal treatment revives graphite for second life applications. Important things to consider here are the interaction of solvent media with the preformed SEI, role of leftover SEI in forming the second-life SEI, and effect of regenerated SEI on second-life electrochemistry. Therefore, the nature of solvent plays a vital role in the overall process. Utilizing water is the most go-to alternative but the obtained electrochemistry from water-washed graphite is below the mark. Organic solvent dimethyl carbonate (DMC) modifies the chemical composition of the interphase in such a way that it improves the second-life electrochemistry. Strong inorganic acid HCl results in the highest carbon purity and makes recovered graphite suitable for non-electrochemical applications. Electrochemically superior DMC-washed graphite is repurposed into dual-ion full cell that delivers an average voltage of 4.5 V and energy density of 110 Wh kg⁻¹.

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Tetrabutylammonium Tetrachloroferrate(III) Complex Derived urchin like Fe₃C/Fe Decorated N doped Carbon as promising bifunctional electrocatalysts for ORR, OER and Zn-Air Batteries in alkaline medium



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Abstract:

Emergence of applicable non-precious metal based robust and economic bifunctional oxygen electrocatalysts for both oxygen reduction (ORR) and oxygen evolution reaction (OER) is crucial for rational design of commercialized Zn–air batteries (ZABs) with safe energy conversion and storage systems. Herein, a novel strategy to fabricate a cost-efficient, bifunctional oxygen electrocatalyst FeC-700(Fe₃C/Fe decorated N doped Carbon), with unique structure has been proposed by carbonization of a new single source precursor (Tetrabutylammonium Tetrachloroferrate (III)) complex. The ORR and OER activity revealed excellent performance ($\Delta E=0.77$ V) of the FeC-700 electrocatalyst, comparable to commercial Pt/C and RuO₂ respectively. The designed temperature tuneable structure provided sufficiently accessible active sites for continuous passage of electrons by shortening the mass transfer pathway, leading to an extremely durable electrocatalysts with high ECSA and amazing charge transfer performance. Remarkably, the assembled Zn–air batteries with the FeC-700 catalyst as the bifunctional air electrode delivers gratifying charging–discharging ability, impressive power density of 134 mW/cm² with long lifespan, demonstrating prodigious possibilities for practical application.

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Borophene Nanosheets as Electrocatalysts for Hydrogen Generation Reaction



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Abstract:

Amidst the energy crunch and global inflation, the search for renewable, clean, and low-cost energy sources has been very intense. Due to its high calorific value (142 MJ/kg), economic hydrogen production is of utmost priority among researchers. Although, expensive catalysts such as platinum and its group member elements limit hydrogen production(1). Therefore, the development of reliable, low-cost catalysts is crucial. Here we report the potential application of boron and borophene (2D nanosheets of boron) as electrocatalysts for hydrogen evolution reaction (HER), as this lightest 2D material has versatile properties compared to other 2D nanomaterials(2). This highly anisotropic, inexpensive layered boron sheets with excellent mechanical strength is proposed to be a prospective electrocatalyst for Hydrogen Evolution (BS) and ultrasonication-assisted hydrothermal (BSH) exfoliation routes and are compared for their electrochemical HER performance using 0.5M H₂SO₄ solution as electrolyte. The borophene developed via two methods are characterised using FTIR, XRD and Raman spectroscopy and the morphology is analysed using HRTEM analysis. The comparatively lower Tafel slopes of BSH (146mV/dec) is attributed to the lower charge transfer resistance and high surface area compared to BS and the pristine bulk boron.

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Two dimensional porous carbon nanostructure developed from tea waste for water purification



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Abstract:

Biomass derived carbonaceous products has been widely used for the removal of organic dyes in the field of waste water treatment. This study focuses on the development of two dimensional carbon nanostructure from the most abundantly available biomass tea waste via KOH activation followed by hydrothermal carbonization. The synthesized product is characterised using SEM, TEM, XRD, FTIR, Raman spectroscopy. Thermal stability of the prepared material was also studied by TGA. Aggregated irregular two dimensional morphology with excellent porosity of the developed carbon nanostructures is confirmed by FESEM. XRD revealed polycrystalline nature of the prepared two dimensional carbon structure. Raman has analysis shows the characteristic bands of carbon with $\frac{I_{D}}{I_{G}}$ ratio of 0.89. The synthesised porous carbon nanostructure shows 97% and 76% of adsorption ability for Methylene blue and Methyl orange dyes respectively for a contact time of 60 minutes. The mechanism behind the adsorption is the strong electrostatic interaction and π - π bonding between adsorbent and adsorbate. Moreover, the porous structure will be a low cost and good adsorbent for cationic and anionic dyes.

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<u>CP-47-EIHE 2023</u>

Effect of dysprosium doping on oxygen reduction reaction activity of NiFe₂O₄



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Abstract:

Direct methanol fuel cells have drawn increasing attention as next-generation energy-conversion devices for electrical vehicles. Transition metal oxides with a spinel structure (AB₂O₄) have received attention as catalysts for oxygen reduction reaction (ORR) because these structures enable good electrical conductivity due to the ready electron hopping between metals at different valence states. Here, we report the synthesis of NiFe₂O₄ and Dy-doped nickel ferrite (NDF) spinel nano crystals, NiDy_xFe_{2-x}O₄ (X=0.2,0.1,0.075,0.05,0.025) denoted as NDF- 0.2, NDF - 0.1, NDF- 0.075, NDF- 0.05 and NDF- 0.025 respectively by co- precipitation method. The structural properties and morphology of the prepared catalysts are studied with the help of XRD, SEM and XPS. The ORR of NiFe₂O₄ and NDF 0.2 exhibits a onset potential of -0.19V and -0.14V vs. Ag/Agcl in alkaline medium respectively. The Koutechy-Levich plot obtained from rotating disk electrode shows a higher electron transfer "n" suggesting a 4 electron pathway for NDF-0.2 nanoparticle.



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<u>CP-48-EIHE 2023</u>



Evalution of Oxygen Reduction Reaction of Transition Metal Doped Rare Earth Metal Oxides Supported on Vulcan Carbon



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Abstract:

Now a days direct methanol fuel cells (DMFCs) are main research of intrest as these are most energy efficient device for extracting power from fuels. Rare earth oxides have been widely investigated for oxygen reduction reaction (ORR) owing to their special 4f shell electronic configurations. In our exepriment we have hydrothermally synthesized Mn-doped Sm₂O₃ (20%Mn@Sm₂O₃) along with bare Sm₂O₃. The synthesized materials were characterized with the help of XRD, SEM and XPS. The ORR performance of all catalysts were evaluated and 20%Mn@Sm₂O₃ material showed better result as comparision to bare counterpart. The study of oxygen reduction potential Vs Ag/AgCl in cyclic voltametry of all theree catalysts were found as -0.18V, and -0.09V for Sm₂O₃ and 20%Mn@Sm₂O₃ respectively in alkaline medium. Furthermore from linear sweep voltametry (LSV) study it shows 20%Mn@Sm₂O₃ is following 4e⁻ for ORR which is better ORR performance than its counterpart.



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CP-49-EIHE 2023



Facile low-temperature synthesis of nanosized highly entropic spinel-type oxide (FeCoNiMnCu)₃O₄ for electrocatalytic application.



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Abstract:

Recently, high-entropy oxides have gained much attention due to the synergistic effects of various metal species. Here, we have synthesised the porous spinel-phase high entropy oxide (FeCoNiMnCu)₃O₄ via a hydrothermal route at a lower temperature. The confirmation of phase composition, the observation of microstructure, and the analysis of the crystal structure distribution of elements were conducted by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDS), respectively. The results show that a single spinel structure (FCC, Fd-3m) was obtained with a uniform distribution of Fe, Co, Ni, Mn, and Cu elements, the typical characteristic of a high-entropy oxide (HEO). The experimental XRD spectrum analysis with the Rietveld refinement methodology shows proper overlap of experimental and computational major (high intensity) characteristic peaks of the spinel phase. This research not only provides a noble and facile route for preparing a nanosized HEO but also gives a blueprint for the development of HEO-based electro-catalysts by integration with cocatalysts such as acetylene black.

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<u>CP-50-EIHE 2023</u>



Designing of an Effective Electrocatalyst with Optimized d-Band Center for Water Oxidation Reaction: a Sabatier Principle Approach



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Abstract:

Minimizing the required overpotential for the electrochemical oxygen evolution reaction (OER) is mostly dependable over the effective strategical modification of standard OER catalysts for large-scale hydrogen production. The LDHs are well-known electrocatalysts for OER and gain special attention for the ease of their synthesis. But due to lacking an effective electronic structure for ion adsorption in intermediate steps, its long-term application is still limited. Here we have developed a facile strategy of decorating the LDH by Ru NPs via the facile Microwave heating method. This decoration has been done by incorporating various amounts of Ru NPs ions like 1, 3, 3.5, 4, and 5%. The bi-metallic LDH material is decorated with



3 % of Ru NPs. It delivers an outstanding OER activity by demanding 249 mV of overpotential at 10 mA/cm². Calculating accumulated charge over the catalyst surface shows that with 3% Ru NPs loading possesses facile OER. The calculated charge versus thermoneutral current density shows a volcanic relationship of adsorption-desorption of all the intermediates. The catalyst having 3% of Ru NPs loading is positioned at the top of the volcano, facilitating the OH adsorption. In addition to

experimental verification, DFT studies have confirmed the same.

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<u>CP-51-EIHE 2023</u>



Recovery of mixed metal oxide from complex lithium-ion battery cathode material as promising catalyst for oxygen evolution reaction



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Abstract:

Lithium-ion battery (LIB) recycling has become a mandate to mitigate potential environmental risk and depletion of valuable metal resources after its end-life. Most common issue of e-waste is improper segregation, which results in complicated e-waste system and hinders complete recycling of LIB cathode into battery regeneration. The complexity in complete recycling is, avoiding incorporation of impurities in the recovered material. One possible solution to this major issue is creating broader application spectrum of recovered material, rather than concentrating only on regenerating in form of battery grade material. Herein we propose a simplemethod for complete recovery of complex e-waste system, where we have recovered valuable metals from complex spent LIB cathode material using mild acid for leaching and cost-effectivereagents for precipitation. The process is optimized with >90% leaching efficiencies of valuablemetal ions of interest. Further utilizing the processed liquor, mix transition metal oxide are regenerated via the complex form of mixed transition metal. The efficacy of mixed metal oxide is evaluated as catalyst for Oxygen Evolution Reaction (OER). A low-cost process for the efficient recovery and reutilization of valuable metal elements are developed to treat spent lithium-ion battery black mass materials.

Keywords: Spent cathode, Recycling Battery, Mixed metal oxide, Oxygen Evolution Reaction

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<u>CP-52-EIHE 2023</u>



A solvent-in-salt type ether based electrolyte with intercalation cathode for rechargeable Fe-ion battery



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Abstract:

With the higher demand for high capacity and cost-effective energy storage technology, the quest for the development of alternative technology to lithium-ion battery will pave a way for the large-scale energy storage technology. Compared to monovalent ion storage as in lithium ion battery, multivalent ion storage (Fe-ion) offers advantages like increase in energy density of intercalation-based electrodes [1, 2]. Along with that liquid electrolytes play a key role in any batteries to allow the conduction of corresponding ions between the cathode and anode. Traditionally, taking into account the ionic conductivity, viscosity and solubility of salt, the salt concentration in liquid electrolytes is typically less than 1.2 mol/L [3]. Here we demonstrated the concept of 'Solvent-in-Salt' electrolyte with higher iron salt concentration in ether based electrolyte for the rechargeable Fe-ion battery. In the present study layered oxides were used as the intercalation cathodes and mild steel sheets as anode delivered a specific capacity of ~ 680 mAh/g at the current density of 30 mA/g. The use of 'Solvent-in-Salt' electrolytes remarkably improved the cyclic efficiency thus enhancing the electrochemical performance with safety. Moreover, when used in Fe-ion battery, the advantage of this electrolyte was further demonstrated in inhibiting the self discharge issue which resulted in extended cycling stability.

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RuO₂/MoS₂ heterostructures for supercapacitor applications



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Abstract:

Rapid development in the field of electronic devices and related technologies demands the development of new materials or effective combination of materials with good electrochemical performance and efficient integration to boost the supercapacitive performance. Compared to carbon-based electrode materials, the storage mechanism in metal oxides are pseudo capacitive in nature, in addition to simple surface adsorption double layer mechanism [1-3].

A heterostructured nanocomposite material consisting of MoS_2 nanosheets and RuO_2 nanoparticles has been synthesized by an easy hydrothermal method and a simple chemical reduction technique followed by a calcination process. The electrochemical performance of the as-prepared RuO_2 nanoparticle dispersed MoS_2 hybrid composite has been evaluated in symmetric two-electrode configuration in 1M KOH electrolyte. At 1 A g⁻¹, the MoS_2 -RuO₂ hybrid electrode exhibits specific capacitance value of 719 F g⁻¹. Moreover, the symmetric supercapacitor based on the composite electrodes retains 100% stability over 10000 cycles, which makes MoS_2 -RuO₂ composite, a promising electrode for energy storage applications.



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Functionalized porous covalent organic framework as promising electrode materials for aqueous supercapacitor.



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Abstract:

Covalent organic Frameworks (COFs) design via covalent bond formation between two organic building blocks and synthesize through variety of approaches with their tuning of pore size, low density, high surface area, good electrical conductivity as well as thermal and chemical stability. Due to these properties COFs are finding extensive range of electrochemical applications in Energy storage devices like supercapacitors and batteries. Here we report the synthesis of novel nitrogen and sulfur enrich triazinethiophene functionalized electrochemically redox active two-dimensional (2D) COFs via reflux and solvothermal methods. The prepared COFs were characterized by SEM, TEM, IR, BET, XRD, SAXS, UV, TGA, DSC and analyzed the properties. The synthesized COFs were made applicable as an electrode material in sustainable aqueous symmetrical supercapacitor. The redox active units present in aforementioned linker found actively participating in charge-storage mechanism. Electrochemical Cyclic Voltammetry of the device shows rectangular shape proving the charge storing mechanism via forming electrochemical double layer process. From the Galvanic charge-discharge COFs based electrodes resulting excellent specific capacitance of 32 F g^{-1} at 0.25A g $^{-1}$ current density and after which no further decrement observed even after 5000 cycles. This study provided a new approach for utilization of redox active COFs for energy storage devices.

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Enhancement of Electrochemical Supercapacitor Performance with Functionalization in Silica based Mesoporous Materials.



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Abstract:

Silica functionalized mesoporous nanoparticles adopting soft polymer infused templates are adopted by the scientific community due to easy sol-gel procedure, low temperature synthetic scheme and effective tunability of the porous structure. Here in, a series of functionalized mesoporous silica (SiO₂-X, $X = OH, Cl, SH, NH_2$ have been synthesized in which amphiphilic block copolymer is used as a templating agent in sol-gel method. The presence of functional groups after completion of synthesis was confirmed by using FT-IR spectroscopy. The prepared functionalized mesoporous silica were characterized by SEM, UVvisible, PL, TGA and DSC analysed the properties. From the CV and UV-Vis measurements, it is confirmed that SiO₂-NH₂ has lowest band gap and produce high value of current over other SiO₂-X materials. The Mott-Schottky and EIS confirmed the *n*-type character as well as good electrical conductivity of synthesized porous silica materials. As the materials having great potential to host the various ions/molecules, hence we have used them to fabricate pseudosupercapacitor using aqueous electrolyte. In the pseudosupercapacitor, the prepared SiO₂-OH and SiO₂-Cl materials are used as electrode materials with H₂SO₄ and KOH as electrolytes. Among these two devices, SiO₂-OH with 1 M KOH electrolyte exhibited excellent power density and specific capacitance along with long cycle stability. Due to porous and ordered structure, materials possess better capacitance and energy density in pseudosupercapacitor. Thus, functionalized mesoporous silica would appear to have tremendous potential for use as high performance pseudosupercapacitor in energy storage devices.

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Fast electrochromic switching and high optical contrast of poly (2,5-dimethoxy aniline) film on flexible PET substrate and its spectral characterizations



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Abstract:

Electrochromism is defined as a reversible change in optical properties of a material as a result of electrochemical oxidation or reduction. Conducting polymers offer the benefits of a fast-switching time, high optical contrast ratio, good processability, and the ability to fine-tune the band gap by modifying the structure compared to inorganic materials. PANI and its derivatives are considered to be especially promising transparent conducting materials for electrochromic display devices like smart window applications. The fabrication of electrochromic device needs electrode of high transparency, uniform surface and low resistance. In the present study highly smooth thin film of poly (2,5-dimethoxy aniline), PDMA, has been electrochemically deposited onto ITO coated PET substrate. Cyclic voltammetry (CV),



UV-Visible spectroscopy, Fourier Transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), were performed for the examination of electrochemical and structural morphology of the electrodeposited PDMA film. Spectro-electrochemical studies reveal that the electrodeposited PDMA film has distinct multichromic behaviour (yellow-green-blue) (Fig-1). The PDMA film (area = $1 \times 1 \text{ cm}^2$) shows maximum optical

contrast of 40 % at 483 nm with a response time of 1.72 s. The PDMA was found to retain 80 % of its optical contrast and 90 % of its original charge density at 1000 double potential steps.

Keywords: PDMA, Electrochromic materials, flexible PET, FE-SEM, and UV-Visible spectroscopy

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Electrodeposition of PEDOT Film on flexible PET and its fast electrochromic properties toward display applications



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Abstract:

The electrochromic property of conducting polymers has received considerable attention recently due to their fast-electrochromic switching, easy thin film formation, light-weight, and compatibility with flexible substrates. Poly(3,4-ethylenedioxythiophene), PEDOT film is prepared on flexible ITO/PET substrate by stepwise galvanostatic route (Fig.1), and their electrochromic properties are examined by cyclic voltammetry (CV), chronoamperometry (CA), and spectro-electrochemical measurements. The electrochromic properties of PEDOT film (multi/dual color changes) on flexible PET substrates were systematically examined in 0.1 M TBACIO₄ and 0.1 M TBAPF₆ by cyclic voltammetry (CV), chronoamperometry (CA), stepwise galvanostatic techniques and UV-Visible spectroscopy. Further electrochromic investigations implied that the PEDOT polymer films showed moderate to high optical contrast, good coloration efficiencies, fast response time, better stabilities, and color persistence as potential electrochromic materials for flexible display devices.



Fig.1: Electrodeposition of PEDOT film on flexible ITO/PET by multistep galvanic route (a), Electrochromic switching behaviour (b) and Percentage transmittance of flexible PEDOT film prepared on PET in 0.1 M TBAClO₄/ACN (c).

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<u>CP-58-EIHE 2023</u>



Hybrid PANI@Fe₂O₃-MXene Nanocomposite for Supercapacitor Applications



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Abstract:

Recently, MXene ($Ti_3C_2X_n$) has become a trending topic in the field of energy storage, due to its high performance, flexibility and ease at which it can form composites with polymers, CNT's, metal oxides and more. Herein, we have synthesized tri-composite of MXene, Fe₂O₃ and conducting polymer PANI, to enhance its electrical conductivity, stability and capacitance. First MXene was prepared using its MAX(TiAlC) phase, subsequently Fe₂O₃-MXene and PANI@Fe₂O₃-MXene composites were prepared. Structural analysis of the prepared materials was performed using characterization techniques such as XRD, FTIR, BET, Raman and TEM. Further to understand its electrochemical properties, Chronopotentiometry, Cyclic voltammetry and Electrochemical impedance spectra were carried out using CH-Electrochemical work station. The specific capacitance of MXene was found to be 205 F/g at 10 mV/s which is enhanced after the addition of Fe₂O₃ and PANI to it with improved retention capacity. Chrono potentiometric studies exhibited an improvement in discharge time too.



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Preparation of GdW/S-GCN composite and its application as electrode material for the sensitive detection of antibiotic in water and food samples.



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Abstract:

The present study elucidates the development of sensor-based nanomaterials to quantify Chloramphenicol (CAP). Dysprosium Molybdate and sulfur-doped graphitic carbon nitride (GdW@S-gcn) are used as transducer material. GdW is synthesized by co-precipitation method and S-gcn is synthesized by thermal polymerization method. The as-synthesized GdW@S-gcn was characterized usingTEM, EDAX, XRD, XPS techniques and the modification of the electrode is confirmed by EIS. The performance parameters such as pH, scan rate, electrocatalytic oxidation of CAP, Interference, repeatability, reproducibility, and stability were optimized for the developed sensor. The developed sensor showed a sensitive response with LOD of 1.25 μ M, LOQ of 41.91 μ M, and sensitivity of 112.26 μ A mM⁻¹cm⁻² for CAP. The proposed sensors find application in a broad concentration range from 100 to 1000 μ M. The results endeavored the possible use of these sensors nevironmental protection and monitoring. Based on the results, it can be claimed that the GdW@S-gcn forms an excellent electrode material for electrochemical detection of CAP.

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Cationic surfactant mediated detaction of mefenamic acid at glucose modified carbon paste sensor in urine and pharmaceutical samples



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Abstract:

In this study, a novel and robust glucose-modified carbon paste electrode (CPE) for the ultrasensitive detection of mefenamic acid (MA) is developed. MA, a non-steroidal anti-inflammatory drug used for its antipyretic and analgesic effects, is harmful to the patient in higher doses. MA is also listed as a chemical pollutant that negatively affects the environment. From this point of view, a sensitive sensor to identify the MA was developed by using a glucose-modified carbon paste electrode in the presence of a cationic surfactant, cetyltrimethylammonium bromide (CTAB). The developed sensor probe was characterized using different electrochemical techniques and then used to study the electrochemical nature of MA. The sensor could detect MA with a linear dynamic range (LDR) of 0.025 to 500.0 μ M and a limit of detection (D_L) of 1.01 nM. Interference from co-existing molecules was found to be negligible. The real sample analysis was performed in human urine samples and pharmaceutical tablets with SWV, and higher recoveries of 92.70-99.16% and 96.0-98.5%, respectively, were obtained. This demonstrates that the sensor can be further used in other biological, pharmaceutical, or environmental samples to detect MA.

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<u>CP-61-EIHE 2023</u>



Graphene oxide/cholesterol nanohybrids for the voltammetric analysis of cetirizine



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Abstract:

Cetirizine (CTR) is second-generation piperazine that belongs to the antihistamines class that helps to reduce allergies. The present research reports on the fabrication of CTR-sensitive sensors for electrochemical detection and quantification. The electrochemical behavior of CTR was studied using a carbon paste-based electrode (CPE) modified with 2D graphene oxide (GO) and cholesterol (CHO). The simple construction of this sensor was achieved by loading the homogenized CHO-GO/CP matrix (cholesterol graphene oxide nanohybrid modified carbon paste) into a polytetrafluoroethylene (PTFE) tube. The surface morphology of the developed sensor array was performed using SEM and AFM. The detection limit of CTR at CHO-GO/CPE was determined to be 9.2 nM. Furthermore, the electrochemical impedance spectroscopy (EIS) study showed that CHO-GO/CPE offered less resistance to charge transfer than CPE. In addition, the physicochemical parameters and the electrode kinetics were evaluated using the effect of the pH of the electrolyte and the scan rate variation study. Furthermore, adding several excipients to the CTR analyte did not affect the CTR's overall electrochemical behavior, confirming the fabricated sensor's anti-interference properties. CTR detection in tablet solutions was investigated to evaluate sensor efficiency for a real-time application, and the results showed remarkable detection with good recovery.

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2D graphene oxide nano sheets-based sensor for electrochemical detection of carbendazim



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Abstract:

The introduction of new pollutants has become an enormous obstruction as these pollutants have adverse effects on humans and the environment. Detecting such contaminants requires a sensitive, selective, and inexpensive technique that can quantify their presence at trace levels. In the present study, we have designed a 2D graphene oxide (GO)-based glassy carbon (GCE) electrochemical sensor (GO/GCE) and employed it in the detection and determination of carbendazim (CRZ). The voltammetric behavior of CRZ was studied using cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques. The SWV was used to quantify and analyze CRZ in actual samples. A better response of CRZ was observed at GO/GCE when pH 4.2 phosphate buffer solution was used as the supporting electrolyte. The SWV technique has been employed in the trace-level detection of CRZ. A linearity plot was obtained for the concentration range from 1.0×10^{-7} M to 2.5×10^{-4} M with a detection limit of 1.38×10^{-8} M. The selectivity of the modified sensor was verified by the interference study of metal ions and other pesticides with CRZ. The agricultural and ecological relevance of the developed method was successfully tested by determining the CRZ in water and soil samples.

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<u>CP-63-EIHE 2023</u>



Hafnium doped tungsten oxide nanorods for electroanalytical detection of perfluorooctanoic acid (PFOA)



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Abstract:

Highly toxic perfluorooctanoic acid (PFOA) has been used extensively to manufacture household products that can harm human health and hygiene, causing environmental pollution. In this research work, a hafnium-doped tungsten oxide (Hf.WO3) modified carbon paste electrode was developed for the first time to study the trace determination of PFOA using electrochemical methods, as these are inexpensive, simple, and selective for the detection of trace-level compounds. The Hf.WO3 nanoparticles were synthesized by a hydrothermal method and characterized by XRD, TEM, EDX, and XPS to understand their structural purity and crystallinity. The effect of electrolyte pH, sampling rate, temperature change, immersion time, and concentration (linearity range from 0.07 μ M to 300.0 μ M) was studied using the CV and SWV techniques. The temperature variation study determined thermodynamic parameters such as enthalpy, entropy and activation energy. The LD for the developed electrode was determined to be 0.018 μ M. The real-time application of the electrode in the determination of PFOA was studied on the spiked soil, water, spoiled vegetable and spoiled fruit samples (% RSD ranging from 2.88 to 5.94), while the interference study showed a high selectivity of the Electrode versus PFOA.

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<u>CP-64-EIHE 2023</u>



Electrochemical detection of diclofenac in urine and commercial tablets samples using XAD-4 sensor



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Abstract:

Amberlite XAD-4 (XAD-4) is a polymeric adsorbent, a crosslinked polystyrene copolymer resin known for its durability, chemical stability, and high surface area. Diclofenac sodium (DIC) is a non-steroidal anti-inflammatory drug (NSAID) with antipyretic and analgesic properties, commonly used in pain-related treatments. Although DIC is an essential and clinically proven drug, it causes serious health problems when administered in overdose, leading to the accumulation in body fluids. Therefore, it is essential to develop a method to detect traces of DIC in various pharmaceutical and clinical samples in order to regulate the optimal dosage. In this study, we developed a new electrochemical sensor to study and detect DIC by modifying the carbon paste with XAD-4 (XAD-4/CPE). DIC showed only an anodic peak and no cathodic peak in the reverse scan, indicating an irreversible reaction mechanism. The developed electrode showed good selectivity, reproducibility, repeatability and sensitivity with a detection limit of 2.71×10^{-8} M. The prepared electrode was employed to directly detect DIC in commercial tablets and urine samples, indicating its broad applicability in clinics and pharmaceutical formulations. Interferences due to the co-existence of chemicals were studied, and the stability of the designed sensor was also studied, confirming its enormous real-world applications.

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<u>CP-65-EIHE 2023</u>



Electrochemical biosensor based on PPO enzyme immobilized on Ag doped Cu nanoparticles and PPy nanotubes for the detection of dopamine.



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Abstract:

Dopamine (DA) is a neurotransmitter and has been responsible for some neurological diseases. Hence, its detection is very essential for the early diagnosis of neurological disease which is caused due to the abnormal level of DA. In the present work we have synthesized silver doped copper nanoparticles (AgDCuNPs) via microwave irradiated green chemical synthesis route. The prepared nano particles were then made into nano composite with polypyrrole nanotubes (PPyNTs). The PPyNTs were synthesized using MO as a template. The synthesized nano composite was characterized by means of XRD, SEM, and TEM analysis. The PPyNTs/AgDCuNPs nano composite were then fabricated onto the graphite electrode (Gr). Finally, the Gr/PPyNTs/AgDCuNPs modified electrode was immobilized with polyphenoloxidase enzyme (PPO). The electrochemical characteristics and catalytic behavior of the as prepared Gr/PPyNTs/AgDCuNPs electrode for the determination of DA were systematically investigated via electrochemical impedance spectroscopy, cyclic voltammetry and potentiometry. The results demonstrate that the developed DA biosensor exhibit a low detection limit, wide linear range, and good sensitivity. The developed sensor also exhibited excellent results for real time detection of DA in the real sample analysis of human blood serum.



Novel triple layered hydroxides of Mg-Ag-Al (LTH) Nano-catalyst for Electroanalysis of Promethazine



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Abstract

A novel electrochemical sensor based on of Mg-Ag-Al (LTH) was confirmed by FE-SEM, EDX and XRD. Mg-Ag-Al (LTH)/GCE has been developed for sensitive and selective detection of promethazine. Electrochemical properties of Mg-Ag-Al (LTH)/GCE has been investigated using cyclic voltametry (CV), differential pulse voltametry (DPV) and amperometry (CA). The CV analysis of promethazine proved the capability of (LTH) Mg-Ag-Al/GC electrode to execute the oxidation reaction. The voltametric and amperometric limit of detection, linear range and limit of quantification of promethazine was found down to CV: 3.5 nM L⁻¹, 50-250 μM L⁻¹ and 10.5 nM L⁻¹, respectively with DPV: 4.2 nM L⁻¹, 50-500 μM L⁻¹ and 12.6 nM L⁻¹. The amperometric LOD were found to be 25 nM L⁻¹. Besides, (LTH) Mg-Ag-Al/GC electrode has also been detecting the promethazine potential for CV; +680 mV and DPV; +660 mV. The (LTH) Mg-Ag-Al/GC electrode was high sensitivity and reproducibility.



Dibutyl Thiourea: Cathodic or anodic inhibitor?



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Abstract:

Corrosion costs range between 3-8% of GDP for many countries globally. Usage of inhibitors is one of the effective ways to alleviate corrosion, however, there is scarcity of benign inhibitors which are as effective as the toxic ones. Study of efficient inhibitors help us understand the mechanism and relation of inhibition to the structure of molecule. Dibutyl thiourea (DBTU) is known to be an excellent inhibitor of steel's corrosion. The extant literature suggests that thioureas are mostly cathodic inhibitors. The mechanism of inhibition i.e. adsorption and charge on the metal surface play important role in the process of designing new inhibitors, owing to the anchoring group's behaviour. Potentiodynamic polarisation and electrochemical impedance studies with circuits fitted, show differences in the molecule's behaviour with concentration, on different steels. Further analyses with surface charge aspects and other techniques like chronocoulometry shall be presented. Gravimetric tests and staged dilution studies may showcase the difference in the inhibitor's behaviour with metallurgy of steel.



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Rapid and Label-free Electrochemical-based Sensing of SARS-CoV-2 Spike Proteins



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Abstract:

Recent, COVID-19 pandemic caused by severe acute respiratory syndrome-coronavirus-2 (SARS-CoV-2), which spread across the globe and ended a million of human life¹. Diagnosis of COVID-19 depends on standard RT-PCR and CT techniques. However, it requires skilled manpower, sophisticated instrumentation, and time-consumption for the detection of infection ^{2,3}. Herein, we have constructed an electrochemical immunosensor platform for detecting receptor binding domains (RBD) of SARS-CoV-2 spike proteins (SP) at an early stage. A facile and cost-efficient sensor platform was devised with electroadsorption of methylene blue (MB) on graphene oxide (GO) modified carbon screen printed electrode (MB-GO/SPE). Selective N-terminal hACE-2 bioreceptor was identified through in silico docking studies enabling higher binding affinity of -20.6 kcal/mol against RBD of SARS-CoV-2 SP. Constructed MB-GO/SPE devised hACE-2 sensor platform exert selective sensing of SP with the support of suitable bio-affinity layer, which was analysed via cyclic voltammetry (CV) and chronoamperometric (CA) studies. CA based quenching of current density with respect to the concentration of SP enabling better sensitivity (0.45 nA/pg mL⁻¹), low detection limit (0.71 pg/mL) with wide linear range (0.001 – 1000 ng/mL). For clinical feasibility, a real patients (nasopharyngeal and oropharyngeal) swab specimens were directly tested with the prepared electrochemical immunosensor platform, and the obtained results are validated with RT-PCR studies, promising for point-of-need analysis.

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<u>CP-69-EIHE 2023</u>



Electrodeposition and Electrocatalytic study of Co-P alloy coatings



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Abstract:

The present study reports the electro-catalytic behavior of Co-P alloy coatings, deposited from a newly formulated bath, using the glycine as additive. A Co-P bath was formulated by conventional Hull cell method. The compositional data revealed that wt. % of P in the deposit has increased with deposition current density. The XRD study demonstrated that solid solution of Co and P were formed in the range of current density studied. Deposition conditions, like current density and pH were optimized for best performance of Co-P alloy coatings against corrosion. The electro-catalytic behavior of Co-P alloy coatings for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) were studied in 1.0 M KOH. Electro-catalytic efficacy of both HER and OER of electrodeposited Co-P alloy coatings were studied by cyclic voltammetry (CV) and chronopotentiometry (CP) techniques. It was found that Co-P alloys deposited, at 1.0 A/dm² (having about 6.2 wt.% P) and 4.0 A/dm² (having about 8.7 wt.% P) are good electrode materials for HER(cathode) and OER(anode), respectively. An inverse dependency of electro-catalytic activity of HER and OER of alloy coatings better electro-catalytic activity were examined using Scanning electron microscopy (SEM), X-ray diffraction (XRD) and Energy dispersive X-ray spectroscopy (EDS) techniques, and results were discussed.

Keywords: Electrocatalytic activity: Co-P alloy, CV and CP study

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<u>CP-70-EIHE 2023</u>



Fresh leachate valorisation through microbial fuel cells (MFCs) for bioelectricity generation



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Abstract:

Dual chambered microbial fuel cell (MFC) configuration was evaluated for the treatment of fresh leachate that generating from municipal solid waste (MSW) handling site. Fresh leachate is having very organic content (90,000 mg COD/L), due to which it cannot be valorised by the microorganisms in MFCs. Five different concentrations (organic loading conditions, OLs) of fresh leachate were evaluated for bioelectricity generation under near neutral pH operating conditions in batch mode operation. OL of 3.20 kg COD/m³ was showed maximum bioelectricity (OCV, 589 mV) generation in 12 days of operation. However, the substrate degradation efficiency was registered maximum with 2.75 kg COD/m³ showed maximum substrate degradation of 67% of COD removal. Closed circuit potential (CCV) of 2.11 was registered during 7th day of operation, which also exhibited the sustainable operational resistance of 300 ohms. The degradation process and bioelectricity generation process were not registered at high with 100% fresh leachate. This might be due to the inhibition of high substrate concentration with high organic matter. The hydraulic retention time was also found to influence by the organic loading concentrations of fresh leachate.

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Modeling a flow cell for electrochemical reduction of CO₂



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Abstract:

The atmospheric carbon-di-oxide is increasing yearly because of rapid economic, technological, and population growth. The significant global CO₂ emission comes from fossil fuels. The widely adopted technique to overcome this issue is CO₂ capture, utilization, and storage. Among them, CO₂ utilization is one of the intriguing fields to explore, where CO₂ is transformed to value-added products. Electrochemical Carbon-di-Oxide reduction is rapidly becoming a more industrially relevant pathway, as this is one of the strong ways to move forward in mitigating climate change. To scale up the process to an industrial scale, it is imperative to perform simulations. However, the main challenge in modeling the system is accounting for multiple reaction pathways, including heterogenous and homogenous reactions and its non-linear dependence on multiple variables on different scales. Due to this, the work on detailed models of porous electrodes coupled with complex kinetics is sparse. In this work, a 1D model of a porous cathode electrode with a diffusion layer was modeled to study the internal properties, namely active surface area, reactant concentration, reaction rate distribution, electrode and electrolyte potential. This model's application gives insight into product distribution by varying electrode properties, and the results were validated with the existing experiments.



Fig : Partial current density of species

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<u>CP-72-EIHE 2023</u>



Redox regulation of anolyte with pretreated bagasse hydrolysate for sustainable bioelectricity generation



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Abstract:

Microbial fuel cells (MFCs) functions based on the electroactive microbial activity on organic matter present in anolyte. Mild acidic to mild alkaline pHs (pH 6-8) was found as effective range for bioelectricity generation by MFCs. The present study was aimed for effective utilization of sugarcane bagasse (biomass waste from sugarcane industry) towards bioelectricity generation. The conversion of organics from bagasse can be made amenable for wastewater treatment by chemical pretreatment. However, the pretreated hydrolysates having extreme pHs, which are not suitable for microbial action in MFCs. In this direction, a sustainable approach was followed, which combines acid and alkaline hydrolysates to bring the resultant hydrolysates are amenable for degradation in MFCs. A maximum of 611 mV of biopotential was generated from bagasse hydrolysate in two chambered MFC configuration using graphite as anodic electrode. The process was found stable during changing the substrates. Current density of 21 mA/m² (100 Ohms) was found maximum and it stable for 3 days in batch mode of operation. Polarization study under different resistances (i-v curves) was showed 300 ohms as the sustainable resistance for dual chamber MFC with graphite as bioanode. Proposed approach opens new avenue for sustainable approach for bagasse valorization for bioenergy generation.

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<u>CP-73-EIHE 2023</u>



Development and characterization of composition modulated multilayer (Sn-Ni) alloy coatings for improved corrosion protection



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Abstract:

Here, we report the electrodeposition and characterization of composition modulated multilayer (CMM) coatings of (Sn-Ni) alloy for better corrosion protection on mild steel (MS). A new electrolytic bath of (Sn-Ni) alloy was formulated using gelatine as the primary additive by conventional Hull cell method. Corrosion study of electrodeposited (Sn-Ni) alloy coatings, deposited over wide range of current density (2.0 Adm⁻² - 5.0 Adm⁻²) revealed that (Sn-Ni)_{4.0 Adm-2} coating is more corrosion resistant, compared to other coatings. By taking the advantage of the fact that periodic modulation in the rate of diffusion of metal ions towards cathode during electroplating allows the development of coating in layered fashion, the corrosion resistance behaviour of (Sn-Ni) alloy coatings was tried to enhance further by CMM technique. The coatings were developed in multilayers by periodic pulsing of direct current (DC) between two values, during the process of deposition. The CMM (Sn-Ni) alloy coatings of different combinations of both composition (by altering the height of pulse) and degree of layering (by altering the duration of each pulse) were developed and their corrosion performances were evaluated by electrochemical AC and DC methods. Corrosion study revealed that CMM coating having (Sn-Ni)_{2/4/120} configuration shows four times better corrosion resistances compared to its monolayer counterpart, deposited from the same bath for same duration. The improved corrosion performance of CMM (Sn-Ni) alloy coatings under optimal conditions was attributed to the increased number interfaces, affected due to alternate layers of (Sn-Ni) alloys having different compositions, surface morphologies and phase structures, confirmed by Scanning electron microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS) and X-ray diffraction (XRD) techniques. The effect of layering on corrosion protection efficacy of CMM (Sn-Ni) alloy coatings were tested, and results are discussed.

KEYWORDS: Sn-Ni alloy, Multilayer coatings, SEM, EDS, XRD study.

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Layer Thickness Dependant HER activity of MoS₂ Nanostructures



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Abstract:

Hydrogen is emerging as an alternative green fuel due to its highest gravimetric energy density and zero-pollutant emission to replace traditional fossil fuel and reduce environmental issues. MoS₂ shows efficient HER performance comparable to that of Pt for their unique layered structure and electronic property. The edge site 'S' atoms in MoS₂ are found to be the catalytic active sites, on the other hand basal plane 'S' atoms are inert. Herein, we report preparation of MoS₂ nanostructures by solvothermal method in which the solvents such as Glycerol and water are taken in different proportions. The XRD studies revealed



activity.

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that interlayer spacing shifts to higher values with gradual increase in Glycerol amount. The morphological analysis of the samples by SEM shows both layered and particle nanostructures. The EDX analysis shows the presence of both Mo and S in the atomic ratio of 1:2. The catalytic activity of the samples towards HER was analysed by a rotating disc electrode method in 0.5M H₂SO₄ solution. The activity of the samples were monitored in terms of onset potential and potential at 10mA/cm⁻² current density. It has been observed that an optimum layer spacing is suitable for efficient HER activity and also revealed that the concentration S precursor plays a vital role in the growth of nanostructures and their HER

<u>CP-75-EIHE 2023</u>



Rapid and direct electrochemical detection of pramipexole using graphitic carbon nitride (gCN) sensor



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Abstract:

Pramipexole (PMXL) belongs to the benzothiazole class of aromatic compounds and is used to treat Parkinson's disease; however, overdose leads to abnormal effects that can trigger severe side effects. Therefore, a sensitive analytical tool is required to detect trace amounts. In this work, we successfully developed an electrochemical sensor for trace detection of PMXL using the voltammetric method. Graphitic carbon nitride (gCN) was synthesized using a high-temperature thermal condensation method. The synthesized nanoparticles were used for surface characterization using TEM, XRD and AFM techniques. The electrochemical characterization of the material was evaluated using the EIS technique to evaluate the solution-electrode interface property. The cyclic voltammetry (CV) behavior of PMXL showed an anodic peak in the forward scan, indicating that PMXL underwent electro-oxidation on the gCN-modified carbon paste electrode (gCN/CPE). A good linearity ranges from 0.05 to 500 μ M was observed for the gCN/CPE produced, and a lower limit of detection (L_D) of 0.012 μ M was achieved for the selected concentration range (0.5 to 30 μ M). The selectivity of the electrode in PMXL detection was investigated by performing an interference study, while the tablet sample analysis demonstrates the sensitive application of the electrode in real-time.

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<u>CP-76-EIHE 2023</u>



Safety and Electrochemical Performance of Single crystal Lithium-rich Layered oxide Cathode for Li-ion Battery Using for Electric Vehicle Applications



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Abstract:

High energy density and high voltage performance of single crystal cathode materials have been using to lithium-ion battery applications. The single crystal Li-rich layered oxide is considered to be most promising next-generation electrode materials for electric vehicle energy storage applications. In this regard, synthesis of layered oxide cathode materials has prepared by solution combustion method. The prepared samples structural and morphological characterizations by XRD, Raman, FE-SEM, and HR-TEM (EDX). The electrochemical performance of electrode materials have been performed by cyclic voltammetry (CV), and Galvanostatic charge and discharge (GCD), and Electrochemical impedance spectrum analysis.

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<u>CP-77-EIHE 2023</u>



Augmenting the surface-active sites of Co-Fe LDH by doping of the Fe²⁺ ions towards effective hydroxide adsorption for the water oxidation reaction: A highperformance OER Electrocatalyst in alkaline medium



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Abstract:

Shortage of energy and environmental pollution due to large usage of fossil fuels has grabbed most of the attention of research scientists to produce green hydrogen by sustainable water splitting reaction. Over the past few years, LDH-based electrocatalysts have gained vast attention as effective electrocatalysts for OER in alkaline conditions owing to their excellent stability under the same electrolyte environment. But lack of proper active sites for OH adsorption inhibits their large-scale application to a greater extent. Here modification of the CoFe-LDH surface is done by doping the active Fe^{2+} ions by adopting a simple wet-chemical approach. The catalyst shows an interesting Fe^{2+} ion dependency towards the OER and a



volcanic relationship between accumulated electronic charge and thermoneutral current density has been observed. The optimized electrocatalysts Fe^{II} -LDH (0.04M) results in a 4-fold increase in TOF value compared to pristine CoFe-LDH, and demands only 268 mV overpotential to reach the current density of 10 mA/cm² compared to Pristine CoFe-LDH ($\eta_{oer} = 345$ mV).

Overall, this study shows an improvisation of the synergistic charge transfer kinetics at the interface by providing a greater number of surface-active sites towards the OH adsorption and an interesting Fe^{2+} ion loading dependency over the LDH surface toward the water oxidation reaction.

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<u>CP-78-EIHE 2023</u>



Electro-polymerization of synthesised BCN for voltammetric determination of Tryptophan in real samples



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Abstract:

Due to their large band gap, boron nitride and related compounds have yet to be thoroughly investigated for potential applications in electrochemical sensing. Here, we report a novel strategy for fabricating a sensing platform by electrodepositing synthesized Boron carbon nitride (BCN) over a screen-printed electrode (SPE). The BCN is synthesized by employing low temperature one-pot solvothermal method. The material is electrochemically polymerized over commercially bought SPEs using cyclic voltammetry. Detailed morphological and chemical analysis of the modified surface is carried out before investigating its electrochemical performance. Compared to the bare SPEs, we witness enhanced electrochemical activity attributed to the increased surface area, facilitated charge transfer, and superb stability and reproducibility. Furthermore, its ability to determine tryptophan is tested in the concentration range of 1 – 400 μ M. Compared to the unmodified SPE, the fabricated electrode showcase a ~ 5 – fold increment in tryptophan peak current with a potential shift of ~ 100mV. Moreover, when tested in the complex matrix containing uric acid, dopamine, and hypo-xanthene, it demonstrated no significant interference. The sensor is further utilized to estimate the tryptophan in real samples (milk, urine) to investigate its practical applications.

Keywords: Boron carbon nitride, Screen-printed electrode, Tryptophan, Voltammetric sensors, Electropolymerization

<u>CP-79-EIHE 2023</u>



Room temperature synthesis of Bismuth Sillenite (Bi₃₆Fe₂O₅₇) for electrochemical oxygen evolution reaction



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Abstract:

Sillenite type members of bismuth ferrite family have been less explored due to roadblock in formation of metastable γ -Bi₂O₃¹. In this work metastable γ -Bi₂O₃ has been stabilised by introduction of Fe into it by inexpensive room temperature coprecipitation method leading to the formation of Bi₃₆Fe₂O₅₇. The detailed physiochemical and electrochemical characterization of the prepared catalyst has been carried out. As synthesized catalyst shows well-defined spherical morphology of about 10 nm in diameter. Bi₃₆Fe₂O₅₇ demonstrated 420 mV overpotential for oxygen evolution reaction (at current density of 10 mA/cm²). The kinetics of the reaction is investigated by Tafel slope, turn over frequency and mass activity measurements^{2,3}. Harnessing unique sillenite structure could pave a way for new horizons for their use as electrocatalysts.

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<u>CP-80-EIHE 2023</u>



Facile hydrothermal synthesis of NdCoO₃@NdO-rGO nanocomposite for energy storage and sensing of an antioxidant drug, alpha lipoic acid



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Abstract:

Rare earth metal oxide composites have recently become irreplaceable and outstanding electrocatalysts because of their interesting properties such as high conductivity, unique and advantageous electronic structure. In this study, a superior electrochemical sensor and supercapacitor nanocomposite material, NdCoO₃@NdO-rGO was prepared in a facile way using the simple hydrothermal method. This material and approach conferred adequate and scalable fabrication of high-performance supercapacitor and electrochemical sensor electrodes. The prepared nanocomposite was characterized using powder X-ray



diffraction, scanning electron microscopyenergy dispersive spectroscopy, fourier transform infrared spectroscopy, thermogravimetric analysis, atomic force microscopy, particle size analyser, and zeta potential. For the first time, NdCoO₃@NdO was used as an electrode material over nickel foam for supercapacitor studies and showed good

specific capacitance. Further, NdCoO₃@NdO-rGO material modified over GCE was used for the electrochemical determination of an antioxidant drug, alpha lipoic acid (ALA). ALA exhibited 28-folds enhancement in the oxidation peak current of NdCoO₃@NdO-rGO modified electrode compared to that bare electrode. A good linearity range was observed between the peak current and concentration of ALA. The applicability of the proposed electrochemical sensor was well demonstrated by analyzing ALA in pharmaceutical formulations and human urine samples. The results of analysis were validated by statistical data treatment.

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CP-81-EIHE 2023



Solar light driven photoelectrocatalytic hydrogen evolution and pollutant degradation by carbon doped Zno nanostructures



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Abstract:

The solar driven photoelectrocatalytic process has been intensively investigated for multifunctional environmental remediation and green fuel generation. A highly efficient photocatalyst based on carbon doped ZnO nanostructures (C-ZnO) were synthesized by a novel microwave assisted electrospinning technique. Polyvinyl alcohol is used as both electrospinning agent and carbon source. The carbon doping extends valence band of ZnO to higher energy region which results in reduced bandgap energy. 10 wt% PVA incorporated C-ZnO nanostructures shows highest photocatalytic activity towards



pollutant degradation. Pure ZnO shows photocatalytic efficiency of 78% while C doped ZnO shows 93% degradation efficiency within 60 min of light irradiation. For, hydrogen evolution reaction, the C doped ZnO shows best activity with a reduced overpotential of only

713 mV at 10 mA/cm² (vs. RHE) and a tafel slope of 62 mV/dec. This significant enhancement in photocatalytic activity can be attributed to the enhanced visible light absorption and reduced charge carrier recombination upon carbon incorporation. The detailed PL, TCSPC and photocurrent response deepens the investigation of separation efficiency of charge carriers. Our present observations provide new insights into the development of photocatalysts that possess multi-function for water-solar energy nexus.

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TiO₂/g-C₃N₄ hybrid photoanodes for PEC water splitting



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Abstract:

Photoelectrochemical (PEC) hydrogen evolution is a promising method to produce renewable energy to tackle the global energy crisis¹. In this work, we report the enhancement in photoefficiency of nanohybrids of titanium dioxide (TiO₂) with graphitic carbon nitride (g-C₃N₄) developed in different weight percentages of g-C₃N₄. Initially, anatase TiO₂ was synthesized via sol-gel assisted hydrothermal method, and carbon nitride(CN) was prepared from melamine by fractional thermal polymerization. Thereafter,TiO₂/g-C₃N₄ nanohybrids in different weight proportions (*viz.* 1,5,10,15,20 wt% of g-C₃N₄ in TiO₂) were synthesized by *in-situ* hydrothermal methods and were optimized using photocatalytic dye degradation studies². The synthesized hybrid samples were systematically characterized using XRD, SEM, TEM, FTIR, and Raman Spectroscopy, and were finally studied for their photoelectrochemical HER performance. TiO₂/g-C₃N₄nanohybrids always showed better PEC performance than bare TiO₂ or g-C₃N₄. This outstanding PEC hydrogen evolution in the nanohybrids is attributed to the reduced recombination of charge carriers facilitated by the synergism between TiO₂ and g-C₃N₄, otherwise unachievable in their pristine individual forms³.

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<u>CP-83-EIHE 2023</u>



Synthesis and application of a 0D/2D nanocomposite for the nanomolar level detection of an antiandrogen drug



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Abstarct:

In this work, Sr@FeNi–S nanostructures were synthesized through a chemical approach. The assynthesized nanostructures were explored for the fabrication of a nanocomposite based potentiometric flutamide (FLU) sensor. Conducting graphene nanoribbons (GnRbs) were used for the strong adsorption of the nanocomposite on a graphite (Gr) electrode. The resulting composite matrix Sr@FeNi–S/GnRbs was further used for the electrochemical detection of FLU. The synthesized nanocomposite was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and FT-IR spectroscopy methods. The synergistic effect of the materials employed in the development of the electrode resulted in an efficient FLU sensor with a low detection limit (20 nM) and a wide linear range of 20–450 nM. These results validated the successful development of an electrochemical sensor with superior analytical performance in comparison to the sensors reported in the literature. The proposed sensor also exhibited good storage stability and reproducibility, and remained unaffected by a few common interferents present in biological samples. The developed sensor was also evaluated for flutamide analysis in real samples with a high percentage recovery (96%), thus validating the possibility of its usage in biomedical applications.

<u>CP-84-EIHE 2023</u>



Hf-doped tungsten oxide as sensing materials for electrochemical detection of paracetamol and salbutamol



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Abstract:

1-D nanostructured metal oxides exhibit high selectivity with efficient catalytic tendencies toward a range of analytes. Tungsten Oxide (WO₃) is known for its catalytic properties, conductivity and stability, which can be further improved by doping. This study addresses the synthesis of hafnium-doped tungsten oxide (Hf.WO₃) nanorods via a hydrothermal process and their characterization using X-ray diffraction, transmission electron microscopy, scanning and transmission electron microscopy, and X-ray photoelectron spectroscopy. The materials developed were used to fabricate an electrochemical sensor by modifying the carbon paste electrode (CPE) used to estimate paracetamol (PAR) and salbutamol (SBM) drugs. The results showed an increased peak current compared to the nascent CPE, indicating easy transfer of the electrons. The catalytic properties, conductivity, and broad surface area of the fabricated 1-D nanostructures have shown remarkable improvement for the detection of the selected analytes. A square wave voltammetric technique was also used to evaluate detection limits of 1.28 nM and 2.42 nM for PAR and SBM, respectively. The estimation of PAR and SBM in biological samples and pharmaceutical dosages of the drugs demonstrated the usefulness of the sensor device for real analytical applications.

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Green synthesis of Zn₂V₂O₇ nanoparticles using *Lawsonia inermis* for supercapacitor application



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Abstract:

In order to meet the enormous demand for electrical energy in today's modernised society, electrode materials that have good potential for storing electrical energy must be developed. The mixed metal oxide family which includes the transition metal vanadates are commonly known as binary metal oxides. This type of materials has recently attracted much interest as active electrode materials in the field of supercapacitors due to their possible multiple oxidation states, layered structure, and the synergistic interaction between two transition metals. In this study, natural henna leaf powder and commercial henna powder were used as novel fuels to successfully synthesize $Zn_2V_2O_7$ nanostructures by simple solution



combustion method.Different analytical methods viz., X-ray diffraction (XRD), fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray fluorescence spectroscopy(T-XRF) were used to characterize the synthesised Zn₂V₂O₇ nanostructures. Cyclic voltammetric and chronopotentiometric techniques were

used to examine the electrochemical performance of $Zn_2V_2O_7$ nanostructures for supercapacitor application. The specific capacitance values of $Zn_2V_2O_7$ nanostructures prepared using natural leaf henna powder and commercial henna powder were noticed to be 883 Fg⁻¹ and 589 Fg⁻¹, respectively, at 1Ag⁻¹ current density in 1M KOH electrolyte.

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Tailoring the structure of NiTiO₃ with TiO₂ to enhance its activity for Oxygen Evolution Reaction



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Abstract:

The current increasing demand of energy has lead scientist all over the world to find alternative renewable sources of energy to curb the need for the continuous depleting non-renewable sources of energy.[1] For the effective utilization of renewable energy economy exploration of the efficient and durable catalysts is the need of the hour.[2] In this work, we have tailored the structure of ilmenite NiTiO₃ with TiO₂. The catalyst was synthesized by hydrothermal method followed by calcination. The detailed physiochemical and electrochemical characterization of the catalyst has been carried out. The resulting NiTiO₃-TiO₂ heterostructure shows an overpotential of 330 mV (current density 10 mA/cm²). The Tafel slope value is 72 mV/dec which indicate faster kinetics towards oxygen evolution reaction. The efficiency of the catalyst was evaluated by chronoamperometry and turn over frequency.[3] The presence of Ni atoms and synergistic effect of the NiTiO₃-TiO₂ results in the enhanced catalytic activity of the resulting catalyst for the oxygen evolution reaction.

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Sensitive Electrochemical Detection of Folic Acid Using Co₃O₄ Modified Carbon Paste Electrode



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Abstract:

A simple electrochemical sensor, Co3O4 modified carbon paste electrode (CPE), was fabricated and utilized for the sensitive detection of Folic acid (FA). FA is an essential complex B vitamin source in making genetic material, red blood cells and human body development. The Co3O4 nanocrystallites were synthesized by a facile hydrothermal method and were characterized using Powder Xray Diffraction (PXRD), Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR). The electrochemical behaviour of FA at Co3O4/CPE was investigated in detail through cyclic voltammetry (CV) and Differential Pulse Voltammetry (DPV). The fabricated electrode showed an acceptable performance in wide concentration range with a detection limit of 0.5 nM towards FA. The developed sensor exhibited good reproducibility and stability.



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An Efficient Electrochemical Sensor for Nitrite Based on a Mesoporous Nickel Cobaltite-Reduced Graphene Oxide (NiCo-RGO) Nanocomposite



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Abstract:

A simple protocol for the preparation nickel cobaltite and graphene-nickel cobaltite composite is described in this paper. NiCo-RGO nanoparticles are produced by self-combustion of the urea-nitrate complexant. Graphene, as expected, inhibits the nanoparticles from clumping together. The production of complex during synthesis is confirmed by electrochemical and spectroscopic analyses of the composites. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used to investigate the electrocatalytic oxidation of nitrite on a (NiCo-RGO) graphite electrode. The DPV approach demonstrated a linear range of 60-860 μ M, with detection limits of 18.0 μ M. For nitrite determination, the method's sensitivity was around 0.06767 μ A μ M⁻¹ cm⁻². Interference, stability, and repeatability were also checked on the sensor. DPV techniques were utilized to examine nitrite levels in soil and juice samples.

Keywords: (NiCo-RGO) composite, electrochemical sensor, cyclic voltammetry (CV), differential pulse voltammetery (DPV), soil and juice samples.

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Novel Mn-Ni Based Selenide Heterostructure for High-Performance All-Solid-State Hybrid Supercapacitors



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Abstract:

Innovative renewable energy sources for energy storage/conversion is the demand of the current scenario in electrochemical machinery.¹ In this context, choosing suitable organic precipitants for tuning the crystal characteristics and microstructures is a challenge.² On the same note, herein a very novel Mn and Ni based selenide based heterostructure (MNS) has been synthesized using a simple two step hydrothermal procedure assisted by sluggish precipitating agent and an effective cappant, followed by intermediated anion exchange. The material was subjected to physicochemical measurements, depicting poly-crystallinity, unique morphology and porous arrangement of crystallites. The material was assessed electrochemically by cyclic voltammetry, chronopotentiometry and electrochemical impedance spectroscopy measurements. The electrochemical studies reveal redox behaviour, supercapacitive chargedischarge, and extremely low charge transfer resistance. Further, the solid-state hybrid supercapacitor (MNS||N-rGO), fabricated with MNS and N-rGO as the positive and negative electrode materials, respectively, delivers excellent rate specific capacity, very low internal resistance, high energy density (~34 W h kg⁻¹) of a typical rechargeable battery and high power density (11995 W kg⁻¹) of an ultrasupercapacitor. The device also shows impressive capacitance retention during long charge-discharge cycles. The physicoelectrochemical physiognomics of novel MNS show that it can be a next-generation material for utilization in high-performance supercapacitors.^{3,4}

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Fabrication of Bi₂O₃||RuCo₂O₄ for Flexible supercapatteries



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Abstract:

Flexible supercapattery became high potential energy storage devices due to their attractive electrochemical performances, notably in favor of high-power density. Fabrication of a supercapattery using Bismuth oxide, and Ruthenium Cobalt oxide in an alkaline medium delivers faradaic and capacitive behavior via a facile one-step hydrothermal method as the binder-free electrode. Herein, the coupling of Bi₂O₃/Carbon cloth as the negative electrode and RuCo₂O₄/Nickel foam as the positive electrode. The fabricated device was assembled using a PVA-KOH gel electrolyte operated within a potential window of 1.6 V and the superior areal capacitance of 4.13 F cm⁻² at 5mA cm⁻². Moreover, the function of the device showed excellent electrochemical stability performances with above 96% coulombic efficiencies and 90% capacitance retentions after 10,000 GCD cycles at a current density of 30 mA cm⁻². Furthermore, the device displays a maximum energy density of 1.47 mW h cm⁻² at a specific power density of 89.24 W cm⁻². The fabricated device in an aqueous electrolyte could power a LED assuring the potential applications for flexible supercapatteries. This combination is a promising electrode for electrochemical energy storage.

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Ni and Mo-Based Chalcogenide Heterostructure as Highly Efficient Electrocatalyst for Oxygen Evolution Reaction



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Abstract:

For the development of hydrogen energy economy, it is crucial to explore highly effective nonnoble metal electrocatalysts for oxygen evolution reaction (OER).¹ Considering this, mixed transition metal chalcogenides are shown as highly active OER electrocatalysts due to their favourable conductivity, high electroactive surface area, and suitable oxygen <u>adsorption energy</u>.² With this motivation, a facile approach has been developed for the synthesis of Ni and Mo-based mixed oxide-sulphide heterostructure using sluggish precipitant. The material has been subjected to thorough physicochemical characterizations, which



reveals discrete crystal structure, ideal elemental composition, and uniquely porous microstructure. Electrochemical studies of the material as an electrocatalyst reveals good redox behaviour, excellent potential stability for OER, minimal charge transfer resistance, and low Tafel slope. Additionally, the material when used as an electrocatalyst displays an excellent rate for OER in an alkaline medium, which exhibits significantly low overpotential value of ~ 400 mV at 10 mA cm⁻

² and shows retention of current for continuous oxygen evolution for 8 hours, which indicates good electromicrostructural stability.^{3,4} Therefore, the material can be an excellent choice as an electrocatalyst for oxygen evolution reaction.

Figure: Polarization curve for Ni and Mo-based mixed oxide-sulfide electrocatalyst

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Bismuth oxide nanoflowers decorate with polyaniline nanowire arrays Bi₂O₃-PANI core-shell electrodes for energy storage device



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Abstract:

We have established for the first-time intertwined material Bi₂O₃-PANI nanostructures constructed through a "seeding approach" on a Ni-foam substrate by a simple, inexpensive, binder-free and one-step chemical bath deposition method. The as prepared Bi₂O₃-PANI electrode demonstrates considerable energy/power density and cycling life. Structure and morphology studies, initially, reveal phase-pure polycrystalline bismuth oxide nanoflowers decorated with polyaniline nanowire arrays. This material upon testing in an electrochemical energy storage system displays supercapattery behaviour. From the power law, an applied-potential-dependent charge storage mechanism is established for the Bi₂O₃-PANI electrode material. A Trasatti plot evidence the presence of inner and outer surface charges. An assembled symmetric supercapattery device with a Bi₂O₃-PANI // Bi₂O₃-PANI configuration demonstrates a moderate energy density and power density. Furthermore, the energy density of the device is comparable to commercial batteries, and the power density also reaches that of symmetric supercapacitors, indicating that the device could be a very promising novel energy storage system for fast and efficient energy storage in the future. From the commercial point of view, these devices were used in series combination and illumination of a color LED panel with full-bright light intensity could be achieved.



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Interaction of catalase enzyme with Tetraalkyl ammonium cations at electrified liquid-liquid interface



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Abstract:

Oxidative stress and related complications are one of the most common forms of physiological conditions that affect public health. To protect living organisms from oxidative stress induced inflammatory damage, certain defence mechanism were adapted. Enzymes such as catalase, superoxide dismutase and glutathione peroxidase were considered as first line of defence against such inflammatory damage¹. Catalase is present in almost all aerobic organism, therefore studying these enzymes is useful in understanding the functioning of enzymes. The casual relationship between amount of these enzymes and inflammatory damage suggests its potential role in quantitative determination of oxidative stress in body. Electrochemical analysis will be helpful in accompanying electron transfer process and helps to understand the nature of these enzymes. However, enzymes being a protein will be challenging for electrochemical analysis due to electrode passivation by bio-fouling. In this regard, a much detailed information can be obtained by studying these enzymes at Interface between Two Immiscible Electrolyte Solution (ITIES) established at the tip of micro-pipette².



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Methodical designing of Pt_{3-x}Co_{0.5+y}Ni_{0.5+y}/C (x=0, 1, 2; y=0, 0.5, 1) particles using a single-step solid state chemistry method as efficient cathode catalyst in H₂-O₂ fuel cells



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Abstract:

A cathode catalyst possessing increased activity for oxygen reduction reaction (ORR) with superior durability is greatly required for polymer electrolyte membrane fuel cells (PEMFCs). Although Platinum (Pt) alloys have been widely studied for ORR, their real time application in fuel cells still remains a challenging task. Chemically ordered Pt alloys have attracted widespread attention due to the unique electronic and geometric factors that boost their electrocatalytic activity. Therefore, it is highly urgent to



fabricate such ordered alloys as efficient cathode catalysts. Herein we report for the first time, a one-step solid-state method for the preparation of $Pt_{3-x}Co_{0.5+y}Ni_{0.5+y}/C$ (x=0, 1, 2; y= 0, 0.5, 1) nanoparticles on carbon support. Different compositions were studied and $Pt_2Co_1Ni_1/C$ was found to be the best performing catalyst. Interestingly,

the mass activity of $Pt_2Co_1Ni_1/C$ was seven times higher than that of commercial Pt/C in an acidic medium, achieving the Department of Energy (DOE) target, 2025. Moreover, a retention in mass activity after 50k cycles confirmed the superiority of this catalyst. Importantly, the peak power density achieved by $Pt_2Co_1Ni_1/C$ under actual PEMFC conditions outperforms the commercially used Pt/C. Thus, this work provides a new approach for the simple scalable synthesis of cathode catalysts for fuel cells.

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Optical <u>sensing of acrylamide based on</u> <u>the fluorescence quenching of rhodamine B</u>



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Abstract:

Acrylamide (AM) is categorised as a class 2A carcinogen, formed by the Maillard reaction of the reducing sugar and amino acid present in food during food processing/cooking, also found in wastewater from industries (food packaging, paper, and textile). The range of human exposure to AM from food and modern industrialization has been estimated to be 0.2 and 1.9 g/kg. respectively. According to scientific reports, AM exposes people to genetic, neurological, and reproductive damage risk. AM toxicity results from the formation of adducts with biomolecules like DNA, neuronal protein, haemoglobin, etc. through soft electrophilic-soft nucleophilic interaction. The hazardous nature of AM produced in food products makes its quantitative and qualitative detection important. This work reports the fluorescence sensing of acrylamide (AM) using Rhodamine B as an optical reporter. Rhodamine B (xanthene dye) is brilliant red with High fluorescence, photostability, and water solubility. Rhodamine B shows an emission spectrum for 4 different excitation wavelengths. At 256 nm excitation, rhodamine B fluorescence intensity is proportionally and selectively quenched by acrylamide (1 mM- 500 mM). This method would be suitable for monitoring water quality and acrylamide contaminants in industrial wastewater effluents.



Image 1: Rhodamine B with various concentrations of AM (1 mM-500 mM).

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Artificial Interphase Formation on Nickel-Rich Layered Oxides to Facilitate High Voltage Cycling of Lithium-ion Batteries



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Abstract:

Nickel-rich layered oxides (LiNixMnyCozO₂, x+y+z = 1, x > 0.6) are one of the most promising cathode materials for high energy-density Li-ion battery due to their high specific capacity (180-220 mAhg⁻¹) and relatively high operating potential (4.3 V vs. Li⁺/Li). But, the practical applications of these materials are limited by the rapid capacity decay and serious safety issues during long-term cycling at high voltage and at high temperature. The major cause of performance degradation is the attack of highly nucleophilic surface oxygens to the electron-deficient carbonyl carbon center of electrolyte solvent. The decomposition products accumulate on the surface which increases the impedance of Li⁺ intercalation. Herein, the strategy of predecomposing LiPF₆ salt via a one-step wet chemical method is applied on commercially availed LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂ cathode material. The alkaline residues on the NMC811 surface reacted with the acidic LiPF₆ salt to form a uniform LiF layer which acts as a protective shield against parasitic surface reactions. This facile low-temperature LiPF₆ treatment improved the capacity retention of NMC811 cells by 80 % over 100 cycles. In summary, high voltage cycling (up to 4.5 V) is achieved via the formation of artificial interphase that enhances the energy density of Li/NMC811 cells.

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Enhanced electrochemical properties in partially Vanadium substituted NVPF cathode material in sodium ion batteries



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Abstract:

Sodium ion batteries (SIBs) have received tremendous attention since a cost-effective substitute to lithium is required to accomplish large-scale applications [1]. Presently, cathodes are the bottlenecks of SIB research as it determines the energy density, rate capability, and voltage of an entire cell and costs about 44 % of the total battery [2]. Na₃V₂(PO₄)F₃ (NVPF) emerged to be the most promising cathode material due to its unique structure of open channels, exceptional ionic conductivity and high average voltage [3] with major shortcomings of usage of high cost Vanadium and poor electronic conductivity [4]. Carbon coated Fe, Cr co-doped NVPF were synthesized using sol gel method and electrochemical investigations of the half cells were done to address the shortcomings. The optimized cathode material has achieved promising high initial capacity of 119.37 mAhg⁻¹ at C/10 and 96.53 mAhg⁻¹ at 1 C without compromising average potential of the cell. The capacity retention of Na₃V_{2-x}Fe_{x-y}Cr_y(PO₄)F₃ after 250 cycles was 92.75% at 1 C in comparison to 78.76 % for as prepared pristine material that can be attributed to enhanced electronic conductivity. Besides, 5 % Vanadium reduction in optimized cathode aided in 8.36 % cost reduction. The results provide the synthesis of cost-effective high performance cathode material for SIBs.



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Proton Exchange Membrane Fuel Cell (PEMFC) Electrocatalyst



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Abstract:

Proton Exchange Membrane fuel cell (PEMFC) is an energy-efficient alternative to combustion engines for automotive and mobile applications. Considerable advances have been made in reducing the cost of the PEMFC in terms of the amount of Platinum (Pt) used for preparing the electrocatalyst and improving the electrode architecture over the last three decades. However, the contemporary Pt/C catalysts are not sufficiently durable under intermittent start-up and shutdown cycles, due to the corrosion of the carbon support and consequent activity loss. From this perspective, carbon-free nanostructured thin-film (NSTF) catalyst layer designs are an attractive option, and recent results show an eight-fold increase in activity over polycrystalline Pt facets (Debe M K. (2012)). Our goal is to develop a carbon-less nanostructured thin film electrocatalyst with enhanced durability and low Pt loading by using the strategy of coating conductive metallic nanostructures with Pt-rich alloy skin.

Along these lines, we propose to use inkjet-printed silver nanostructures (Parmar et al. (2014)) as substrates for platinum electrodeposition. The initial experiments were carried out on commercial silver thin films to gain deeper insights into the electrodeposition of platinum and nickel on silver. To achieve this, we modified the self-terminating electrodeposition of platinum on gold protocol to address the issues related to silver leaching and obtain repeatable and reproducible deposition. Preliminary experiments indicate that the Pt/Ni alloy catalyst synthesized on thin silver films has Electrochemical Surface Area (ECSA) of $5m^2 / g_{Pt}$ and exhibits <40% loss of activity over 30,000 ex-situ potential cycles. The durable nature of the deposited platinum film is promising and we are currently extending this technique to fabricate such platinum rich alloy overlayers on printed silver nanostructures.

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Microwave Assisted Recycling of Spent Li-ion battery electrode material into Efficient Oxygen Evolution Reaction Catalyst



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Abstract:

Owing to the high utilization of Li-ion battery (LIB) in the industrial sector and subsequent production of waste from cycled LIB endows with the shortage of critical metals and environmental pollution. Herein, we demonstrate an efficient strategy for the conversion of spent LIB for the recovery of valuable metals through a facile microwave-assisted hydrometallurgical technique for the large-scale production of catalysts towards oxygen evolution reaction (OER). After performing a series of recycling procedures with the variation in H₂SO₄ concentration, H₂O₂ dosage, and microwave parameters, the optimum condition for the leaching are 60 °C, 30 min, 0.5 M H₂SO₄, 50 W microwave power, 3 vol % H₂O₂ to achieve Li: 89.07 %, Co: 94.57 %, Ni: 94.25 % and Mn: 100 %. Further coprecipitation reaction leads to the formation of mixed metal hydroxide containing a majority of α -Co(OH)₂ phase with traces of Ni and Mn. The recovered α -Co(OH)₂ exhibits pronounced OER activity with an overpotential of 131 mV to achieve 10 mA/cm² current density and Tafel slope of 80.2 mV/dec surpassing all the synthesized mixed metal, commercial Co(OH)₂ and benchmark electrocatalyst (IrO₂). The recycling strategy using the microwave technique provides a pathway for low-cost recycling of waste material for the large-scale production of efficient electrocatalyst towards a sustainable future.

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Oxygen evolution incorporating phosphorous doped carbon composite with CoTiO₃ as an effective electrocatalyst



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Abstract:

The incessant incineration of the finite fossil fuels has shifted focus to renewable energy resources like hydrogen. The slow kinetics and enormous overpotential requirements for the anodic oxygen evolution reaction (OER) of the Electrocatalytic water splitting process to generate H₂ obstructs the practical application of the overall water splitting process. Porous carbon materials with high specific surface area and good conductivity along with heteroatom doping is reported to bring out best results as catalysts for various applications.^[1] Perovskite composites CoTiO₃/graphene and CoTiO₃/NrGO played out as good OER catalysts. Phosphorous doped carbon composite with CoTiO₃ (PC-CoTiO₃) composite was synthesized to substitute costly and less stable benchmark catalysts and characterized by XRD, UV-DRS, FT-IR, FE-SEM, TEM and XPS. PC-CoTiO₃ was demonstrated as an efficient electrocatalyst with enhanced activity towards OER as displayed by the lower overpotential of 405 mV at 10 mA/cm² in 1M KOH (CoTiO₃: η_{10} : 560 mV) due to the higher ECSA and lower tafel slope. Electrochemical Impedance spectroscopy (EIS) analysis revealed that the charge transfer resistance (R_{et}) in PC-CoTiO₃ reduced phenomenally compared to that of CoTiO₃. The catalyst showed promising durability till 10 h at 10 mA/cm².

Keywords: Oxygen evolution reaction, Electrocatalytic water splitting, Renewable energy resources.

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Rationalizing the Effect of Cobalt and Nickel substitution in Layered manganese Oxide towards Oxygen Reduction Reaction



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Abstract:

With the soaring demand for energy supplies, there is an increasing demand of sustainable energy conversion and storage technologies like fuel cells and metal-air batteries in which Oxygen reduction reaction (ORR) is the primary cathodic reaction. Till now, platinum (Pt) based materials are extensively used as most efficient ORR catalyst. However, platinum's scarcity and poor durability have limited its practical applications. Manganese-based oxides have captured much attention because of their natural abundance, wide variation of crystal structure, variable Mn oxidation state, and nontoxicity. We report the electrochemical activity of layered δ -MnO₂, along with their Co-and Ni-doped counterparts prepared by molten salt method. The interlayer K⁺-ions were exchanged by H⁺-ions by acid treatment. The linear sweep voltammetry (LSV) studies of the samples revealed that the catalytic activity of doped δ -MnO₂ are lower than the pristine one in terms of limiting current density, half-wave potential, and onset potential. However, enhanced activity has been observed for their proton-exchanged counterparts. On multiple cycling the ORR stability continues to degrade which is a serious issue. Further work is in under progress to understand the factors responsible for the higher activity and retain the ORR stability in both doped and pristine δ -MnO₂.



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Pulse Electrodeposited Copper on Copper for Electrochemical Reduction of CO₂ to Hydrocarbon



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Abstract:

Many feasible methods and strategies were studied for mitigation of CO_2 in the atmosphere. Electrocatalytic reduction of CO_2 to produce value-added chemicals and fuels powered by renewable energy input has been a promising route to solve increasing environmental problems[1]. Despite the extensive research into catalytic materials for CO_2RR , only Cu-based catalysts have been shown to yield highly faradaic C_2 + products. Consequently, a lot of work has been put in, both experimentally and theoretically, to figure out how to maximise the FE to C_2 + products on Cu while reducing the FE to C_1

products (CO, HCOOH, and CH₄) and H₂ [2][3]. Copper alloys, copper composites and copper on copper modified catalysts provide various morphology and grain size which leads in formation of C₂ products[4,5]. Pulse electrodeposited Cu on Cu electrodes were prepared in our work to improve copper electrode features such as morphology, selectivity, stability, and electrochemical performance to increase the efficiency of C₂ formation. For prepared catalyst cyclic voltammetry



studies, impedance spectroscopy and electrolysis with CO_2 has been studied and supported with its characterization of XRD and SEM. Figure.1 shows the SEM image of Pulse electrodeposited Cu on Cu were dendrite like morphology was observed.

Figure: SEM image of Pulse electrodeposited Cu on Cu

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<u>CP-103-EIHE 2023</u>



Self-enhanced solid state ECL sensing platform of SiO₂ PEI NPs and its application in detection of spermine



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Abstract:

The electrochemiluminescence of the synthesized solid-state SiO₂ PEI NPs were studied with chemically modified $[Ru(bpy)_3]^{2+}$ that contains nafion, by the electrostatic interactions between positively charged $[Ru(bpy)_3]^{2+}$ and the negatively charged cationic-exchange polymer in the nafion. The *in-situ* generation of amine radicals from the PEI matrix, leads to the better stability with an appreciable enhancement in the ECL emission for the solid-state ECL matrix. Spermine comes under the category of biogenic amine, which is one of the main biomarkers for early-stage cancer diagnosis. Furthermore, the developed SiO₂ PEI NPs/[Ru(bpy)₃]²⁺/Nafion was used to detect spermine molecule in 0.1 M PBS at physiological pH conditions with the limit of detection of 12.2 nM.



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<u>CP-104-EIHE 2023</u>



Development of Battery-Supercapacitor hybrid device using LiMn_{1.5}Ni_{0.5}O₄-high surface area carbon composite as cathode and carbon coated Li₄Ti₅O₁₂ as anode



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Abstract:

Battery-Supercapacitor hybrid device has been recently attracted enormous attention in order to utilize the high energy of lithium-ion batteries and high power of supercapacitors in a single device. Here, we have demonstrated the study of a composite materials consisting of lithium-ion battery and supercapacitor type as cathode and a lithium-ion battery type as anode for lithium-ion hybrid capacitor. The composite cathode utilizes redox as well as adsorption mechanism to store ions additionally leading to more capacity whereas nanostructure anode can store Li ion through faster diffusion process. The LIC hybrid device designed using pre-lithiated carbon coated lithium titanate as the battery-type anode and Lithium nickel manganese oxide- high surface area carbon composite as the cathode. In which the use of high voltage LNMO and c-LTO enables to achieve higher cell voltage, avoids SEI formation and also no lithium plating. It delivers energy densities of 37 and 29 Whkg-1 at power densities of 220 and 6300 W kg-1, respectively in anode: cathode mass configuration of 1:1. When the full cell is cycled at 1 A g-1 it retains $\sim 70 \%$ specific capacitance retention till 4,000 cycles.

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<u>CP-105-EIHE 2023</u>



Fe Doped NiCo₂Se₄ Nanorod Array: Efficient Electrocatalyst for Overall Electrochemical Water-Splitting



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Abstract:

The development of efficient, affordable, and earth-abundant bifunctional electrocatalysts is of vital importance for the water-splitting reaction.¹⁻³ Hydrogen gas is found as an alternative source of green and sustainable energy.^{4,5} In this work, we have fabricated NiCo₂Se₄ and Fe-doped NiCo₂Se₄ through a simple hydrothermal route on the surface of carbon cloth. The developed electrocatalyst was thoroughly investigated by various techniques like powder XRD, XPS, FESEM, ICP-AES, and TEM analysis. The optimized Fe_{0.2}NiCo_{1.8}Se₄ has worked finest for hydrogen and oxygen evolution in an alkaline medium; it entails an overpotential of 148 and 166 mV *vs.* RHE to obtain 50 mA/cm² current density for HER and OER, respectively. The Tafel slope values for HER and OER are 85.7 and 56.3 mV/dec, respectively. This catalyst is stable under an alkaline medium for 48 hours. The best HER and OER activity recommend the

catalyst as a bifunctional in an alkaline medium, and the developed cell consists of doped sample requires 1.51 V to generate a 10 mA/cm^2 current density with 24 hours of stability. The Fe_{0.2}NiCo_{1.8}Se₄ catalyst has Faradaic efficiency of 89.9 % for overall water splitting. The nanorod morphology has a specific role in enhancing the electron transportation and conductivity of Fe_{0.2}NiCo_{1.8}Se₄. This research provides us a simple approach for the synthesis of Fe doped ternary



NiCo₂Se₄ nanorod array on the surface of carbon cloth, which is highly active and stable for water-splitting in an alkaline medium.

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<u>CP-106-EIHE 2023</u>



Development and Feasibility of High-Performance Sodium ion Battery through Doping and Surface coating onto electrochemical active material



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Abstract:

SIBs became an alternative to LIBs because sodium is the sixth most abundant element in the Earth's crust and the electrical storage mechanism of SIBs and LIBs are basically the same except for their ion carriers. In this work, a good capacity retention in SIB through Manganese rich NaMn_{0.9}Fe_{0.1}O₂ (NMF-91) cathode as an electrode has been achieved. We synthesized O3 type NaMn_xFe_{1-x}O₂ 9 composite through combustion process by varying the composition of Mn and Fe such as NMF-55 (Mn: Fe = 50:50 wt.%), NMF-64, NMF-73, NMF-82 and NMF-91 (Mn: Fe = 90:10 wt.%). Electrochemical studies for these different composites is compared using NMF as working electrode, Na metal as reference electrode and NaClO₄ in EC: PC (1:1 wt. %) Solvent as electrolyte. Whereas, NMF-91 (NaMn_{0.9}Fe_{0.1}O₂) delivers the highest capacity of 150 mAh g⁻¹ at C/20 current rate with 70% capacity retention and 80 mAh g⁻¹ at 10 C rate. With the increasing Mn content in NMF the capacity increases and Fe gives the structural stability of the NMF. This Cobalt and Nickel free O3 type NMF Composite acts as buffer, volume change due to expansion and shrinkage of M-O bonds in MO₆ octahedra during cycling is suppressed and the rate performance of SIBs is improved.

Acknowledgements:

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Optical Immunosensor for the detection of clinical biomarker related to renal disease



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Abstract:

Creatinine is one of the most common and specific biomarkers for renal diseases, usually found in the serum and urine of humans. Hence, detecting creatinine in clinically relevant ranges in a simplistic and personalized manner is interesting and important. In this direction, an optical sensing device has been developed for simple and point-of-care detection of creatinine. The developed biosensor was able to detect creatinine quantitatively based on optical signals measured through a change in color. The sensor has been integrated with a smartphone to develop a palm-sized device for creatinine analysis in personalized settings. The fabricated sensor has been thoroughly characterized by FTIR, AFM, and controlled optical analyses. The difference in color intensity and creatinine concentrations show an excellent dose-dependent correlation in linear concentration range. Several interfering molecules, such as; albumin, glucose, ascorbic acid, citric acid, glycine, uric acid, Na⁺, K⁺, and Cl⁻, were tested using the biosensor, where no cross-reactivity was observed. The utility of the developed system to quantify creatinine in spiked serum samples was validated and the obtained percentage recoveries were found.

<u>CP-108-EIHE 2023</u>



Development of a Chemo-Nano Sensor Surface for Ultrasensitive Detection of Lead in Surface Water



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Abstract:

Lead is considered to be one of the highly poisonous and most commonly present heavy metal ions in environmental samples. It can promote serious medical conditions involving nervous, cardiac, genital, and mental disorders due to the exposure to even a very small amount of it. Thus, the detection and measurement of trace levels of lead ion (Pb2+) in natural sources such as water, agriculture, and medical samples is highly important. In this direction in the following study we have represented a nano-chemo tuned sensor system that can detect Pb2+ ion at a trace level in water in presence of other heavy metal ions. The sensor is electrochemically characterized and imposed to a self-reporting construct involving a flexible electronic chip. The sensor surface was engineered using highly conductive gold nanoparticles and metal complex nanohybrid. The promoter metal complex shows a coordinative ion exchange characteristic specific for lead ions that further promotes a selective and robust detection of lead in real water sample. The recorded limit of detection (LOD) is 0.0016 μ M (0.33 ppb) with a wide dual dynamic range of 0.006 μ M to 0.25 μ M (1.24 – 51.69 ppb) and 40 μ M to 150 μ M. This value is within the recommended limit by the World Health Organization (WHO) for drinking water (10 ppb). The recovered concentration of the sensor is found to be > 90% in spiked real water samples. The chip shows improved sensor robustness and reusability alongside an ultrafast response time of ≤ 1.0 sec.

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<u>CP-109-EIHE 2023</u>



Electrochemical analysis of theophylline at cholesterol modified graphene oxide sensor



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Abstract:

Theophylline (THP) is the most effective bronchodilator, a derivative of xanthine, and is prescribed for severe breathing problems. The THP concentration can be accepted up to a level of 5 to 20 gL-1 for plasma, and deviation in the range can cause adverse effects including tachycardia, seizures, vomiting and central nervous system excitation. Therefore, the development of a method to detect traces of THP in real samples is essential to regulate the optimal dosage. In this study, we developed a new electrochemical sensor to probe and detect THP by modifying the carbon paste with the matrix of cholesterol (CHE) intercalated graphene oxide (GO), i.e. (CHE-GO/CPE). The THP showed only an anodic peak in the forward scan and no peak in the reverse scan, indicating an irreversible reaction mechanism. The developed electrode showed good selectivity, reproducibility, repeatability and sensitivity with a detection limit in the nanomolar range. The prepared electrode was used for the direct detection of THP in commercial tablets, indicating its broad applicability in pharmaceutical formulations. Interferences due to co-existence of chemicals were studied, and the stability of the designed sensor was also studied, confirming its enormous real-time applications.

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Utility Scale Battery Energy Storage System–Technoeconomic Perspective



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Abstract:

Around 75% of India's electricity is generated through coal-based thermal power plant. Combustion of fossil fuels coal emits significant amount of CO₂ that is a contributor in global warming. To combat global warming and as a part of the net zero carbon, India has targeted to install 500GW renewable energy (RE) by 2030. Solar and wind energy are intermittent in nature and integration of utility-scale energy storage systems (ESS) are required to store and utilize round-the-clock.

Globally, pumped hydro energy storage system (PHESS) is widely used as large-scale ESS to support grid. However, it has location, Capex (capital expenditure) and response time-based constraints. Several approaches are being made to develop battery energy storage systems (BESS) for utility purpose as an alternate to PHESS.¹ The basic performance characteristics of BESS for utility-scale application are highenergy efficiency, longer life, low self-discharge, high depth of discharge and less environmental hazard. Besides low Capex and Opex are also desirable to make this affordable. Amongst the different battery chemistries for utility-scale, high temperature molten salt/metal (Na-S, Ca-Sb), metal-ion (LIB, NaIB), redox flow (VRFB, Zn-Br₂, Fe-Cr) batteries are popular and have of commercial interests.

Calculated levelized cost of electricity $(LCOE)^2$ of various batteries shows that there is trade-off between Capex and battery performance. In this article, challenges and scopes of BESS for integrating with RE are discussed based on their techno-economic advantages and challenges.

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<u>CP-111-EIHE 2023</u>



Ni Nanoparticle Decoration on PANI (Ni@PANI) for Enhanced Ammonia and water Oxidation Reactions.



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Abstract:

The electrocatalytic direct oxidation of ammonia and water splitting represents a sustainable route from the point of view of environmental protection and H_2 generation. Particularly, the development of low-cost and efficient electrocatalysts grew attention to large-scale clean-energy production. Herein, method for synthesis of Ni@PANI nanosheets is reported by using polyaniline (PANI) directing structure macromolecule at room temperature for electrocatalytic direct ammonia and water oxidation reactions. Nano-sized domain of polycrystalline powder sustained with particle size, as well as elemental composition was confirmed by using X-ray diffraction spectra (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX) and transmission electron microscopy (TEM). Variable oxidation states, with non-stoichiometric Ni-O, confirmed from X-ray photoelectron spectroscopy (XPS), ultra-violet visible spectroscopy (UV) signifies that two absorption bands associated with benzenoid rings into quinoid rings, bending modes of vibrations in Furrier transform infra-red spectroscopy (FTIR) confirms that Ni interactions with PANI chains, thermo-gravimetric analysis (TGA) and Raman Spectra reflects higher stability with Ni-N with supportive C-backbone. electrocatalyst has been showing excellent results for OER and AOR due to availability of additional anchoring sites and cooperative interactions of both Ni and PANI confirmed from morphological and electrochemical studies. The cyclic voltammetry and electrochemical impedance of Ni@PANI nanosheets having higher sensitivity and better activity at ultralow potential of



1.24 V vs. RHE for a current density of 10 mA/cm² oxidation of ammonia (AOR). Chronoamperometric (i-t) measurement shows proposed Ni@PANI nanosheet-based system is having stable and long-term current performance at a potential of 1.24 V vs. RHE towards the AOR. This work affords noble metal-free electrocatalyst for novel appliances and remarkable consequence as Ammonia determination and hydrogen generation.

Fig.1 Schematic representation of Ni@PANI synthesis with respective electrocatalytic activity.

<u>CP-112-EIHE 2023</u>



Polymer sensing system over laser-induced graphene for creatinine detection



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Abstract:

This study developed a method for sensing creatinine over the Laser induced graphene surface using a polymer sensing technology i.e. Molecular Imprinting. The functionalization of the LIG surface aids in the selective and sensitive detection of creatinine. This technology is particularly cost-effective in terms of manufacturing processes that do not require expensive equipment, and the modest outcomes that a PoC device may deliver. The fabrication process schematically shown in Figure 1(a). Several stages are involved in the fabrication process, including laser engraving on the polyimide surface, drop casting over

the LIG surface with synthesized coating, and ultimately enclosing the surface with acrylic well. The electrochemical characterization was carried out for the analysis. The cyclic voltammetry was conducted for validating the functionalization of LIG as shown in Figure 1(b). The EIS technique was conducted over the fabricated device for creatinine detection over the frequency range of 1 to 100 Hz with a distinguishable concentration range of 100 μ M to 500 μ M shown in Figure 1(c). This



sensing system was specifically designed for creatinine detection where Figure 1 (b-c) confirmed the same results. This Sensing system in a versatile and simple method demonstrates considerable potential in a wide range of functional requirements.

Figure: (a) Fabrication Process for the creatinine sensor (b) Cyclic Voltammetry for the validating functionalization of LIG (c) EIS analysis for the different concertation of the Creatinine.

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<u>CP-113-EIHE 2023</u>



Enhanced Photoelectrochemical Water Oxidation Behavior of Mo-doped BiVO₄ semiconductor



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Abstract:

The present study reports the fabrication of Molybdenum (Mo) doped BiVO₄ photoanodes by electrodeposition followed by thermochemical reaction. Doping with electron-rich elements (Mo) in metaloxide photoelectrocatalyst, BiVO₄, notably doubles its activity for water oxidation. The 20% Mo doped BiVO₄ film was optimized with the best photoelectrochemical activity. To improve the charge transfer



capacity and generating the oxygen vacancy on photoanode, semiconductor has been playing as a donor contributor where as it can also perform as the recombination centre for the photo-generated charges. By doping into the semiconductor with reducing the recombination by enhancing the separation of photoexcited electron-hole pairs can decrease the charge transfer resistance for water oxidation performance. An incident photon-to-current efficacy (IPCE) of the

20% Mo doped BiVO₄ electrode is enhanced from 36% to 46%. The donor density N_D value of each of the SC materials is calculated from the slope of the respective M-S plots, it is found to be of the order of 0.48 x 10^{16} / cm³ which increase three times for optimized level of doping. XRD measurements confirm that crystal size is decreased after Mo doping than undoped material.

Figure: Variation of energy conversion efficiency (% η) and fill factor (%FF) of Undoped and Mo doped BiVO4 semiconductor

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J. H. Kim, Y. Jo, J. H. Kim, J. W. Jang, H. J. Kang, Y. H. Lee, D. S. Kim, Y. Jun, J. S. Lee, ACS Nano, 9(2015) 11820.



Outstanding performance of commercial-level massloading 2D WS₂ for symmetric supercapacitors



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Abstract:

Today's modern world is heading fast towards a severe energy crisis. It is now a high time to implement new environment friendly initiatives to overcome the approaching crisis. Supercapacitors are one of the most promising energy storage devices owing to their intrinsic performance advantages. 2D WS₂ Transition



stability over 10,000 charge discharge cycles.

metal dichalcogenides are considered promising constituents in energy storage devices due to their large surface areas, high theoretical capacitance and occurrence of efficient redox reactions at their surfaces. Here we designed a nano flower like morphology based WS₂ via a facile and effective hydrothermal method, without adding any dopants or composites. An exceptional high performance super capacitor behaviour were found for the commercial mass loading nano-flower like WS₂ with 100 %

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Poonam, K. Sharma, A. Arora, S.K. Tripathi, J. Energy Storage. 2019, 21, 801–825.

<u>CP-115-EIHE 2023</u>



Highly Sensitive Electrochemical Detection of Biomolecules



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Abstract:

The development of electrochemical sensors continues to be a surging area of electrochemistry. We successfully implemented the fabrication of different voltammetric sensors for the sensitive and selective detection of a variety of biomolecules. The important molecules are Dopamine, Epinephrine, Serotonin, Ascorbic acid, Uric acid, Tyrosine, Tryptophan and Acetaminophen. The electrode material's



[.] DPVs of various concentrations EPN (9–0.6 μ M), UA (5–0.1 μ M) and TYR (12–1 μ M) in 0.1 M PBS of pH 7.0 at ZnO/RGO16/CPE (a), E neentrations EPN (32–1.1 μ M) in presence of 0.7 μ M UA and 6 μ M TYR (b), Ipa vs concentration of EPN (inset of Fig. 13b), DPVs 2 μ M) in presence of 6 μ M EPN and 6.4 μ M TYR (c), Ipa vs concentration of UA (inset of Fig. 13c), DPVs of TYR (30–2.5 μ M) in presence of $37 \,\mu$ M UA (d) and Ipa vs concentration of TYR (inset of Fig. 13d).

chemistry impacts an electrochemical sensor's characteristics, including sensitivity, selectivity, and reproducibility. Metal oxides, sitesubstituted metal oxides and composite nanomaterials are the commonly used modifiers in electrode preparation. Each modifier causes significant changes in the oxidation and reduction potential of analytes allowing for reliable and precise analyte detection even when a variety of other compounds are present. The practical applicability of the developed

sensors was demonstrated by real sample analysis in blood plasma and urine. We achieved very low detection and quantification limits in the range of nanomolar and even picomolar levels, which will be useful in a variety of scientific areas.

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<u>CP-116-EIHE 2023</u>



Optimization of Zn-Modified Bismuth Molybdate Semiconductor for Highly Efficient Photoelectrochemical Water Splitting



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Abstract:

One of the greatest challenges in the field of photo-electrochemistry is to develop novel photocatalysts with excellent solar-light-harvesting capacity and separation efficiency of photo-induced charge carriers. Bismuth molybdates are found to be very fascinating materials due to their narrow band gap energy, high chemical stability and suitable valence band potential makes it a good visible light active photocatalyst but its application is marred by low quantum yield and poor charge separation efficiency. In this work, we have developed Zn^{2+} modified bismuth molybdate thin film using a simple drop-cast method. Activity of the semiconductors was tested through linear sweep voltammetry under chopped illumination in presence 0.1 M Na₂SO₄ solution for water oxidation and in 0.1 M Na₂SO₃ - 0.1 M Na₂SO₄solution for

sacrificial oxidation. The optimized thickness of zinc modified bismuth molybdate yields a photocurrent density of 237μ A/cm² using linear sweep voltammetry [1]. The synthesized samples were characterized various analytical by (SEM, RAMAN). techniques Electrochemical impedance and action spectra suggest significant photon to current conversion efficiencies of the material under



UV-visas well as for visible illumination. In addition, the Zn modified bismuth molybdate photocatalysts maintained good stability at least for an hour and also most importantly, it is visible light active.

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Investigations on Ni based Alloys for Hydrogen Evolution Reaction in Alkaline Media



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Abstract:

The development of adequate and inexpensive electrocatalysts for electrochemical hydrogen production is of utmost importance to meet the world's growing demand for energy and to overcome the challenge of global warming. In this study we report non-noble Ni based binary alloys, coated on Ni foam through an in-situ, one-step electrodeposition approach. The synthesized Ni-Mo/NF(NiMo) and Ni-P/NF (NiP) are capable of delivering a current density of 10 mA cm⁻² at a small overpotential of 34 mV and 40 mV respectively in alkaline medium. Which demonstrates the excellent HER activity of the electrode. Moreover, the electrode exhibited favourable catalytic durability through different stability tests. The remarkable electrocatalytic activity of NiMo and NiP can be ascribed to the synergistic effect of Mo, P, and Ni elements, the large active surface area, and high electrical conductivity of this electrode, which is a result of the binder-free synthesis method of the coating [1] .The outstanding HER performance of NiMo electrode, along with its cost-effective and scalable synthesis approach, highlights the significant potential of this electrode to be utilized in commercial water electrolyzers.



Fig1: Linear sweep voltammetry studies of the electrocatalysts

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CP-118-EIHE 2023



An Unsteady-state, One-dimensional Model for Predicting the Performance of Lithium-ion Batteries



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Abstract:

Electrical energy storage is one of the critical technologies to achieve carbon neutrality. Green energy generated by solar rays and wind needs to be stored in batteries to make it available during the night and for a stable grid supply. Millions of electric vehicles are already in the market using battery storage. Lithium-ion batteries, due



to their high capacity of energy storage and fast discharge, are being used worldwide for consumer electronic applications, electric-vehicle applications and small-to-medium size utility scale electricity storage. There has been a vast development in the lithium-ion batteries since the last 20 years. However, there are still enough room for improvement to lower the cost and improve the storage capacity and safety, which call for a rapid prototyping. The development of an optimized battery design for a particular

application involves a large amount of time and experimental effort. Computer simulations using various types of mathematical models have been extensively used in new battery development leading to a great savings of time and materials. In this work, an unsteady-state, one-dimensional battery model simulates a lithium-ion cell. The cell consists of three sections: the negative electrode of graphite material, a polymer electrolyte separator, and a positive



electrode made of lithium manganese oxide. The process of electron and Li-ion transfer during the electrochemical reaction in the battery is schematically shown in Figure 1. The simulation results are compared with the experimental data for different C-rate factors. Effect of electrode particle size, porosity, and resistance due to surface layer are also reported.

Figure-1 shows that the maximum discharge capacity of 17.5 Ah/m^2 is obtained for a current density of 1.75 A/m^2 (0.1 C). It can also be seen that the 3 V discharge capacity decreases slightly when applying a 1C discharge current and dramatically when going above that. At 4C, the battery delivers approximately 50% of the theoretical capacity before it reaches a cell voltage of 3V. **References:**

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<u>CP-119-EIHE 2023</u>



Facets-Directed Epitaxially Grown Lead Halide Perovskite-Sulfobromide Nanocrystals Heterostructures and Their Improved Photocatalytic Activity



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Abstract:

Lead halide perovskite nanocrystals heterostructures have been extensively studied in the recent past for improving their photogenerated charge carriers mobility. However, most of such heterostructures are formed with random connections without having strong evidence of epitaxial relation. Perovskitechalcohalide are the first in this category, where all-inorganic heterostructures are formed with epitaxial growth. Going beyond one facet, herein, different polyhedral nanocrystals of CsPbBr₃ are explored for facet-selective secondary epitaxial sulfobromide growths. Lattice matching induced these epitaxial growths, and their heterojunction have been extensively studied with electron microscopic imaging (Figure 1). Unfortunately, these heterostructures did not retain the intense host emission because of their indirect band structures, but such combinations are found to be ideal for promoting photocatalytic CO₂ reduction. The pseudo-Type-II combination helped here in the successful movement of charge carriers and also improved the rate of catalysis. These results suggest that facet-selective all-inorganic perovskite heterostructures can be epitaxially grown and this could help in improving their catalytic activities (Figure

 $2).^{1}$



Figure 1. TEM image of CsPbBr3-Pb4S3¬Br2 heterostructures. **Figure 2.** Products generated after 2h of photocatalytic CO₂ reduction using pristine CsPbBr₃ and its heterostructure with Pb₄S₃Br₂

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Morphology Driven Activity of Layered Manganese Oxide towards Oxygen Reduction Reaction



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Abstract:

Oxygen reduction reaction (ORR) is the primary cathodic reaction for sustainable energy conversion and energy storage systems. Platinum based electrocatalysts are promising candidates to overcome the high activation barrier and sluggish ORR kinetics. Due to high cost of Pt, efforts have been made to replace it with cheaper alternatives. Manganese oxide has gained much attention because of its natural abundance, wide variation of crystallographic structure, variable Mn valency, non-toxicity. Thus, in the current work, layered Manganese Oxide(δ -MnO₂) was synthesized by different methods (Molten salt, McKenzie, Sol-Gel and Hydrothermal) and their respective ORR activity was compared. The XRD pattern of the samples match with δ -MnO₂ (JCPDS-18-1035). The linear sweep voltammetry (LSV) studies revealed that sample prepared by molten salt method possess remarkable activity in terms of onset potential, halfwave potential, limiting current density, n value and showed layered nano-flakes like structure whereas the samples prepared by Mckenzie and hydrothermal showed interwoven layers with honeycomb like morphology. The nano-flakes like structure with more exposed surface can be ascertained for the higher activity. But degrading ORR stability on multiple cycling is major challenge. Therefore, further work is required to understand the factors responsible for the higher activity and stability issue in the samples.



Figure : LSV curves of each materials at 1600 rpm in O₂ saturated 0.1M KOH
CP-121-EIHE 2023



Performance of polymer electrolyte membrane water electrolysis using dendrimer protected platinum catalyst



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Abstract:

The technology known as polymer electrolyte membrane water electrolysis (PEM WE) is regarded as a crucial step in the process of creating high-purity hydrogen from water and zero carbon emissions [1]. Electrolyzer industries efforts are aimed at reducing system complexity in order to enable system scale-up, lowering capital costs through less expensive materials and sophisticated stack manufacturing processes [2]. The goal of this work is to mitigate the use of platinum (Pt) for hydrogen evolution reaction in a single-cell PEM water electrolyzer. To this purpose, Polyamidoamine dendrimer encapsulated platinum metal (D-Pt) incorporated into multilayer graphene oxide (MLG) was synthesized as a cathode catalyst for HER. The performance evaluation and degradation of Dend-Pt in a single-cell PEM WE were systematically scruitinized using the standard electrochemical techniques. The amount of Pt was determined to be between \sim 1-2 wt.% on MLG support. The loaded Dend-Pt for single cell water electrolysis is 0.025 mg cm-2, which



is 40 times lower than the commercial Pt/C loading (1 mg cm⁻²). The MLG/D-Pt NPs catalyst exhibits a maximum current density of 12 A cm⁻² mg_{Pt}⁻¹@2 V while the commercial Pt/C catalyst only exhibits a maximum current density of 0.9 A cm² mg_{Pt}⁻¹@2 V.

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CP-122-EIHE 2023



Electrodeposited Molarity Dependent Bismuth Oxide Binder Free Flexible Electrode and ASSD (Bi2CuO4//AC) Supercapacitor Device



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Abstract:

Supercapacitors have attracted a lot of attention in recent years because of their great power density, extraordinarily extended cycling lifetime, outstanding cycling stability, and excellent safety liability. The present research investigates the bismuth oxide nano-materials were synthesized using electrodeposition method. Thin film electrodes were synthesized using bismuth nitrate as ingredient dissolved in distilled water deposited for molarity variations samples wereannealed at 573 K.

XRD of all deposited sample revels polycrystalline nature with tetragonal crystal structure. The FE-SEM revels Spruce Leaf-like Morphology. The CVs study of the bismuth oxide films in 1 M KOH



showed maximum SC of 239.26 F/g at scan rate of 2 mV/Sec. The SE of 42.36 Wh/kg¹, SP of 13.56 kW/kg¹ was calculated at 40 mA/cm² current density. The Electrochemical characterization of Asymmetric solid-state device (Bi₂CuO₄//AC), properties are investigated. The greatest specific capacitance of the asymmetric solid-state device (Bi₂CuO₄/AC) determined using

cyclic voltammetry at a scan rate of 5 mV/Sec was 93.53 F/g. At a current density of 10 mA/cm², the specific energy of 29.32 Wh/kg and the specific power of 3.36 kW/kg were estimated. All CV curves shows mixed capacitive nature. Nyquist plot is used for the observation of internal resistance of the optimized electrode.

Keywords: Electrodeposition; Thin Film; Flexible Electrode; Bismuth Oxide, ASSD.

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CP-123-EIHE 2023



Sensing of caffeine in real samples using Cu-MOF derived CuO nanoparticle decorated amorphous carbon as an electrochemical platform



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Abstract:

In recent times, development of an efficient electrode material for the determination of caffeine content in beverages and other related sources becomes essential [1,2]. In this work, for the first time, a novel electrochemical sensor based on carbonized Cu-4,4'-bipyridine-trimesic interlinked metal-organic framework (CBT-MOF) was prepared [3], characterized by various surface analytical techniques and employed for the effective sensing of caffeine. Copper-4,4'-bipyridine-trimesic acid interlinked MOF



(CBT-MOF) was prepared by simple solvo-thermal method and it was carbonized at different temperatures. The superiority of CBT-500 may be associated with rise in the Conductivity of the copper oxide nanoparticles by increasing the carbonizing temperature at 500 °C. which enhances the electron transfer kinetics between the analyte

and the copper oxide nanoparticle. Increase in temperature above 500 °C, (CBT-600 and CBT-700), results in lower conductivity, thereby decreasing the electron transfer kinetics between the electrode/electrolyte



interface. As expected, the amperometric detection of caffeine on fabricated electrode material provided a linear dynamic range from 1 to 10 μ M with a low detection limit and higher sensitivity of 0.0190 μ M and 0.0848 mA μ M⁻¹ cm⁻². Further, the fabricated electrode material remained stable, leading to a promising sensor material for the analysis of caffeine in coffee samples.

Figure: a) amperometric i-t response registered with increasing caffeine concentration (1 to 10 μ M) at CBT-500/GCE in 0.1 M PBS, b) the corresponding calibration curve for amperometric caffeine sensor and c) amperometric determination of caffeine (0.1 M PBS) in commercially available coffee powder, obtained in Tamil Nadu, India.

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<u>CP-124-EIHE 2023</u>



One pot synthesis and characterization of binary and ternary metal organic frameworks (MOFs) as tri-modal catalysts for thiophene electrooxidation, water splitting and 4-nitrophenol reduction



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Abstract

Because of their large specific surfacearea, high porosity, and changeable pore size, metal organic frameworks (MOFs) are emerging as electrocatalysts in various fields of energy resources and bio-sensors [1,2]. In this work, we report a one-pot synthesis of trimetallic MOF (Co-Ni-Al-MOF), as well as bimetallic

MOFs (Co-Ni-MOF, Co-Al-MOF, Ni-Al-MOF) using Co, Ni, as well as Al metal salts and BTC and 4,4'-bipyridine as linkers [3], their characterization using various analytical techniques and explored them as tri-modal catalysts for various redox processes. Electrochemical studies using linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS) on Co-Ni-Al-MOF showed the lowest onset potential of 1.36 V with a lesser Tafel slope of 181 mV/dec and charge transfer resistance value (R_{ct}) of 447 Ω for the effective electroxidation of thiophene. Further catalytic activity studies towards water splitting revealed that



Co-Ni-Al-MOF displayed superior catalytic activity towards HER and OER at a lower overpotential of 174 and 220 mV with Tafel slope of 108 and 97 mV/dec respectively (Fig. 1). Moreover, the catalytic activity was assessed towards the reduction of 4-NP to 4-aminophenol (4-AP), where Co-Ni-Al- MOF exhibited exceptional activity with a minimum reduction time of 8 mins bearing a high rate constant value.

Figure: (a) LSV curves of Ni-Al-MOF, Co-Al-MOF, Co-Ni-MOF, Co-Al-Ni-MOF, and commercial Pt-C electrocatalyst at a scan rate of 5 mV/s in 1.0 M KOH, (b) Tafel slope, (c) EIS spectra of the catalysts, (d) CA study of Co-Al-Ni-MOF for 24 h.

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<u>CP-125-EIHE 2023</u>



Effect of Ni Doping on the Oxygen Evolution Reaction Performance of Co₃O₄



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Abstract:

Oxygen evolution reaction (OER) is one of the essential reaction occurring in many energy conversion and storage technologies ¹. The mechanism of OER is somewhat complex due to the involvement of four electron-proton coupled reactions. Therefore the development of effective and stable OER catalyst is urgently required in order to facilitate the reaction and promote the evolution kinetics ². In this work, we have prepared Co₃O₄ with different concentration of Ni (X% Ni-Co₃O₄, X = 0, 2, 4, 6 and 8) by hydrothermal method and annealing treatment and evaluated as the OER electrocatalyst. Ni substitution remarkably enhances the OER activity. The electrocatalytic performance and physical shape of Co₃O₄



depends on the Ni substitution level. The 4 wt % Ni-Co₃O₄ nanoparticles can reach to a higher current density at a lower overpotential and required an overpotential of 390 mV to achieve 10 mA/cm² and the corresponding Tafel slope was 65.7 mV/dec. The results imply that proper Ni doping greatly enhances the OER activity due to the synergistic effect between Ni and

Co and the unique branched morphology. These findings suggest that transition metal oxide with low doping concentration will inspire the design of low cost and highly active electrocatalyst for OER.

Figure: (a) XRD pattern, (b) FT-IR spectra (c) polarization curve at a scan rate of 5 mV/s and (d) Tafel plot of X% Ni-Co3O4 (X = 0, 2, 4, 6 and 8)

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Metal oxide and Chalcogenides incorporated Graphene Sponge for enhanced water splitting



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Abstract:

Owing to several important properties, BiVO₄ is the promising photoanode material for the photoelectrochemical (PEC) water oxidation reaction, however the poor charge transfer, transport and slow surface catalytic activity limits to achieve the expected high theoretical efficiency. In the present investigation graphene sponge (GS) has been incorporated with BiVO₄ matrix. The PEC performances have been evaluated by fabricating the photoanodes by coating the material over FTO plates. Enhancement in the performance has been observed compared to the unmodified BiVO₄. In addition to the enhancement in the surface area of the catalyst the graphene sponge has the additional role in entanglement of the catalyst materials and the direction electron transfer, which has enhanced the catalytic performance significantly. The investigations like chopped light voltammetry, transient photoexcitation was carried out to evaluate the steady state and kinetic parameters of the catalysis process. It has bee observed that both the charge transfer and transport kinetics have been improved on graphene sponge incorporation. The Graphene Sponge and MoS₂

composite based cathode has bee fabricated for electrocatalytic hydrogen evolution. The catalytic performance has been enhanced by about 53% with the incorporation of GS along with MoS₂. The stability of the material has been improved due to the presence of stable GS network. The typical PEC performance due to the incorporation Gs along with BiVO₄ has been shown in Fig 1.

Fig.1 the chopped light voltammetry plot of BiVO4 photoanodes before and after different modifications.



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<u>CP-127-EIHE 2023</u>



Electro oxidation of methylorange on the surface of poly(ribo-flavin) by using carbon paste electrode



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Abstract:

This research describes the use of poly (Riboflavin) modified carbon paste sensor (PRFMCPS) to estimate the behaviour of electrochemical and to evolve an electrochemical procedure for detection of methyl orange (MO). The determination and estimation are performed through a cyclic voltammetry (CV). The surface morphology of the electrochemical sensor was characterised by field emission scanning electron microscopy (FE-SEM). PRFMCPS creates an electrocatalytic contact on the oxidation of MO. PRFMCPS properties were estimated using parameter such as pH solution, detection limit, and scan rate by means of CV. Electrochemical oxidation of MO in 0.2 M phosphate buffer solution (PBS) of PH 6.5 was examined in water sample by the application of PRFMCPS.



Investigation of Carbon Quantum Dots as an Aqueous Electrolyte for Energy Storage Devices



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Abstract:

The facile accessibility of electroactive species to the surface of graphene-based supercapacitors is crucial. Here, we report the potential of carbon quantum dots (CQDs) as an electrolyte for graphene-based supercapacitors. The aqueous CQDs electrolyte properties are explored and compared with other commonly used aqueous electrolytes. A gravimetric capacitance of 155 F/g at a current density of 1 A/g is achieved with an aqueous 25 mM CQDs electrolyte having 0.43 S/cm ionic conductivity. The energy density of as-fabricated device is calculated to be ~55 Wh/kg at a power density of 3200 W/kg with 1.6 V potential window (PW). Also, our approach comprises a solution-based flexible and free-standing CQDs-polymer



gel (f-CPG) electrolyte film formation. The f-CPG film reveals an ionic conductivity of 0.48 S/cm and a high dielectric constant (972) with low dielectric loss (~12) at 2 MHz frequency, at room temperature. The f-CPG electrolyte film exhibits a considerable electrochemical

performance with gravimetric capacitance, energy, and power densities of 140 F/g, 50 Wh/kg, and 8534 W/kg at 2 A/g, respectively. The CQDs electrolyte could be an excellent choice for energy storage devices.

Keywords: carbon quantum dots, electrolyte, flexible CQDs film, graphene supercapacitor

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Effect of Morphology Variations in CuS electrode material for Na-ion capacitor



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Abstract:

The electrochemical performance of copper sulphide (CuS) as an anode material for a Na-ion capacitor (NIC) is closely related to its morphology. Some CuS nanomaterials have improved Na+ ions transfer in addition to having a high capacitance. Here, various CuS nanostructures, including nanoparticles (0D), nanotubes (1D), hexagonal coins (2D), cross-linked nanotubes (3D), and worms, are synthesized by simple chemical routes and investigated for NICs in aqueous system. Cross-linked nanotubes (CLNTs) exhibit the highest gravimetric capacitance of 275 F g⁻¹ at 0.5 A g⁻¹ in three electrode configurations, as compared to other CuS nanostructures. The cavity of intricate CLNTs is effectively accommodating the volume change of CuS and help to avoid the discharged products from dissolution. The symmetric configuration of NIC with CLNTs shows a gravimetric capacitance of 315 F g⁻¹ at 1 A g⁻¹, followed by device fabrication with maximum working potential of 2.5 V. The device glows a red LED of 1.6 V and able to hold charge for ~111 seconds at 1 Ag⁻¹. The remarkable electrochemical results on CLNTs CuS obtained here suggest that it may be possible to develop and produce attractive CLNTs nanostructured materials for Na-ion Capacitors.



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<u>CP-130-EIHE 2023</u>



Synthesis and characterization of Si:MoSe₂ nanostructures for hydrogen Evolution reaction



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Abstract:

The systematized design of two-dimensional (2D) nanocatalysts for sensible energy-efficient reactions is quite a puzzling prospective aspect in energy-related applications. In this current work, we used a top-down strategy to synthesize silicon (Si) nanoparticles using a high-energy mechanical ball milling technique. In hydrothermal reaction, these Si nanoparticles were introduced into the 2D MoSe₂ matrix sequence based on varying the percentages of silicon (0 to 15 %) vs Se content. The high crystalline phases of the synthesized 10% Si:MoSe₂ exhibited the sheet-like morphology and silicon inserted layered structure. The pristine MoSe₂@CC & Si:MoSe₂@CC electrodes were prepared by tape casting method. During HER reaction, the miniscule insertion of Si into MoSe₂ matrix amplified the current density until 10% addition and moved the reduction curves towards lower onset overpotential (76.23 mV) in addition to the significant Tafel value (112.3 mV/decade). Furthermore, the rationally constructed functional electrode (Si:MoSe₂@CC) showed strong physicochemical stability, which can be used in future sustainable energy generation and storage devices.



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<u>CP-131-EIHE 2023</u>



One-Step Electrodeposited Cobalt Doped Bismuth Nanoparticles on Flexible Copper Substrate: Influence of Bismuth and Cobalt ratio variation for ASSD Device



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Abstract:

Energy generating and storage arrays are urgently needed in today's globe due to the rising energy consumption and population growth. The usage of supercapacitors as a high-power source for numerous electronic products is one of the efficient alternative methods for storing energy. Using bismuth and cobalt nitrates as the main ingredients, dissolved in distilled water, thin film electrodes were created by adjusting the ratios during the electrodeposition process. In a muffle furnace, prepared samples



were annealed at 573 K. Utilizing techniques such as XRD, FTIR, FE-SEM, Elemental mapping, EDX, XPS, CV, CP, and Impedance spectroscopy, physical and electrochemical characterizations of deposition potential variation dependent materials were investigated. In 1 M KOH, prepared samples were subjected to electrochemical analysis at various scan

speeds ranging from 1 to 100 mV/s. At a scan rate of 2 mV/s in 1 M KOH and in the potential window of 0.75 V to 0.75 V vs. Ag/AgCl, the greatest value of specific capacitance (SC) was recorded at 1698.0 F/gm. Charge-discharge behaviour of the improved electrode was investigated using the chronopotentiometric technique at various current densities. The computed maximum values of specific energy and specific power were 51.78 Wh/kg and 2.14 kW/kg at 10 mA/cm², respectively. The internal resistance of the improved electrode is seen using the Nyquist plot. On a flexible copper substrate, an asymmetric-solid-state flexible (ASSD) device was constructed using activated carbon as the negative electrode and cobalt-doped bismuth oxide as the positive electrode. No additional materials, such as a binder, separator, or packing material, were employed in the gel experiment save PVA/KOH as the electrolyte.

Keywords: Electrodeposition; Thin Film; Electrode; Cobalt-Bismuth Nanoparticle, ASSD.



A hybrid machine learning model for prediction of cobalt metal-organic framework-based ZIF-67 as corrosion inhibitor for X65 pipeline steel in CO₂-saturated brine



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Abstract:

Co-MOF based metal organic framework was synthesized by reacting a metal ion (cobalt nitrate hexahydrate) with an organic ligand (2 methyl imidazole) *via* a wet chemical method. The resulting material was characterized using detailed analytical methods and further was used as a self-assembly corrosion inhibitor in CO₂ environment. Prior to the study, design of experiment was done considering a hybrid machine learning algorithm- adaptive neuro fuzzy inference system (ANFIS). The empirical data was



Electrochemical measurement

derived from the electrochemical studies. The observed results showed that Co-MOF could significantly impede the corrosion rate of X65 steel and protect it from CO_2 corrosion. Increasing the concentration of Co-MOF in the test solution increased the inhibition efficiency up to 97 % at 0.1 wt. % Co-MOF with a mixed-type inhibition mechanism. From the standpoint of statistics, the explanatory model aligned credibly with high degree of accuracy

using ANFIS model. The overall findings confirmed a dense hybrid coating of the synthesized Co-MOF on X65 steel as responsible for the inhibition of the CO₂ corrosion.

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Alternative approach for highly sensitive and freeinterference electrochemical dopamine sensing



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Abstract:

In biological fluids, the dopamine (DA) concentration provides vital information about neurodegenerative disorders [1, 2]. An accurate DA determination, testified by a real sample is crucial for the prevention or early diagnosis and monitoring of these syndromes. Herein we report an improved approach for sensitive and free-interference DA electroanalysis. AgNPs were successfully attached to the surface of individual pristine MWCNTs. The resulting nanocomposite exhibited enhanced electron transfer properties, good electrocatalytic properties towards DA and great abilities to limit the UA oxidation in-situ. The properties of thus synthesized nanocomposite (AgNPs@MWCNTs) were subsequently combined with excellent capabilities of graphene oxide (GO) to attract DA while repelling AA and UA via electrostatic interactions [3], to fabricate an electrode material (GO-AgNPs@MWCNTs). Physico-chemical characterization confirmed the successful synthesis of AgNPs@MWCNTs, GO and GO-AgNPs@MWCNTs. The resulting sensor showed good repeatability, high sensitivity and complete suppression of UA and AA interferences. Calibration in the concentration range of 0.5 - 6.5 μ M in the presence of 300 μ M of AA and 500 μ M of UA revealed a linear response (R² = 0.99944) with a detection limit of 2.58 nM (S/N = 3). Moreover, the proposed sensor shown good long-term stability and satisfactory recoveries in human blood serum.

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<u>CP-134-EIHE 2023</u>



Design and development of electrodeposited Pd-thin film electrodes for acetaminophen detection



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Abstract:

The present work is mainly focused on the preparation of eco-friendly electrodeposited flexible electrode using ammonia complex without any surfactant additives. Herein, Pd electrodeposition was carried out on carbon cloth (CC) and applied for electrochemical sensing applications. Further, cathode



current efficiency and rate of film growth were calculated using Faraday's law of electrolysis which helps to improve the quality of deposited Pd. The surface morphology, crystalline structure, topography, elemental

composition and oxidation state of elements were analysed by FESEM, XRD, AFM and XPS characterisation techniques. The electrochemical sensing performance towards acetaminophen (ACAP) in neutral medium (pH 7.0) were evaluated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). PdCC modified electrode shows an enhanced electrocatalytic activity for the oxidation of ACAP with lower oxidation potential with a wider linear range of $5 - 6000 \mu$ M along with an LOD of 0.942 μ M. The PdCC modified electrode has achieved good stability, reproducibility, reusability and anti-interference ability towards the sensing of ACAP.

Figure: DPV response of bare CC and PdCC with the existence of 1 mM ACAP and (B) DPV concertation effect.

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<u>CP-135-EIHE 2023</u>



Co₃O₄-CuO Supported AgNPs Nanocomposite as a Potential Material for Supercapacitor Application



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Abstract:

In the present work, hydrothermal synthesis of Co₃O₄-CuO oxide composite thin film substrate material with greener deposition of silver nanoparticles over oxide support has been illustrated successfully. The synthesized material was characterized by using different analytical techniques including XRD, FE-SEM, HR-TEM and XPS. As prepared Co₃O₄-CuO@AgNPs composite material was used for the



modification of glassy carbon electrode. The Supercapacitance of application the newly synthesized composite material was studied using cyclic voltammetry (CV), galvanostatic charge-discharge test and electrochemical impedance spectroscopy (EIS). The composed catalytic material exhibited excellent Supercapacitance and charge-discharge activity in

alkaline medium. Furthermore, the composed material showed superior stability towards supercapacitance for different cycles.

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<u>CP-136-EIHE 2023</u>



Layered Porous Graphitic Carbon Nitride Stabilized Effective Inverse Spinels, Spinels and Perovskites as Bifunctional Electrocatalyst



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Abstract:

Developing efficient, low-cost and non-noble metal oxide based nanohybrid material as bifunctional electrocatalyst is highly desirable approach in the promotion of clean energy harnessing and to minimize environmental issues. Accordingly, we proposed an interfacial engineering approach to construct layered porous graphitic carbon nitride $(g-C_3N_4)$ stabilized $-Co_2SnO_4$ inverse spinel or $-Ni_xCu_1$. $_xFe_2O_4$ spinel or -perovskite-type NiSnO_3 or $-NiWO_4$ nanohybrid materials as highly active bifunctional electrocatalyst. Herein, the different morphologies metal oxides nanohybrids stabilized with layered porous g-C₃N₄ has been synthesized with enhanced surface area via simple one-pot hydrothermal method. Besides, the detailed structural and morphological characterizations were carried out using powder XRD, XPS, FE-SEM, HR-TEM, FT-IR and BET analysis. Briefly, XPS analysis has revealed the existence of strong coupling bond at the interface between definite proportion of g-C₃N₄ nanosheets and metal oxides, act as heterojunction stimulates electron transport channel to explore the exceptional performances in HER, OER, Overall water splitting and in methanol oxidation.



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<u>CP-137-EIHE 2023</u>



Meniscus-confined electrochemical additive manufacturing (MC-ECAM) technique for metallic nanostructures



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Abstract:

Micro- and nano-printing of cost-effective addressable metallic nanostructures has been a long endeavour in terms of both scientific understanding and industrial needs. Herein, a simple and efficient meniscus-confined electrochemical additive manufacturing (MC-ECAM) technique with a faster deposition speed (1 mm/s⁻¹) is designed. A stable meniscus bridges the nozzle to the conductive substrate to precisely control metal deposition by reduction (M ^{z+} + M ^{e-} \rightarrow M⁰) of metal on the substrate. Various metal such as gold, silver and copper nanostructures are printed without any additional post-printing steps. The precise electron microscope characterizations show well-oriented metallic nanostructures are successfully printed via MC-ECAM. Furthermore, the XRD results revealed the formation of pure metallic nanostructures which remained unchanged after 10 months in the atmosphere. An underlying mechanism for the remarkable stability and corrosion resistance of MC-ECAM printed metallic nanostructures is proposed. MC-ECAM enabled precise additive control over a metallic nanostructure, enabling programmatic synthesis of metallic structures with the desired shapes and properties.



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<u>CP-138-EIHE 2023</u>



Aqueous Alkaline hybrid Zinc/TEMPO Flow Battery: A High Voltage Green Energy Storage Device



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Abstract:

Aqueous organic redox flow batteries (AORFBs) have gained special attention for large-scale energy storage due to several specific advantages such as synthetically programmable high oxidation/reduction redox potentials, abundance in nature and great solubility. However, the low cell voltage aqueous based electrolytes limited energy density. The hybrid RFB inherits the advantages of both aqueous and non-aqueous systems, displaying promising properties for next-generation RFBs such as a large potential window and high energy density. The limiting cell voltage of the hybrid neutral Zinc/TEMPO polymer hybrid flow battery is 1.4 V, resulting in a poor energy density. We have used freshly alkaline $Zn(OH)_4^{2-}/4$ -hydrox TEMPO (4HT) as a hybrid RFB system, which has a high cell voltage of 2.097 V and an energy density of 25.32 Wh L⁻¹. At 40 mA/cm⁻² current density, the high rate GCD profile of alkaline $Zn(OH)_4^{2-}/4$ HT demonstrates 90% coulombic efficiency and 60% energy efficiency. Further, the alkaline-based Zn/4HT exhibits a remarkable capacity retention of 99.99% over 100 cycles and an energy density of 25.32 Wh L⁻¹. The complete physio-chemical and electrochemical characterization of Zinc/TEMPO hybrid redox flow cell will be discussed in detail.

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Binder free Aluminium doped MoS₂@CC electrode for supercapacitor



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Abstract:

Aluminium doped MoS2 electrode is directly grown on carbon cloth using facile hydrothermal method. The formation of MoS₂ was confirmed by X-ray diffraction (XRD) and Raman spectroscopy analysis. Field Emission Scanning Electron Microscope (FESEM) and High-Resolution Transmission Electron Microscope (HRTEM) images exhibited the flowerlike morphology and layered structure of MoS2, respectively. X-ray photo electron spectroscopy (XPS) identifies the presence of constituent elements and their chemical state. The potential of the prepared electrodes is tested using three electrodes, symmetric two electrodes and asymmetric two electrode systems in 1M Na₂SO₄ electrolyte. Three electrodes system yielded a specific capacitance of 111 F/g at a current density of 1 A/g with an energy density of 10 Wh/kg at a power density of 175 W/kg. The asymmetric supercapacitor yielded a specific capacitance of 45 F/g at current density of 1 A/g and an energy density of 3.62 Wh/kg at a power density of 424.5 W/kg. The asymmetric capacitor yieldes at a current density of 2A/g.



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<u>CP-140-EIHE 2023</u>



Electrochemically Generated Cu(I) Catalyzed Click Chemistry: Triazole Synthesis and Insights into their Photophysical Properties



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Abstract:

The most well-known "click" reaction is highly effective and selective catalyzed by copper(I) catalyst and hence called Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC). A five-membered di-substituted triazole is produced via 1,3-dipolar cycloaddition reaction between a terminal alkyne and an organic azide. Herein, we report the electro-click (e-CLICK) reaction catalyzed by electrochemically generated copper(I) catalytic species. The reaction was carried out under constant potential electrolysis (-0.25 V vs. Ag/AgCl) with copper (II) nitrate and 2,2'-bipyridine serving as pre-catalyst and ligand respectively. The reaction accommodates electronically different organic azides to afford 1,2,3-triazoles in good synthetic yields with excellent 1,4-regioselectivity. Compared to traditional click chemistry, the developed e-CLICK methodology avoids the use of external reducing agent such as sodium ascorbate. Absorptive properties of the resulting triazole products were assessed by UV-visible spectroscopy.

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Cerium-based metal organic framework as corrosion inhibitor for Cu alloy in chloride environment



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Abstract:

The synergistic effect of a metal ion/cluster (cerium nitrate hexahydrate) with an organic linker (2 methyl imidazole) as a hybrid corrosion inhibitor for Cu alloy in chloride environment was investigated. Detailed characterization of the Ce-MOF was achieved *via* series of analytical test and was further evaluated using complete electrochemical approach based on polarization study and electrochemical impedance spectroscopy. The results reveals that the synthesized Ce-MOF inhibited Cu corrosion in severe marine environment. From the electrochemical point of view, Ce-MOF acted as a mixed type inhibitor and the increase in the charge transfer resistance is dependent on the systematic increase in the Ce-MOF for polarization and impedance studies, respectively. Also, the surface analysis *via* FE-SEM, AFM and XPS evidence the presence of a hybrid coating on the Cu surface, thus protecting it from further surface dissolution in harsh marine environment.

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<u>CP-142-EIHE 2023</u>



The effect of Benzotriazole, 8-Hydroxyqunoline and €-2-(2,3,4 trihydroxybenzylidene)hydrazinecarbothioamide on the corrosion of AA 7075 in 3.5 % NaCl environment



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Abstract:

The present research studies highlight the effect of (E)-2-(2,3,4 trihydroxybenzylidene) hydrazinecarbothioamide (THC) on the corrosion of AA7075 in 3.5% NaCl. The results are compared with benzotriazole (BZT) and 8-hydroxyquinoline (HQ) which are frequently reported as corrosion inhibitors

for iron, aluminum, and copper alloy. Electrochemical impedance spectroscopy and potentiodynamic polarization studies were performed to study the effect of BZT, HQ, and THC on the disintegration of AA7075 in a 3.5% NaCl aqueous solution. Corrosion studies are performed for various exposure durations at $30\pm1^{\circ}$ C. The maximum corrosion inhibition efficiency of



BZT, 8-Hq, and THC is 44 %, 94.3 %, and 99.66 %, respectively. The samples were immersed in the corrosive media with and without inhibitors for seven days. The resultant specimens were examined using FE-SEM and 3D profilometry to verify the inhibition performance of the organic molecules on the substrate. In addition, XPS was employed to find the inhibitor layer on the substrate.

Keywords: AA7075, BZT, HQ, THC, 3.5 % NaCl, EIS, Potentiodynamic polarization.

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<u>CP-143-EIHE 2023</u>



Co- doped Cubic NiO Nanoflakes: Facile, one-step synthesis, effective doping and excellent supercapacitor performance



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Abstract:

We have synthesized highly porous cobalt doped NiO nanostructures with systematic doped ratios such as $Co_{0.1}Ni_{0.9}O$, $Co_{0.2}Ni_{0.8}O$, $Co_{0.3}Ni_{0.7}O$, $Co_{0.4}Ni_{0.6}O$ and $Co_{0.5}Ni_{0.5}O$ through a facile, low cost, one step solution combustion method^{1,2}. The synthesis strategy requires no post calcination treatment and the products of high quality are obtained in very short time. It was found that the process of doping does not alter the phase structure of pristine cubic NiO³, but it obviously influences the textural and morphological properties, more importantly, enhances the electrochemical properties of pristine NiO. The maximum specific capacity exhibited by Co doped sample, $Co_{0.4}Ni_{0.6}O$ is 746 C/g, which is far superior to undoped NiO (295 C/g). An asymmetric device fabricated using $Co_{0.4}Ni_{0.6}O$ electrode as the positive electrode and activated carbon as the negative electrode delivered an energy density of 32.7 Wh/kg at a power density of 261 W/kg. The performance of cobalt doped NiO nanostructures suggests its potential in the field of energy storage.



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<u>CP-144-EIHE 2023</u>



Development of selective and sensitive electrochemical sensor for the determination of antihistamine drug



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Abstract:

A novel electrochemical sensor based on of Mg-Ag-Al (LTH) was confirmed by FE-SEM, EDX and XRD. Mg-Ag-Al (LTH)/GCE has been developed for sensitive and selective detection of promethazine. Electrochemical properties of Mg-Ag-Al (LTH)/GCE has been investigated using cyclic voltametry (CV), differential pulse voltametry (DPV) and amperometry (CA). The CV analysis of promethazine proved the capability of (LTH) Mg-Ag-Al/GC electrode to execute the oxidation reaction. The voltametric and amperometric limit of detection, linear range and limit of quantification of promethazine was found down to CV: 3.5 nM L^{-1} , $50-250 \mu M L^{-1}$ and 10.5 nM L^{-1} , respectively with DPV: 4.2 nM L^{-1} , $50-500 \mu M L^{-1}$ and 12.6 nM L^{-1} . The amperometric LOD were found to be 25 nM L^{-1} . Besides, (LTH) Mg-Ag-Al/GC electrode has also been detecting the promethazine potential for CV; +680 mV and DPV; +660 mV. The (LTH) Mg-Ag-Al/GC electrode was high sensitivity and reproducibility.

Keywords: Modified GCE, Mg-Ag-Al (LTH), Promethazine, Limit of detection and Voltametric methods.



Fluorine-free synthesis of Tantalum carbide: Enhanced HER activity and Nitro compound reduction



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Abstract:

The electrochemical process is one of the sustainable ways to produce hydrogen which is considered to be a clean energy source. Herein, we report the preparation of 2D Tantalum carbide MXene prepared via fluorine-free etching method and its application in catalysis. It is well-known that owing to their layered structure, MXene shows better catalytic activities and hence they find applications in catalysis and electrocatalysis. Ta₂AlC (MAX phase) and Ta₂C (MXene) were evaluated for their electrocatalytic application in the hydrogen evolution reaction and further, the reducing behavior of Ta₂C towards the reduction of *p*-nitrophenol to *p*-aminophenol in the presence of NaBH₄ was tested. In both studies, Ta₂C showed improved catalytic performance and stability.

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<u>CP-146-EIHE 2023</u>



Biocompatible Redox Nanosystem for Inflammation Management via free radical scavenging and Electrochemical Immunosensing of Interleukin-6



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Abstract:

Cascade of free radical generation affects body homeostasis further trigger release of pro/antiinflammatory cytokines such as IL-6 (interleukin-6) augmenting inflammation^{1,2}. Emerging redox-active nanosystems encompassing antioxidative phytochemicals with free radical scavenging and electrochemical transduction properties can be of prime importance in inflammation disease management. Additionally,



biocompatible nanosystem are advantageous for implantable matrix for real-time monitoring of inflammation. Herein, we have synthesized triad (biocompatible, redox-active, and free-radical scavenger) nanosystem (*dia.* 12-18 nm) by two step microwave/sonochemistry assisted hybridization of anti-oxidative polyphenol (kaempferol) ligand in molybdenum tri-oxide matrix, a metalloprotein co-factor, named as molybdenum tri-oxide hybridized kaempferol

nanoparticles (MoHK NPs). Mechanistic studies revealed a strong electrostatic/H-bond formation between $Mo^+-O^-=C4/Mo=O-OH-C5$ with increase oxidation and decreased coordination number enabled enhanced redox activity. MoHK NPs acted as a potent free radical scavenger both *in vitro* and *ex vivo* on inflammatory cell (RAW 264.7). Further, *in situ* ECIS (Electrical cell substrate impedance sensing) based biocompatibility studies ensured applicability of MoHK NPs as an implantable matrix and further employed as transducer for IL-6 immunosensing in layer-by-layer fabricated electrochemical platform. Observed clinical range of detection in serum samples (fM-nM) with high selectivity, sensitivity (0.63 fM/mA/cm²), and low detection limit (~0.91 fM), enabled its potential utility in anti-inflammatory theranostics.

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Enhanced Energy Storage by Ternary Composite of Metalloid Induced Porous Polyacrylonitrile / polyvinylpyrrolidone Carbon Nanofiber, NiCo-MOF and Conducting polymer for Free-standing Symmetric Supercapacitor



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Abstract:

Porous carbon nanofibers (PCNFs) produced from polyacrylonitrile (PAN)/polyvinylpyrrolidone (PVP) hybrid nanofibers with different doping levels of metalloid were developed with NiCo-MOF, and the fabricated electrode was modified with a conducting polymer by electrochemical polymerization and was used as free-standing, high performance electrodes for symmetric supercapacitors. Effects of metalloid



(MA) doping level to polymer mixture, stabilization/carbonization process on chemical structure and morphology of PAN/PVP, PAN/PVP-MA hybrid nanofibers and PCNF/NiCo-MOF/CPT were investigated by X-

ray diffraction spectroscopy (XRD), Raman spectroscopy, Fourier transform infrared (FT-IR), field emission scanning electron microscopy (FE-SEM). It was proved by XRD, FT-IR and FE-SEM analyses that PAN/PVP-MA and PCNF/NiCo-MOF/PEDOT hybrid nanofibers were successfully produced and

carbonized. In addition, the electrochemical performance of free standing symmetric supercapacitors with PAN/PVP, PAN/PVP-MA and PCNF/NiCo-MOF/PEDOT electrodes



was analysed by cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), and electrochemical impedance spectroscopy (EIS) methods. Specific capacitance of PAN/PVP-MA CNF (PCNF) and PCNF/NiCo-MOF/CPT were determined by two electrode assembly. The fabricated substrate electrodes have delivered good energy density, power density and improved rate capability.

Figure: (a) SEM image of ternary PCNF hybrid composite, (b) Elemental carbon mapping of PCNF hybrid composite, (c) Cyclic voltammetry of composite PCNF/NiCo-MOF/CPT//PCNF/NiCo-MOF/CPT symmetric capacitor, (d) Galvanostatic charge discharge of PCNF/NiCo-MOF/CPT//PCNF/NiCo-MOF/CPT.

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<u>CP-148-EIHE 2023</u>



Synthesis of DyM/S-GCN composite and its application as electrode material for the sensitive detection of antibiotic.



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Abstract

The present study elucidates the development of sensor-based nanomaterials to quantify Chloramphenicol (CAP). Dysprosium Molybdate and sulfur-doped graphitic carbon nitride (DyM@S-gcn) are used as transducer material. DyM is synthesized by co-precipitation method and S-gcn is synthesized by thermal polymerization method. The as-synthesized DyM@S-gcn was characterized usingTEM, EDAX, XRD, XPS techniques and the modification of the electrode is confirmed by EIS. The performance parameters such as pH, scan rate, electrocatalytic oxidation of CAP, Interference, repeatability, reproducibility, and stability were optimized for the developed sensor. The developed sensor showed a sensitive response with a LOD of 1.25 μ M, limit of quantification LOQ of 41.91 μ M, and sensitivity of 112.26 μ A mM⁻¹cm⁻² for CAP. The proposed sensors find application in a broad concentration range from 100 to 1000 μ M. The results endeavored the possible use of these sensors in environmental protection and monitoring. Based on the results, it can be claimed that the DyM@ S-gcn forms an excellent electrode material for electrochemical detection of CAP.

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Facile Synthesis of Pd@Ag-Zn-rGO Nanocomposite and it's Selective Electro-Catalytic Application in Ethanol Oxidation



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Abstract:

In the present work, two step facile approach was developed for the synthesis of Pd@Ag-Zn-rGO nanocomposite material via incineration and sol-gel method. The synthesized material was characterized by different characterization methods such as XRD, FE-SEM, HR-TEM, and XPS etc. Electrochemical analysis was studied by using electron impedance spectroscopy. The application of the composed material was investigated for the electro-oxidation of ethanol in alkaline medium by using cyclic voltammetry technique. The proposed catalytic material showed excellent current density with high stability towards ethanol oxidation.



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Wearable glove based electrochemical sensor for rapid and point of care detection of Chikungunya virus



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Abstract:

Flexible biosensors are an increasingly important field of research and development. Rubber gloves are a viable option in this context because of their flexibility, cost, disposability, and scope for integration. On the other hand, an electrochemical detection is fully compatible with flexible biosensors. Therefore, prepared high response nanomaterials play a crucial for fabrication of wearable sensors. Zinc oxide nanomaterials are considered as a preferable active sensing material because to their superior biocompatibility, broad electrochemical window, and chemical inertness. Here in the present study, an



extremely conductive zinc oxide nanorods were created using a simple, inexpensive approach. Scanning Electron Microscopy, X-ray Diffraction, FTIR analysis and UV-Vis Spectrophotometer were used to characterize zinc oxide nanorods in terms of their morphology. Further, aptamers are employed as the biorecognition element because they acquire specificity, higher binding affinity, and better target discrimination. This specific, and sensitive assay, as well as the usage of aptamer in point-of-care testing near the patient, can be

employed as a rapid and early diagnostic tool. The entire process was monitored using cyclic voltametric and linear sweep voltametric responses. With this highly sensitive glove-based biosensor with 1ng/ml limit of detection was achieved. Our findings imply that the developed glove-based aptamer biosensor can be employed in a variety of quick diagnostic procedures for the detection of Chikungunya virus infection.

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Stabilizing low-Co content based LiNi_{0.7}Mn_{0.2}Co_{0.1}O₂ layered cathode using Cu²⁺substitution



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Abstract

Layered structure $Li[Ni_xMn_yCo_{1-x-y}]O_2$ (NMC721, x=0.7, y=0.2)and LiNi_{0.7}Mn_{0.2}Co_{0.08}Cu_{0.02}O₂(NMC721-Cu) were prepared using solid-state process. The electrochemical charge storage performances were investigated using Li-ion half-cell configurations. All the prepared samples were subjected to various structural and morphological characterizations such as X-ray diffraction analysis, XPS, HR-TEM, FESEM, and Raman spectral analysis. XRD refinement studies revealed that the doped (Cu²⁺) element occupy the inter-slab spacing of the NMC721 layered crystal structure. Substituting the Cu2+ ions in the bare NMC721 structure helped to improve the structural stability and specific capacity of the NMC721 cathode. The maximum specific capacity of 162 mAh g⁻¹ (at 0.1C) vs. Li/Li⁺ for the NMC721-Cu cathode was obtained, which is far better than the bare NMC721 (130 mAh g^{-1} at 0.1C). Thus, the effect of doping in the nickel-rich, layered cathodes will be considered a futuristic candidate for highenergy Li-ion battery applications.

Keywords: Layered structure, solid state synthesis, copper doping, high voltage, high capacity, and high energy density



Graphical Abstract:

<u>CP-152-EIHE 2023</u>



Origami-based aptasensor using gold decorated zinc and graphene nanocomposites to detect polyvalent antigen of dengue virus spiked in human serum



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Abstract:

The development of point-of-care devices based on paper-based origami biosensors is currently of great interest. These devices highlight how the foldability of paper enables the development of sensitive, selective, user-friendly, intelligent, and sustainable analytical devices for the diagnosis of various diseases.



Here, for the very first time, we have demonstrated electrochemical aptasensor-based detection of polyvalent antigen of dengue virus using the paper-folded technique called origami and combining it with aptasensor leads to the development of new notation called OBAs i.e., origami-based aptasensor which offers numerous

benefits to the developed platform, such as, it helps to protect the sample from the air-dust particles, to make it confidential, provide closed chamber to the electrodes. In this work, nanocomposites was also synthesized which enhance the signal of the proposed sensor. Herein is low-cost, simple, and effective OBAs is constructed without using any expensive leaser cutter and 3D printer machines which successfully detected the polyvalent antigen of dengue virus in spiked human serum showing a good range from 0.0001mg/ml to 0.1mg/ml with a LOD of 0.0001mg/ml. This single-folding ori-aptasensor exhibits excellent sensitivity, specificity, and remarkable performance in human serum assay and could be used in point-of-care testing of different viral infections for remote locations, and developing nations, as well as applicable during outbreaks.

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Graphite recovery from spent lithium ion batteries.



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Abstract:

With the massive increase in the demand of electronic devices such as mobile phone, laptop, vehicles and computer the utilization yield of Lithium batteries gradually increases. Consequently, the occurrence of spent lithium batteries increases as well. The graphite content in Li ion batterie is between 15% to 21%. The wide usage of natural graphite in various field will induce graphite scarcity in the future and price fluctuation of the later. Therefore, recycling graphite from spent Li batterie will not only prevent the graphite scarcity, but will also be economically beneficial, reduced environmental pollution and be a material of choice for sustainable development of related industries. This work investigates effective method for recovery of graphite from Spent Li ion batteries trough thermal, and acid treatment method. The regenerated graphite was characterized using XRD, FETEM, FETEM and FTIR method.



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<u>CP-154-EIHE 2023</u>



A novel hierarchical porous activated carbon-organic composite cathode material for high performance aqueous zinc-ion hybrid supercapacitors



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Abstract:

Zinc-ion hybrid supercapacitors (ZIHSCs) are among the most promising electrochemical energy storage technologies because of their high energy density, environmental sustainability, low price, and inherent security. Hence, we have developed a novel energy storage system that uses a hierarchical porous activated carbon with redox-active organic materials as an active hybrid cathode material for ZIHSCs. The large surface area of chitosan-derived activated carbon (Ch-C), the fast electron transfer mechanism of bis-glycinyl naphthalene diimide (H₂BNDI), and zinc's bivalent nature all together contribute to the high energy density of redox-active zinc-ion hybrid supercapacitors (RAZIHSCs). The fabricated device exhibited an outstanding energy output of 250 Wh kg⁻¹ @ 0.1 A g⁻¹ and a power output of 9.5 kW kg⁻¹ @ 10 A g⁻¹ due to the additional pseudocapacitive behaviour arising out of the redox-active H₂BNDI material. Additionally, 100 % coulombic efficiency and 80 % capacitance retention are still attained after 10000 cycles at a high current density of 5 A g⁻¹. As a result of the complex chemical reactions between Zn²⁺-ions and H₂BNDI moiety in the composite cathode, the proposed RAZIHSCs demonstrated a lower self-discharge rate (23 % in 25 h) with extremely low leakage current density (15 mA g⁻¹).

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Surface engineering of Hollow Carbon Tubes via Heteroatom Doping Approach for Electrochemical Detection of Diphenyl Amine



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Abstract:

To design and develop a facile synthesis of hollow tubular carbon-based materials with higher catalytic performances are remains challenging. Herein, self-sacrificing template strategy is employed for the construction of graphitic layer wrapped hollow carbon nanotubes (CNT) encapsulated with nitrogen and sulphur heteroatoms. Surface engineering of nitrogen and sulphur codoped mesoporous hollow carbon nanotubes (NSCNT) is described, and synergistic effect of heteroatom doping and porosity tuning upon the electrochemical performance is demonstrated for the effective detection of diphenyl amine (DPA). Differential pulse voltammetry was employed as an electrochemical tool to assay DPA using NSCNT-0.5/GCE with an increased sensitivity of 3-fold compared with bare. Benefitting from abundant catalytic active sites and faster electron transfer kinetics, the NSCNT altered electrode covered a wide range of concentration 5-500 µM and achieved a lower LOD with appreciable sensitivity. Moreover, the impact of negligible effect on DPA sensing which clearly makes it as ideal sensing device feasible for technical analysis. Real sample analysis was scrutinizing the excellent efficiency and reliability of proposed sensor with fruit samples for the detection of DPA with peerless recovery range. The strategy developed herein reveals a feasible path for enhancing the electrochemical applications.

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<u>CP-156-EIHE 2023</u>

Electrochemical studies of the complex of U(VI)-1hydroxy 2-pyridone



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Abstract:

Hydroxypyridones are considered as the most promising agents for the treatment of iron overdose diseases. It forms a stable bidentate chelating complex with Fe(III), Al(III) and with other actinide ions (Pu(IV), Th(IV)) [1]. A recent publication by Wang et al. shows its application in the decorporation of U(VI) ions [2]. The objective of the present investigation is to understand the electrochemical behaviour of uranyl complex with 1-hydroxy 2-pyridone (1,2-HOPO, Fig1a(inset)). Cyclic voltametric (CV) studies were done in a three electrode system (WE: GC, CE: Pt, RE: Ag/AgCl) at different nitric acid concentrations with the ligand (1,2-HOPO), U(VI) ion and the metal-ligand complex. The corresponding CV at pH 2.0 is



Figure: (a): CV of the U(VI)/Ligand/Complex, (b) Scan rate variation of the complex

shown in Fig. As can be seen from Fig. 1a, a negative shift in the reduction potential (97 mV) is seen in the complex corresponding to U(VI)/U(V) couple whereas a broad peak resulted in the U(V)/U(IV) couple. The negative peak shift suggests the formation of U(VI)-HOPO complex in the solution. Diffusion coefficient of U(VI)-HOPO complex was found to be 6.2×10^{-7} cm²/s from the scan rate variation experiment (Fig.1b).

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Promising dual-doped Porous Carbon Materials as Metal-Free Electrocatalyst for Oxygen Reduction Reaction



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Abstract:

Designing of cost-effective electrocatalyst with excellent catalytic activity for oxygen reduction reaction (ORR) is one of the crucial parameters in the development of clean and sustainable fuel cells and metal-air batteries. This work demonstrates the synthesis of dual-doped porous carbon materials as a high performing metal-free electrocatalyst. A Cyclotripolyphosphazene based polymer was utilised to derive the asprepared carbons at different temperatures. As expected, the resulting nitrogen and phosphorus-doped porous carbons have large specific surface areas, high nitrogen content with phosphorus contributing synergistically for enhancement of the catalytic activity towards Oxygen reduction reaction. The optimized catalyst obtained by carbonization at 800 °C exhibits superior ORR performance as compared to the state-of-the-art Pt/C or Pt-based catalysts as judged by high onset potential, positive half-wave potential and high diffusion-limited-current density. Furthermore, the remarkable electrochemical stability of the optimized material, appreciable tolerance towards methanol poisoning and a near four-electron pathway for oxygen reduction in alkaline medium (0.1 M KOH) unambiguously demonstrates that the metal-free electrocatalysts.



Figure. Comparative LSV curves of the optimized catalyst and commercial Pt/C catalysts

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Nitrogen and Sulfur Enriched Porous Carbon Materials with Trace Fe as an Efficient Oxygen Reduction Electrocatalyst



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Abstract

The replacement of Pt-based catalysts with non-precious metal-based electrocatalysts has become an urgent need for the commercialization of metal-air batteries and fuel cells. Our work is based on designing a non-precious metal-based electrocatalyst that can effectively be used as a substitute for the precious Pt-based catalysts. The synthesized electrocatalyst is porous carbon material containing Nitrogen (N), Sulfur (S), and trace Iron (Fe) moieties which makes it a compatible electrocatalyst for improving the sluggish kinetics of Oxygen Reduction Reaction (ORR). The optimized catalyst appeared to have a high surface area and large porosity. The optimized catalyst displayed a positive onset potential and a high diffusion-limited current density along with the favoured 4-electron pathway for ORR. Further, it exhibited superior methanol tolerance and long-term durability compared to Pt/C. This remarkable catalytic ORR activity and electrochemical stability collectively makes our designed catalyst competent for energy conversion and energy storage devices.



Figure. Comparative LSV curves of the optimized catalyst and commercial Pt/C catalysts

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Redox speciation of Uranium at 2D-MXene/GC modified electrode for electrochemical sensing



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Abstract:

A new family of two dimensional (2D) nanomaterials, called MXenes (first discovered in $2011^{[1]}$), have emerged as a exciting electrodic materials for energy storage and electrochemical sensing due to their unique physical, chemical, and electrical properties. MXenes have a generic formula $M_{n+1}X_nT_x$ (n = 1~3), where M represents an early transition metal, X is C and/or N, and T_x refers to surface-terminating functional groups (such as O, -OH or -F). Compared to other 2D materials, MXene possess high electrical conductivity, excellent hydrophilicity, good chemical and thermal stability, high surface areas, tuneable and abundant surface functionalities and faster access to analyte. Therefore, Mxene can be utilized as effective transducers for molecular sensing and is ideal for constructing high performance electrochemical sensors. Uranium (U) high concentration in the environment is known to pose serious health hazard to mankind. Advancement of sensor for speciation and monitoring at low concentration level of U is essential to understand its mobility and reactivity in environment and to analyse swipe samples collected from equipment or environs of nuclear facilities for nuclear forensic applications. MXenes are stable in the cathodic potential window, therefore, it can work a promising sensing material for U. MXene $(Ti_3C_2T_x)$ is synthesized in our lab by selectively etching of Al from Ti₃AlC₂ using HF and characterized by XPS, which indicates presence of terminal -OH groups. As-synthesized MXene (3 mg/ml) was used to modify GC electrode. Cyclic (CV) [Fig. 1] and differential pulse voltammetry (DPV) of U were performed at varying pH and scan rates (v) at MXene/GC. Results indicates (i) two reductive peaks at -0.288 and -0.846 V, which are assigned as two consecutive single electron transfer of U(VI)-U(V) & U(V)-U(IV) conversion with cathodic shift in peak potential (E_p) and enhancement in peak current (i_p) at MXene/GC than GC, (ii) Enhancement in i_p with v along with linearity between i_p vs. \sqrt{v} [Fig. 2], implies diffusion-controlled reduction of U, (iii) more current density at pH 4.5, which may be due to more chelating efficiency of -OH of MXene (iv) Diffusion coefficient (D₀), $\alpha n \& k^0$ of U were determined to be 5.25 x10⁻⁵ cm²/sec, 0.65 and 2.5×10^{-4} cm/sec, respectively while detection limit was found as $(1\pm 0.06)\times 10^{-7}$ M. DFT studies provide the binding modes of MXene with U and corroborates the CV results.



Fig. 1: CV of U (10⁻⁴ M) at GC & MXene/GC; pH 4.5

Fig. 2: (a) CV with v variation (b) $i_p vs. \sqrt{v}$ plot



Waste cotton cloth derived carbon cloth for high performance lithium sulfur battery



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Abstract:

Low cost, non-toxicity and abundant resources have driven the attention of the battery research



fraternity towards sulfur based energy storage systems. In particular, the lithium sulfur battery with a high theoretical capacity (1675 mA h g⁻¹) and energy density 2600 (Wh kg⁻¹) has become the most promising contender for next generation of renewable energy storage devices and is expected to replace the current lithium ion battery systems. However, the practical application of lithium sulfur batteries is constrained by the insulating nature of the sulfur and its end products. Moreover, the polysulfide shuttle effect leads to rapid capacity fade and premature failure of these batteries. The conventional lithium-

sulfur battery employs an aluminum current collector which does not actively participate in the electrochemical reaction leading to a significant reduction in the energy density. Furthermore, the planar geometry provides poor interfacial contacts and is not robust under stressed conditions restraining the use of such devices in flexible energy storage system. In the present work, we prepare a carbon cloth current collector with optimized electrical properties from waste cotton cloth. The fibrous architecture with enhanced electrical conductivity provides efficient channels for electron transport leading to better activation of sulfur. In addition, the 3-dimensional fibrous architecture acts as a matrix for physically confining the active material and inhibiting the shuttle effect. Moreover, the internal void volume between interwoven fibers provides space for good electrolyte uptake and shortens ion diffusion paths. Therefore, the synergistic result of good contact, rapid electron transport and fast ion diffusion results in higher initial discharge capacity and better life cycle of lithium sulfur battery. Additionally, the flexible current collector opens possibilities for development of flexible and wearable energy storage devices.

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Integration of oligonucleotide nanocomposites with crosslinked hydrogel network for fouling-insensitive electrochemical sensing



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Abstract:

Electrochemical affinity (antibodies/DNA) sensors are potential to be used in clinical analysis, their utility in analysing biological samples (blood/serum) are still challenging with the non-specific binding (NSB) on the sensor surface. Proteins/albumins present in the blood/serum samples forms a passivating layer through NSB on the electrode surface which in turn lead to sensor fouling. To mitigates the NSB on the sensor surface, antifouling agents were employed on the electrode modification^{1,2}. Here, the reported work includes the gold nanoparticles (AuNPs) and self-assembled thiol modified aptamers specific for progesterone steroidal hormone³. Antifouling biolayer were synthesized by incorporating the natural polymer of chitosan and semi-synthetic polymer of hydroxyethyl cellulose which launch as hydrophilic hydrogel through the genipin crosslinking mechanism. Functionalized aptamer and AuNPs was integrated with the hydrophilic biolayer of hydrogel for the progesterone aptasensor fabrication. Square wave voltammetry was used to investigate the binding characteristics of the progesterone aptasensor can measure a physiological condition in the real-time samples.

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<u>CP-162-EIHE 2023</u>



Electrolysis of aniline-containing waste water yields polyaniline and hydrogen with negligible energy consumption



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Abstract:

Energy and the environment are two of the most important issues in modern society. They are important for the world's economic and social sustainable growth. [1,2] In 2018, non-renewable and harmful conventional energy sources like coal, petroleum oil, and natural gas make up 79.5% of the energy economy. [3] The issue has prompted a worldwide push to find renewable and clean alternatives to fossil fuels. In an effort to replace less desirable fuels with more desirable ones, hydrogen produced via electrolysis of water is being explored as a potential clean fuel with high energy density. The large overpotential of the oxygen evolution process, however, restricts its usefulness (OER). By switching out OER for aniline electrochemical polymerization, hydrogen fuel can be produced from wastewater. When compared to the OER, the potential of aniline electropolymerization drops dramatically to 1240 mV at a current density of 30 mA cm⁻² even with a carbon paper electrode. Furthermore, the Faradaic efficiency of hydrogen production is close to 100%. As-prepared polyaniline performs well as electrochemical capitative materials. This work provides an efficient and low-energy access to co-generate hydrogen and polyaniline in a convenient step by starting with toxic and environmentally unfriendly wastewater.

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Arsenic remediation from contaminated drinking water via sacrificial metal-based reactor column



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Abstract:

The widespread arsenic contamination in ground water, either from anthropogenic or natural sources, is a serious problem in many parts of the world. The main concerns related to arsenic in groundwater are its toxicity and carcinogenicity. The objective of our work is to develop the Point of Use (POU) column for remediation of arsenic contaminated water with the exit concentration below the permissible limit of $10 \mu g/L$ [1]. Experiments were conducted both in batch and column mode with different reactive media such as Fe, Zn, Cu-Fe and Cu-Zn. In this study, 10% active material was used as reactive media for removing 1 mg/L of pollutant at different flow rates (10, 30, 50 mL/min). The effect of arsenic on the corrosion rate of the selected reactive media was investigated by analysis of Tafel diagrams with arsenic concentration of 1 mg/L. The total arsenic, pH, oxidation-reduction potential and total metal ions in the exit stream of the reactor was monitored as a function of flow rate and duration for which the reactor column is operated. Based on the test results, iron and galvanically coupled copper-iron system performed best and identified as the efficient, sustainable process for arsenic mitigation in contaminated water.

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One pot fabrication of CuO-CuFe₂O₄@rGO nanostructure for electrochemical sensing application of paracetamol



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Abstract:

In the present study, the facile and synergistic approach for electrochemical sensing of paracetamol (PA) drug was demonstrated by hydrothermally synthesized copper oxide-copper doped ferrite supported on reduced graphene oxide (CuO-CuFe2O4@rGO) nanohybrid composite fabricated glassy carbon electrode. The surface texture and structural information was analysed through FE-SEM, HR-TEM, and X-ray diffraction techniques, while electrochemical sensing application of paracetamol oxidation was investigated by cyclic voltametry method. The average crystallite size of CuO-CuFe₂O₄ was calculated from XRD data and found to be 35.45 nm. The fabricated sensor exhibited higher sensitivity of 970.26 μ A.mM⁻¹.cm⁻² alongwith lower limit of detection (LOD) and limit of quantification (LOQ) of 7.0 μ M and 25 μ M with linear dynamic range of 10-1200 μ M. Furthermore, the CuO-CuFe₂O₄@rGO modified sensor showed excellent selectivity, long-term stability and reproducibility towards electro-oxidation of paracetamol drug. Moreover, it can be efficiently applied for the analysis of paracetamol in biological samples. Finally, the synthesized nanocomposite material validated to be competent electrocatalyst for electrochemical sensing application of paracetamol.



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Synthesis & Characterization of NiM Composite as Cathodic Material in Mg Seawater Batteries



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Abstract:

Owing to the rising demand for clean energy technologies, there is an increased interest in harnessing energy from inexhaustible sources like seawater. A high specific energy Magnesium Seawater Battery (Mg SWB) combines Mg oxidation as anodic reaction with Hydrogen Evolution Reaction (HER) as cathodic reaction. Such batteries are potential energy storage devices for deep sea applications. Pt is a



suitable catalyst for HER, but its high cost becomes an economic burden for commercial applications. Hence, the development of cost-effective catalysts which can boost the performance of HER is the need of the hour, to realise Mg SWB technology on a commercial scale.

Nickel based electrodes possess excellent water splitting capabilities. In this study, we fabricated Ni-based electrodes for HER using simple electrodeposition techniques. Nickel based composite catalysts (NiM, M=

Co, Cu) were electrodeposited on Titanium (Ti) substrate and their catalytic performances for HER in seawater were analysed using electrochemical techniques such as Linear Sweep Voltammetry and Chronopotentiometry. The optimised electrodes are used to assemble Mg SWBs. From the preliminary analysis, it is observed that TiNiCo is a good electrode with an onset potential of -400 mV and a Tafel slope of 203.47mV per decade. The results of this study are aimed at providing an alternative power source with high specific energy, environment adaptability and low cost for underwater applications.

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Graphene based nanosensor for selective and sensitive detection of ketamine drug



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Abstract

Ketamine is one of the most commonly abused drugs around the world and poses a severe risk to social stability and human-health. There is a significant need for quick, accurate, portable, and simple detection techniques for a variety of substances of interest in various matrices, including police samples, biological fluids, hairs, and beverages. Electrochemical sensors have gained much interest among researchers due to their various advantages such as low cost and good specificity, particularly (SPBE) screen-printed paperbased electrode biosensor. Here, we reported an electrochemical paper-based analytical device (EPAD) for the detection of recreational drug; Ketamine. Using a paper-based electrode reduced the electrode's production costs, while graphene oxide nanoparticles (GO-NPs) assisted in amplifying the signals generated in the cyclic voltammetry system when ketamine was present. This EPAD was developed by immobilizing Ketamine Aptamer on graphene oxide nanoparticles (GO-NPs) electrodes. The morphology in terms of size and shape of GO-NPs was done by Transmission Electron Microscopic (TEM) and Scanning Electron Microscopy (SEM) was done to characterize the nanoparticles. The abuse of ketamine, however, is growing to the point where it has become a major problem. This is because, in addition to being used for recreational purposes, this tasteless, odourless, and colourless drug also facilitates sexual assaults when it is mixed with drinks. The developed sensor showed low LOD of about 0.01 µg/ml and linear range was between 0.01-6 µg/ml. This work provides a reliable diagnostic method for distant places with limited resources, and will also help people who cannot afford expensive medical tests and have limited access to power and trained personnel.

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Reliability and Durability Study of Lithium-ion Battery: Electrochemical Impedance Spectroscopy Technique



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Abstract:

Lithium-ion battery (LIB) degradation and health monitoring are investigated through life-cycle testing and failure analysis. Aging is the most common problem for lithium-ion battery on under various conditions such as temperature, vacuum, Load conditions, and local humidity conditions. The state of health of the LIB is measured through the capacity and power fade which is occurred due to the loss of Lithium-ion Inventory, loss of anode/cathode active material, loss of electrolyte, and resistance increment. However, these losses are directly affected or depend on the side reactions, Electrode particle cracking, solid electrolyte interface (SEI) film formation and thickening, Graphite exfoliation, and Structure Disordering under the operating condition. The present work is focused on the electrochemical impedance spectroscopy (EIS) study of coin LIB at three different frequencies mainly (i) 100 kHz to 0.01 mHz, (ii) 100 kHz to 1.0 mHz, and (iii) 100 kHz to 100 mHz. EIS data in terms of Nyquist and Bode plot of the electrode system is used to evaluate the establishment of a solid electrolyte interface (SEI) and the charge transfer reaction on the electrode's surface. According to Bode analysis, the SEI produced from either effectively reduces the surface heterogeneity of the cathode and anode electrodes.

Keywords: Aging mechanism, Capacity fade, Power fade, Electrochemical impedance spectroscopy, Solid electrolyte interface

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Surface enhanced IR-spectroelectrochemical analysis of self-assembled monolayer modification and interfacial electron transfer reactions



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Abstract:

Redox active self-assembled monolayers (SAMs) are widely used as test systems for validating classical and semi-classical electron transfer models.¹ Kinetic data is almost always extracted using purely electrochemical techniques, but these methods are very insensitive to time-dependent changes in the SAM that extend beyond the redox centre.² Furthermore, it is very difficult to prepare layers with sufficient homogeneity and the absence of lateral interactions that lead to kinetic dispersion.³ In this work, the electron transfer kinetics of 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) monolayers have been studied using both a chronocoloumetric method and surface sensitive infrared spectroelectrochemistry (attenuated total reflection surface enhanced infrared absorption spectroscopy, ATR-SEIRAS).⁴ Redox active self-assembled monolayers (SAMs) are constructed by covalently attaching 4-amino-TEMPO to preformed monolayers of different chain length alkanoic acid thiol monolayers leading to redox-active SAMs that



exhibit very little kinetic heterogeneity. The chronocoloumetric analysis reveals asymmetry between the forward (oxidation of the radical to the nitrosonium cation) and reverse (reduction to the TEMPO radical) reactions. Direct evidence of conformational changes in the layer upon oxidation (reduction) are extracted from ATR-SEIRAS studies. Oxidation of the TEMPO radical leads to a chair-chair flip in the piperdinyl ring. The nitrosonium conformer pushes the N=O⁺ centre away

from the electrode and into a polar environment. Conformational differences in the reduced and oxidized species are cited as the reason for kinetic asymmetry in the TEMPO/TEMPO⁺ redox system.

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WO₃/CDs an Photoanode for Photoelectrochemical Water Splitting



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Abstract:

Hydrogen (H₂), due to its high energy density, is a potential replacement for fossil fuels. It can be generated in a greener way by utilizing water and solar energy, with photoelectrochemical (PEC) water-splitting.¹⁻³ In this study, 2D nanosheets of WO₃ developed and their activity in PEC water-splitting is investigated in order to produce green hydrogen. Low charge transfer rates in WO₃ limit its effectiveness as a photoanode. One method for boosting charge transfer rates is sensitization using carbon dots (CDs). In comparison to bare WO₃, the impedance analysis reveals that WO₃/CDs have reduced charge transfer resistance. After sensitization, an increase in charge transfer rates causes an improvement in PEC activity. When compared to bare WO₃, the best heterostructure, WO₃/CD-2 photoanode, displays a roughly 1.22 times increase in photocurrent density. While WO₃/CD-2 can create 1.93 mA/cm² at 1.39 V vs. Ag/AgCl, bare WO₃ nanosheets can only produce 1.58 mA/cm² at this potential. Additionally, the increased carrier density in the heterostructure is observed in Mott Schottky analysis. The enhancement in PEC water-splitting is due to the increase in light absorbance, low charge transfer resistance, and photogenerated charge carrier separation.

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Role of Torque Power on Lithium-Ion Battery Degradation



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Abstract:

क्त सेवा में मुद्द

Lithium-Ion Battery (LIB) is one of the most important and advancing energy storing systems due to its high gravimetric and volumetric energy density. Torque is a crucial factor and it has always varied in electric vehicles (EVs). EVs produce maximum torque where the vehicle needs to respond immediately to move forward and it will significantly affect the performance of the battery life.

The present study focused on the capacity fade and power fade when the torque is continuously changed by changing the vehicle's gear ratio. Electrochemical Impedance Spectroscopy (EIS) is used to understand the resistance and capacitance of the battery which is carried out at the scan rate of 100 kHz to 0.01 Hz. The surface morphology of the battery is examined using a Scanning Electron Microscope (SEM) and Atomic Force Microscopy (AFM). The effect of gear ratio and torque directly affected the resistance and capacitance in the EIS plot.

Keywords: Lithium-Ion Battery (LIB), Gear ratio, Torque, Electrochemical Impedance Spectroscopy (EIS), Solid Electrolyte Interface (SEI), Scanning Electron Microscope (SEM), Atomic Force Microscopy (AFM)



Effect of lightning on metal degradation



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Abstract:

Lightning is the visible discharge of electricity that occurs when a region of a cloud acquires an excess electrical charge, either positive or negative, that is sufficient to break down the resistance of air. Lightning is usually associated with cumulonimbus clouds (thunderclouds). The potential difference between cloud and ground is of the order of 10 to 100 million volts, and the peak currents in leaders are typically about 30,000 amperes. The peak temperatures in the return-stroke channel are on the order of 30,000 °C. Since the entire lightning process takes place in the order of milliseconds, an Impulse voltage surge creates a blistered structure on the metallic surface. Study of Corrosion Kinetics Lightning affected Metals is necessary to understand how metals are subjected to corrosion, which gives an understanding of how microscopy changes when affected by lightning. This effect is studied in microcosm, in which super capacitor is used to dissipate charge onto the metal surface. In the present work, a strategically lab-designed method is implemented on copper, mild steel, and aluminum to study Corrosion behavior on lightning-affected metals. An electrochemical corrosion examination was carried out in the Coastal environment. XRD, SEM (EDS), and AFM characterization tools are used after the corrosion test of each sample.

Keywords: Lightning discharge, Electrochemical corrosion, Microcosm study

<u>CP-172-EIHE 2023</u>



Electrochemical impedance spectroscopy (eis) study of api steel under flow conditions in CO₂ saturated environment



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Abstract:

The internal corrosion of pipelines in the oil and gas transportation industries is quite challenging. It is always a threat to the integrity of materials. This is more complex when the nature of the flow is turbulent which can cause damage and may further result in thinning of the wall which can cause leakage and huge economical losses and environmental problems. In the present work, electrochemical impedance spectroscopy (EIS) of API X70 pipeline steel has been studied in static as well as flow conditions (close loop system) at the elbow section with a flow velocity of 2.5 m/s in CO₂ saturated environment. EIS study was carried out at the frequency range of 0.1 Hz to 10 kHz. The EIS plots were fitted using an equivalent circuit and the impedance kinetics parameters such as polarization resistance and capacitance value were obtained, it was observed that the polarization resistance (R_P) is significantly low in flow condition as compared to static condition. The computational fluid dynamics (CFD) approach was used to determine the shear stress value in the elbow section. The post-corrosion topography of the samples and corrosion product was analyzed through a Scanning electron microscope (SEM) equipped with EDAX and Raman spectroscope.

Keywords: Electrochemical impedance spectroscopy, Close loop system, Computational fluid dynamic (CFD), Polarization resistance (R_p) .



Development of nano composite intumescent fire resistance coating



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Abstract:

Intumescent coatings is composed of ammonium polyphosphate, pentaerythritol and melamine which are widely used in the field of passive fire protection for structural steel. This study focused to understand how the role of two different Nano fillers (CeO₂ and TiO₂) separately and together at different wt.% will affect the fire into the matrix of an intumescent coating. Different combination of Nanocomposite intumescent coating was prepared at different wt% of these two fillers. Fire test is performed for the bare and coated samples at different temperature. Char is collected after Fire test and it is examined using Scanning electron microscope (SEM) equipped with EDAX, Time vs Temperature curve is carried out to observe the fire performance of different fillers and X- Ray Diffraction is used for phase identification of a crystalline material after the fire test at different temperatures. Thermal performance of the coating was studied by using Thermo Gravimetric Analysis (TGA) and Fourier Transform Infra-Red (FTIR) is used to observe chemical properties of the extracted char.

Keywords: Intumescent coatings, fire protection, Char formation, Nano fillers.



Electrochemical impedance spectroscopy behavior for thermal barrier coatings integrity



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Abstract:

Thermal barrier coatings (TBCs) are characteristic attributes to enhance the durability and longevity of metal parts in gas turbine engines. In-house synthesized rare-earth-based Samarium strontium aluminate (70% Al₂O₃ + 30% Sm₂SrAl₂O₇) composite coating is been identified as an alternative material for TBCs. The Al₂O₃ + Sm₂SrAl₂O₇ composite TBCs are developed using atmospheric plasma spraying (APS) on a bond-coated Inconel 718 substrate. Further, surface modification is carried out using a Laser treatment of APS-coated TBC to improve oxidation, hot corrosion, and high-temperature erosion. The objective of this paper examines impedance kinetics such as various resistances and capacitance behavior of APS-coated and laser-treated TBCs using an Electrochemical impedance spectroscopy (EIS) technique. Interestingly, it is well correlated with high-temperature oxidation characteristics with the impedance kinetics and found that higher resistances and low oxidation rate for the laser-treated samples over the APS TBC. It is due to the elimination of surface defects after the surface modifications.

Keywords: Thermal barrier coatings, Impedance, Samarium strontium aluminate, Oxidation

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Electrochemical sensing of Methamphetamine employing Silver-Zinc Oxide Nanocomposite



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Abstract:

Drug abuse is a widespread issue that requires a multidisciplinary response. There is a significant need for quick, accurate, portable, and simple detection techniques for a variety of substances of interest in various matrices, including police samples, biological fluids, hairs, and beverages. Biosensors are a viable option for onsite drug detection. Here, we present the development of an electrochemical paper-based analytical device (EPAD) for the detection of methamphetamine as a recreational drug (Meth). Meth is a stimulant that young people use as an addictive narcotic, and it needs to be caught soon since it may be a hazardous substance. The suggested EPAD has the advantages of being simple, affordable, reliable, and recyclable. This EPAD was developed by immobilizing methamphetamine binding Aptamer on Ag-ZnO nanocomposite electrodes. The sensor showed low LOD of about 0.01 μ /ml and linear range was between 0.01- 6 μ g/ml. This research will benefit those who can't afford expensive medical tests and don't have easy access to power or skilled workers by providing a dependable diagnosis approach for distant places with little resources. The designed EPAD could prove to be very effective in case of forensic diagnostic applications and it offers many good features of being rapid, sensitive and selective.



<u>CP-176-EIHE 2023</u>

Theory for IMPS on Rough and Finite Fractal Dye Sensitized Solar Cell



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Abstract:

A generalized theoretical model of intensity modulated photocurrent spectroscopy (IMPS) for the random morphology in a dye sensitized solar cell (DSSC) under uniform illumination is developed. The generalized IMPS expression for the disordered semiconducting/conducting glass interface of a DSSC is obtained in term of power spectral density of roughness. Influence of surface roughness on the dynamic response of DSSC originate due to the coupling of characteristic phenomenological and morphological length scales. A detailed analysis of IMPS response is performed over finite self- affine fractals to highlight roughness induced anomalies and cause of photocurrent enhancement. The IMPS of a rough DSSC exhibit three characteristic frequency regimes: lifetime of charge carrier dependent low frequency regime, surface irregularity dependent intermediate power-law regime and diffusion controlled high frequency regime. Finally, our theory facilitates the understanding of dynamics and kinetics of charge carriers under the influence of ubiquitous surface disorder.

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The Theory of Pulse Voltammetries on Roughness Electrodes: Multistep Reversible Charge Transfer Mechanism



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Abstract:

Theoretical model for voltametric response of multistep reversible charge transfer mechanism at rough electrode including unequal diffusivities of electroactive species is developed in this work. An explicit mathematical expression relating the staircase (SCV), cyclic staircase (CSCV), differential pulse (DPV), and square wave (SWV) voltametric response of finite fractal electrode to the statistical morphological characteristics is obtained. The fractal characteristics, viz. fractal dimension (D_H), lower length scale of fractality(1) and topothesy length(I_{τ}) and found to dominantly control the various voltametric techniques responses of a multistep charge transfer mechanism. The height of the voltametric peaks corresponding to each charge transfer step is found to increase with increasing roughness. In CSCS, the anomalous intermediate scan rate window of Randles-Sevcik plot shifts with the number of charge transfer The peak current for charge transfer step occurring at lower potential has an early onset of the step. influence of morphology i.e., the anomalous regime window shifts at lower scan rate compared to those occurring at higher potential values. The differential techniques show roughness induced current enhancement for all peaks without affecting the position of the peak potential. Thus, roughness helps to overcome the major drawback of low Faradaic current in these techniques and improves their application for analytical and sensing purposes.

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<u>CP-178-EIHE 2023</u>



PANI -wrapped MOF as cathode host with MOF modified separator for performance improvement of Li–S batteries



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Abstract:

Lithium-sulfur batteries are attractive choice for the next-generation energy storage device for electric transportation because of their superior theoretical capacity (1675 mA h g⁻¹) and energy density (2600 Wh kg⁻¹). Additionally, sulfur has high natural abundance (~3% of earth's mass), environmentally friendly and low cost. The shuttling of lithium polysulfde (LiPS) during cycling is integral problem in these batteries which leads to huge capacity fading with cycling and obstruct their practical applications. To deal with these issues, PANI/ MOF (metal organic framework MIL-101(Cr)) is used as cathode host while MOF alone used as separator modifier. The unique cathode structure with large specific surface area of MOF and a conductive coating of PANI ensures a high loading of S, trapping of LiPS and take care of conductivity issue of elemental sulfur. MOF modified separator serves as a barrier to retrain the diffusion of LiPS within the vicinity of cathode which further maximizes cycle life and minimizes capacity fading by enhancing the active mass utilization. Consequently, the cathode showed discharge capacity of 627mAhg⁻¹ after 20th cycle at 100mAg⁻¹current density. After 100th cycle, its shows capacity of 420mAhg⁻¹ or responding to a low fading rate of 0.33 % per cycle.



Fig. SEM image of MOF (b) Cycling performance of PANI/MOF/S

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Investigation of layered β-Co(OH)₂ for Supercapacitor application



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Abstract:

Two-dimensional layered β -Cobalt hydroxide Co(OH)₂ was synthesised via facile one pot hydrothermal method. The obtained product was subjected to x-ray diffraction(XRD) and Fourier transform infra-red (FTIR) spectroscopy for structural and functional properties. The XRD pattern confirmed the formation of pure Co(OH)₂. From the FTIR spectroscopy, the material exhibited a strong vibration of hydroxide bond accompanied with nitrate ions that were intercalated in the basal spacing between the hydroxide layers. Further the as-prepared material was subjected to FESEM which confirmed the formation of nanorods that were systematically assembled into flower-like morphology. The electrochemical analysis was conducted using conventional three electrode system with reference electrode as Ag/AgCl dipped in 3.5M KCl solution, counter electrode as platinum electrode and slurry of the as-prepared material on the graphite foil as working electrode where it reveals the pseudocapacitive nature of the material. Using galvanostatic charge-discharge studies, the specific capacity was roughly determined as 314 F g⁻¹ at a specific current of 0.5 A g⁻¹ which indicates that this could be an appealing candidate for futuristic supercapacitor electrodes.



Figure 1: (a, b) SEM images of as prepared β -cobalt hydroxide at different magnifications.

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<u>CP-180-EIHE 2023</u>



Electrochemical Corrosion Phenomenon and Prospect of Green Corrosion Inhibiting Coating for Carbon steel in Marine Environment



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Abstract:

Life has been severely harmed by corrosion progression over time, which also has an impact on the mechanical, economic, and environmental elements of material services. Electrochemical reactions, such as corrosion, involve the transfer of electrons from one substance to another from one location to another both oxidation and reduction processes occur during electrochemical reactions; oxidation reactions raise the valence number of a substance by eliminating particles and making it positively charged. In various respects, the corrosion inhibition property of a green corrosion inhibitor additive derived from carbonaceous biomass on carbon steel in 3.5 wt% NaCl solution was investigated using the potentiodynamic polarization (*PDP*) technique and electrochemical impedance spectroscopy (*EIS*). The results showed a decrease in corrosion rate up to 89% with respect to uncoated carbon steel specimens. this development has made several attempts to comprehend this disaster, offering consistent cost-cutting controls and mitigating remedies. This overview examines electrochemical corrosion mechanisms and the potential for material selection to address a variety of problems.

Keywords: Electrochemical, Green corrosion inhibitor additive, Oxidation

<u>CP-181-EIHE 2023</u>



Carbonaceous Biomass-derived Graphitic Carbon-based Composite to Mitigate Corrosion of Carbon Steel



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Abstract:

Corrosion mitigation of metals has been an interesting research area for years. According to the National Association of Corrosion Engineers, the global loss due to corrosion is about 2.5 trillion USD, equivalent to 3.4% of the global GDP (2013). Therefore, developing and introducing new materials and techniques to inhibit corrosion is always necessary. This research investigates the utilization of graphitic carbon-based composites as corrosion inhibitors for mitigating corrosion in carbon steel. For this purpose, boron nitride and the waste-derived graphitic carbon composite mixture were synthesized. The corrosion inhibition performance of graphitic carbon-based composite as an additive in industrial grade epoxy coating was monitored and compared using electrochemical impedance spectroscopy (*EIS*) and potentiodynamic polarization (*PDP*) technique in 3.5 wt% NaCl solution. The results exhibited more than 97% improvement in corrosion rate compared to uncoated carbon steel surfaces. Moreover, the hydrophobic nature of the coating surface was also investigated.

Keywords: Carbon steel, Corrosion, Anticorrosive coating, Electrochemical techniques.

CP-182-EIHE 2023



Electrochemical characterization of solutions of UO₃ dissolved in new DES



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Abstract:

Deep eutectic solvents (DES), the new solvent systems are finding widespread studies and applications since the work of Abbott ^[1,2] on biodegradable and cheap DES choline chloride and urea. Two new deep eutectic solvents, were prepared using i.e.2-methylimidazole (C₂mim) was mixed with hydrogen bond donors, phenylphosphinic acid (PA) and diglycolic acid (DGA) to form DES and are referred to as DES-PA and DES-DGA. Oxide of uranium, i.e. UO₃ was dissolved in these DES separately and characterized by cyclic voltammetry. This might be the first ever report on electrochemistry of an actinide ion in the new DES. Figure 1. (a) DES-DGA (b) DES-PA gives the CV plots of UO₃ dissolved in two DES solvents along with blanks with bare DES. It can be seen that clear reduction peak at -0.502 V and -1.129



V were observed in DES-DGA and DES-PA, respectively realted to reduction of uranium species. The oxidation peak was found at 1.104 V and 0.486 V in DES-DGA and DES-PA, respectively. According to our

previous work ^[3] and through electrochemical caluction, the reduction peaks can be assigned to U(VI) to (V) with irreversible nature. The CV plots for both DES (a: DESPA, b: DES-DGA) for the solution of the uranium trioxide as a function of scan rate were also recorded, which indicates the enhancement in peak current (i_p) with scan rates and thus corroborates the diffusion-controlled reduction of uranium species in both DES. From the plots of peak current vs. square root of scan rate, the diffusion coefficients (D₀) were determined to be 1.24×10^{-8} and 0.96×10^{-8} cm²/sec in DGA and PA, respectively. In addition, α n and rate constant (k^0) of dissolved uranium species in both DES were also evaluated. The D₀ of uranium species in both DES is lower than the aqueous medium, which may be due to solvent and speciation effect.

Figure: Cyclic voltammetry plots of dissolved UO_3 in (a) DGA (b) PA containing DES

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A new cobalt complex for homogenous hydrogen generation



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Abstract:

Hydrogen generation through electrocatalytic route is a promising alternative of green fuel. Cobalt is known as an active metal for electrocatalytic hydrogen generation. Several cobalt complexes have been evaluated for electrocatalytic hydrogen generation¹. In this study, the complex of cobalt with 2,6-Bis(methylhydroxy) pyridine (BHPy) is prepared and is evaluated for electrocatalysis.

The complex was characterized by single crystal XRD. The electrochemical studies were performed in DMF/water medium. The cyclic voltammetry data shows an irreversible cathodic peak at -1.84 V versus Fc^+/Fc (Fig. 1). With increasing trifluoroacetic acid concentration, the cathodic peak increases, showing the catalytic behaviour of the complex (Fig. 1). The catalytic efficiency was determined by controlled potential electrolysis at -1.85 V (Fig. 2). The turn over number was found to be 44.7 and turn over frequency 10.73 hr^{-1} with faradic efficiency of 75%





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<u>CP-184-EIHE 2023</u>

Electrodeposition of Ni on Al-Brass for corrosion protection



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Abstract:

Aluminium brass is being used in seawater for cooling purpose. Nickel electrodeposition on Albrass surface has been explored for corrosion protection of the surface. Al-Brass coupons were polished and degreased before electrodeposition. The Watts type bath consisting of 7.5 g NiSO₄.6H₂O, 1g NiCl₂.6H₂O and 1 g H₃BO₃ in 50 ml water has been used for electrodeposition [1]. The potentiostatic pulse



deposition has been carried out for 1000 cycles using different pulse parameters. The pulse deposition parameters were varied to optimize the coating for better corrosion resistant. The electrochemical measurements have been carried out 0.5 NaSO₄ Μ medium. in Impedance spectra and Tafel plot have been analysed to find out the corrosion behavior (Figure). It was observed that pulse on at -1.2 V (10 ms ton) and pulse off at -0.5 V (200

ms t_{off}) were optimum parameters for electrodeposition. The coupon electrodeposited with optimum parameters shows around 10 times more charge transfer resistance (R_{ct}) as compared to others. Tafel analysis also shows lower corrosion rate for this coupon. SEM image also confirms full coverage single layer fine coating with these optimum parameters.

Figure: Electrochemical measurements on the each electrodeposited Al- brass surface A: Impedance Spectra, B: Tafel Plots, Black: Polished surface without Ni, Red: $-1.0 \text{ V } t_{on}(10\text{ms})$, $-0.50\text{ V} t_{off}(200\text{ms})$, Green: $-1.1 \text{ V } t_{on}(10\text{ms})$, $-0.50\text{ V } t_{off}(200\text{ms})$, Blue: $-1.2 \text{ V } t_{on}(10\text{ms})$, $-0.50\text{ V } t_{off}(200\text{ms})$, Cyan: $-1.2 \text{ V } t_{on}(10\text{ms})$, $-0.50\text{ V } t_{off}(100\text{ms})$; \circ : Experimental data, -: Fitted data

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<u>CP-185-EIHE 2023</u>



Chemical Assisted Engineering of Unzipped Multiwalled Carbon Nanotube and rGO Nanocomposite for the Sensitive Detection of Picloram



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Abstract:

Picloram (4-Amino-3,5,6-trichloropyridine-2-carboxylic acid) is a chlorinated herbicide that has been discovered to be tenacious and relatively durable in both soil and water. It is known to have an adverse and unpleasant effects in humans such as skin rashes, sore throat and eyes, burning and itchy skin, frequent headaches, lethargy, eyesight and memory degeneration, pain and numbness in feet and hands, and perhaps even joint problems that resemble arthritis. Determination of picloram is profoundly effective because of its bioaccumulation and persistent nature. Therefore, a sensitive, rapid and robust detection system is essential to detect traces of this molecule in agricultural and environmental samples. In this study, we have constructed an unzipped multiwalled carbon nanotube (UZMWCNT) and reduced graphene oxide (rGO) nanocomposite on a gold-nanoparticles (AuNPs) modified glassy carbon electrode (UZMWCNT+rGO/AuNPs/GCE) for the analysis and sensitive detection of picloram in collected samples obtained from the agricultural field. The synthesized nanomaterials and the developed system were subjected to characterization techniques such as Square Wave Voltammetry (SWV), Linear Sweep Voltammetry (LSV), Electrochemical Impedance Spectroscopy (EIS), Chronoamperometry and benchtop scanning electron microscopy (BT-SEM). The engineered sensor surface showed a low limit of detection and a broad linear range. The response time recorded was less, and the efficacy of the proposed sensor system was studied using rice water and soil samples collected from the agricultural field. Due to its simplicity of manufacturing and sample pretreatment procedures, the sensor probe could be deployed for on-site detection of picloram.

<u>CP-186-EIHE 2023</u>



An impedimetric immunosensor for detection of alkaline phosphatase in serum using electrochemically engineered graphene oxide and chitosan/silk fibroin scaffold composite



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Abstract:

Serum, saliva, and other bodily secretions contain a phosphate-cleaving enzyme called alkaline phosphatase (ALP), which plays an essential role in a wide variety of essential physiological processes. Serum ALP levels in healthy adults range from 20 to 140 U/L; in infants, children, and pregnant women, ALP levels are slightly higher. Clinical ranges above 350 U/L have been associated with liver and bone diseases. In the present work, we have shown the detection of alkaline phosphatase (ALP) via a label-free electrochemical impedance spectroscopy (EIS) technique using graphene oxide (GO), chitosan/silk fibroin scaffold composite. The graphene oxide and scaffold composite were deposited sequentially on the screen-printed carbon electrode (SPCE) and subsequent treated with antibody against ALP (anti-ALP) and ALP. Many different methods, including XRD, FE-SEM, EDX, FTIR, and electrochemical analysis, have been used to characterise the sensor probe. EIS has been used to assess the biosensor's analytical performance after fabrication where the obtained linear dynamic range was found to be 50-1000 U/L. Furthermore, the developed system has been tested against biological sample i.e., human serum for detection of ALP.

<u>CP-187-EIHE 2023</u>



Designing an Engineered Nanodendritic Sensing Probe for Acetaminophen Detection in Human Urine



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Abstract:

Metallic dendrites, a type of three-dimensional nanomaterial with a fern-like appearance, have been shown to have superior catalytic activity owing to the presence of a larger active surface area provided by its three-dimensional bulged-out structures. These dendrites are a hierarchical self-assembled array of primary, secondary, and terminal branches with a high density of sharp ends, ridges, and edges. Furthermore, less fouling has been observed due to the substantially higher active surface area. Several monometallic dendrites based on Ag, Cu, Co, Au, Pt, Ni, and other metals have been synthesized and their catalytic behaviour has been studied. However, due to remarkable biocompatibility, Au-based dendritic structures have been extensively researched and exploited in electrochemical sensing. Besides nanodendrites, multiwalled carbon nanotubes (MWCNTs), a class of carbon nanomaterials, are also widely being used in the fabrication of biosensor due to its conductivity, greater surface area, chemical stability, good mechanical strength, and high catalytic activity. We have created a biomimetic sensing matrix for acetaminophen detection based on multi-walled carbon nanotube-gold nanoparticle (MWCNT-AuNP) and gold nanodendrites (AuND) composites. The nanoengineered surface has been thoroughly characterized electrochemically to show its ability for ultrasensitive detection of acetaminophen. These kinds of integrative studies can enhance the sensor's analytical capabilities and pave the way for the design of pointof-care bioelectronic devices.

Keywords: Gold Nanodendrites, AuNPs, Acetaminophen, Clinical Bioanalysis

<u>CP-188-EIHE 2023</u>



Effect of Second Phase Particle Size variation on Microstructure, Mechanical and Corrosion Behaviour of Electrodeposited NiW-Diamond Nanocomposite Coatings



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Abstract:

In the present work, as an alternative to hard chrome plating, Ni-W-diamond nanocomposite coatings were prepared by sediment co-electrodeposition from Ni-W plating bath, containing suspended diamond particles of various sizes (0.5 μ m, 2 μ m and 8 μ m). To study the effect of diamond particle size variation on nanocomposite coatings, micro-hardness, wear and corrosion tests were performed and compared. Surface morphology of the deposited coatings was investigated under FESEM. The measured micro-hardness was found to be increasing with increase in the particle size. A maximum micro-hardness of 1892±57 HV_{100gf} was obtained for nanocomposite coating with 8 μ m particle size. Comparison of potentiodynamic polarization curves of NiW-diamond nano-composite coatings with different particle sizes carried out in 3.5wt% NaCl solution at RT are shown in the Fig.1.A distinct shifting of corrosion potential towards anodic direction could be visible with increase in diamond particle size. For 8 μ m size particle, E_{Corr} values obtained were -0.310V vs. SCE and 4.34E-6 A.cm⁻² respectively.



Fig.1 Tafel plots of Ni-W-diamond nanocomposite coatings in 3.5wt% NaCl solution at RT.

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Bimetallic Pt-Co/CNT Electrocatalyst for Aqueous SO₂ Electrolysis



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Abstact:

Hybrid-Sulfur (Hy-S) cycle is a promising thermochemical cycle for hydrogen generation by water splitting, using concentrated solar energy or futuristic high temperature nuclear reactors [1]. In this cycle the hydrogen generation step is the aqueous SO₂ electrolysis, in which electrooxidation of SO₂ occurs at the anode and hydrogen evolution reaction at the cathode. Bimetallic Pt-Co and conventional Pt dispersed on carbon nanotubes are prepared via sequential wet impregnation followed by chemical reduction. The prepared materials are characterized by powder XRD, FTIR, Raman and FESEM-EDX. The electrocatalytic activities of both Pt/CNT and Pt-Co/CNT are evaluated for half-cell reactions involved in aqueous SO₂ electrolysis by recording the linear sweep voltammetry (LSV) and cyclic voltammetry (CV) of the two electrocatalysts in acidic electrolytes. Representative CV patterns of the Pt/CNT and Pt-Co/CNT for SO₂ electrooxidation is shown in Fig. 1. Evidently, better performance of the bimetallic catalyst for the above reaction is established.



Fig. 1. The cv curves of the Pt/CNT and Pt-Co/CNT electrocatalysts in 0.1 M Na₂SO₃ electrolyte

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<u>CP-190-EIHE 2023</u>



Development of g-C₃N₄ modified electrode for the determination of aclonifen and its environmental application



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Abstract:

Environmental monitoring of water and soil pollutants is associated with a variety of human activities. Escalating demands are therefore emerging for environmental analysis of emerging pollutants, which require the need for more sensitive and selective analytical techniques to alleviate pollution issues. Electroanalytical techniques viz., cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques are the widely preferred approaches for quantitative assessment of pollutant such as herbicide aclonifen (ACF). The sensing device was constructed for the detection of ACF using graphitic carbon nitride coated onto glassy carbon electrode (g-C₃N₄/GCE). The sensing material was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). Electro-kinetic parameters such as heterogeneous rate constant, transfer coefficient, activation energy, and the number of protons and electrons involved in the reduction of ACF have been determined. The SWV technique was employed to detect ACF at trace level concentration. Linearity was observed over the range of 1×10^{-5} M – 8×10^{-7} M with a limit of detection at 1.28 nM of the analyte. Biological, agricultural and environmental relevance of the method developed was successfully applied to the monitoring of ACF in wastewater as well as in actual soil samples.

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<u>CP-191-EIHE 2023</u>



Environmental analysis of fungicide carbendazim using TiO₂ nanoparticle modified carbon paste electrode



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Abstract:

Pesticides pollution is a regular and increasing issue, strongly connected with the growing number of food-satisfying agricultural operations. In reality, Pesticides are used intensively in a wide range of plants. The present study to investigate the environmental analysis of CBZ fungicide in water and soil samples using the electrochemical technique. The sensing device was designed to detect CBZ using TiO₂ nano- particles modified carbon electrode (TiO₂/CPE) in cyclic voltammetry (CV). The impact of pH, a significant increase of peak current of CBZ in 7 pH phosphate buffer solution (PBS) as compared to the other pH solution (3 to 11.2). Farther, to investigate physiochemical properties and thermodynamic properties of CBZ by CV and square wave voltammetry (SWV) techniques. The obtained results show low detection value (LOD) 3S/M and limit of quantification value (LOQ) 10S/M. To apply the developed electrode on the detection of amitrole in water and soil sample.

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<u>CP-192-EIHE 2023</u>



Detection of herbicide, molinate at ZnO nanoparticles modified electrode and its environmental application



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Abstract:

In this work, electrochemical detection of molinate herbicide was studied by developing a novel sensor based on carbon paste incorporated with zinc oxide (ZnO) nanoparticles using cyclic (CV) and square wave voltammetric (SWV) techniques. Molinate exhibited one well resolved peak at pH of 3.0 phosphate buffer solution (PBS), which was irreversible. The lowest possible detection limit of 1.03×10^{-8} M was achieved in the concentration range of 0.002 mM to 0.25 mM. The modifying ability of ZnO nanoparticles was responsible for such a low-level sensing in water and soil samples.

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<u>CP-193-EIHE 2023</u>



Electrochemical detection and determination of mefenamic acid at silver-doped TiO₂ nanoparticles modified electrode



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Abstract:

A simple sensitive voltammetric method to detect and to determine a nano level anthranilic acid derivative, mefenamic acid has been developed using different voltammetric techniques in pH 5.0 phosphate buffer solutions with ionic strength 0.2M. An enhancement of oxidation peak current for an analyte on the modified paste was observed followed by characterization with atomic mass spectroscopy analysis. The control of various parameters on the drug oxidation current like accumulation time, amount of modifier, pH, scan rate, and concentration was also evaluated. The analytical applications were studied by square wave voltammetry technique. A suitable electro-oxidation mechanism for mefenamic acid at nanoparticles silver-doped titanium dioxide modified carbon paste electrode was proposed. The oxidation peak currents of mefenamic acid concentration were studied using square wave voltammetry technique in the range 1.0 x 10⁻⁸ to 3.0 x 10⁻⁶ M with a lower detection limit 1.94 nM compared to earlier reported practice. The modified sensor showed an excellent physiological feature, large surface area, remarkable stability, reproducibility by simple preparation process. The proposed method was successfully employed for the determination of mefenamic acid in pharmaceutical and biological samples with good recovery values.

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<u>CP-194-EIHE 2023</u>



Electrochemical behavior of diclofenac sodium at core shell nanostructure modified glassy carbon electrode



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Abstract:

In this contemporary study, a novel core-shell nanostructures modified electrochemical sensor based on glassy electrode was engineered which achieved enhanced sensitivity towards Diclofenac. The electrochemical behavior and applications of Diclofenac (DCF) was determined by applying discrete voltammetric techniques. The surface characteristics and morphology of the sensing surface was analyzed by X-ray diffractometer (XRD), transmission electron microscope (TEM) and atomic force microscope (AFM). The proposed modified working electrode showed strong electro catalytic activity and electro oxidation towards DCF with higher peak enhancement as compared to the unmodified electrode. In addition, the modified electrode possesses some unique characteristics such as appropriate charge transfer rate, enduring stability, repeatability and reproducibility. The various parameters affecting the peak enhancement such as pH, modifier amount, accumulation time, scan rate and concentration impacts were studied. The electro- oxidation of DCF was studied by cyclic voltammetry (CV) and effect of concentration variation was studied using square wave voltammetric technique in the concentration range of about $0.01 \mu M - 300 \mu M$ and with lower LOD and LOQ values. The applicability of the proposed method was checked by quantification of DCF in pharmaceutical formulations and human urine samples.

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A novel sensor for a anti-inflammatory, theophylline drug at TiO₂ nanoparticles modified electrode



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Abstract:

A simple modified sensor has been proposed using titanium dioxide (TiO₂) nanoparticles for the electro-analysis of theophylline (TP) in phosphate buffer solution (PBS). The surface was characterized by atomic mass spectroscopy (AFM). The electro-oxidation of the drug was studied by employing techniques such cyclic voltammetry (CV) and square wave voltammetry (SWV). The heterogeneous rate constant was calculated and a suitable electrochemical oxidation mechanism was also proposed. The concentration variation of the drug showed good linear response with lower detection limit value. The influence of physic-chemical parameters like scan rate, pH, accumulation time, and amount of the modifier, excipients, metal ions and concentration on the voltammetricbehavior of an analyte were studied. To test its analytical applications, it was applied to determine drug in pharmaceutical and urine samples with good recovery values.

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Improved Corrosion Resistance of Picosecond laser Surface Textured Ti₆Al₄V Biomaterial



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Abstract:

Surface texturing and thin film coating are two popular methods of improving the corrosion properties of metallic biomaterials e.g., Ti6Al4V-alloy commonly employed in load-bearing applications [1, 2]. In this submission we present the experimental results that clearly show the advantage of laser surface textured of Ti6Al4V biomaterial with a pristine sample in respect to its corrosion properties. Appropriate focusing of the emission of a pulsed frequency doubled Nd YAG laser (30 ps pulse duration, 10Hz, 12mJ/pulse) onto the Ti6Al4V surface resulted in a distinct grid like microstructure. The electrochemical analysis of both pristine and textured samples was performed in simulated body fluid using a three-electrode cell after recoding open circuit potential for 2 hours.



Fig. 1 SEM images of (a) pristine, inset: WCA = 78°, (b) Laser textured, inset: WCA = 126° and (c) Electrochemical potential curve of pristine and textured Ti6Al4V sample

Figs. 1a and 1b show surface topography of pristine and laser treated samples and laser induced hydrophobicity is evident from the increase in water contact angle from 78° for pristine to 126° post laser treatment (insets of Fig. 1a & 1b). The E_{corr} of Ti6Al4V increased from -0.59V to -0.49V and passivation current (I_{pass}) decreased from -5.55A/cm² to -7.25A/cm² after laser surface texturing (Fig. 1c). This clearly shows that the corrosion resistance of Ti6Al4V sample can be improved significantly by laser surface texturing.

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<u>CP-197-EIHE 2023</u>



Bimetallic Nickel-Ferrous Spherical Nanoalloy: Highly Efficient Electrocatalyst for Hydrogen Evolution Reaction



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Abstract:

The development of highly effective catalysts for the hydrogen evolution reaction (HER) in acidic media is critical for improving electrochemical energy conversion in fuel cells and the simple synthesis of hydrogen as an ideal energy carrier via water splitting. Finding an easy way to make alloys is crucial because the majority of metal alloys that have been created so far are bimetals. Here, spherical ferrous nickel nanoalloys (FeNi-1 alloy NCs) have been produced at room temperature using the usual precipitation procedure. As the produced nanoalloy was examined by X-ray diffraction, FE-SEM, HR-TEM, and XPS, it was discovered that Fe-Ni alloy NCs had a spherical shape. These techniques also disclosed the valence states and chemical composition of the Fe-Ni-1 alloy NC's Fe, Ni, C, and O components. Additionally, alkaline electrolytes and manufactured Ni, Fe, FeNi, and FeNi-1 alloy NCs with different Ni:Fe ratios were used to demonstrate the electrochemical hydrogen evolution process (HER). These NCs were examined



using a linear sweep voltammetry (LSV) test, overpotential to obtain a current density of 10 mA cm2 and a potential of -0.374 V vs. RHE, demonstrating a higher electrochemical activity on FeNi-1 alloy. Faster electron transfer was observed in electrochemical impedance spectroscopic (EIS) tests due to better conductivity, intermediate stability, and higher urea molecule adsorption rates. With the help of these investigations, new renewable energy-generating technology will be created that is highly effective at reducing water pollution and has a long history of energy sustainability.^{1,2}

Keywords: Environmental green hydrogen production, Ni-Fe nanoalloys, hydrogen evolution reactions and electrocatalysis.

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Electrochemical detection of Ascorbic acid using Conductive Polymers



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Abstract:

Vitamin C is a water-soluble compound found in living organisms. It is an essential nutrient for various metabolism in our body and also serves as a reagent for the preparation of many materials in the pharmaceutical and food industry. Electrochemical sensors for ascorbic acid based on polyaniline (PANI). The polymers are characterized by different physicochemical characterization techniques such as FT-IR, XRD, UV-Vis and morphology was investigated by FE-SEM and HR-TEM. The electrodes prepared with polyanilines was used to investigate sensing ability for ascorbic acid (AA) by different electrochemical techniques such as cyclic voltammetry (CV), electrochemical impendence spectroscopy (EIS) etc. Electrochemical sensing study was conducted at different pH (4,7, & 9) and at different scan rates. PANI shows best sensing towards ascorbic acid. Electrochemical sensing of AA was successfully achieved using



PANI at onset potential -0.019V vs SCE in pH 7. The enhanced AA electrochemical properties of PANI modified electrode in our work can be attributed to the improvement of electroactive surface area of PANI. This work shows that the PANI hold the prospect for sensitive and selective determination of AA in practical clinical application.

Keywords: Electrochemical sensors, ascorbic acid, Polyaniline (PANI).

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<u>CP-199-EIHE 2023</u>



Nickel-Ferrous Derived Spherical Nanoalloy as an Efficient and Stable Electrocatalyst for Urea Oxidation Reactions



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Abstract:

The development of highly efficient electrocatalysts for treating urea-rich wastewater is an important problem in environmental management and energy production. Herein, Ferrous Nickel spherical nanoalloy (FeNi-1 alloy NCs) has been fabricated by using the standard precipitation approach at room temperature. As synthesized nanoalloy was characterized by X-ray diffraction revealed the formation of FCC structure of Fe-Ni alloy NCs, field emission electron microscopic analysis was observed Fe-Ni alloy NCs is a spherical shape nanoalloy, and HR-TEM revealed an average size is ~33.09 nm, X-ray photoelectron spectroscopy showed Fe, Ni, C and O-components in the Fe-Ni-1 alloy NCs chemical

composition and valence states. Furthermore, the electrochemical urea oxidation reaction (UOR) has been demonstrated as synthesized Ni, Fe, NiFe, and FeNi alloy NCs with different Ni:Fe ratios in alkaline electrolytes were investigated by using linear sweep voltammetry (LSV) test, overpotential to obtaining a 10 mA cm⁻² current density and potential of 1.27 V vs. RHE showing



a higher electrochemical activity on FeNi-1 alloy NCs compared to FeNi, Ni, and Fe NPs, which could be due to altered electronic structures, synergetic and electronic effect in nanoscale. Electrochemical impedance spectroscopic (EIS) studies exhibited faster electron transfer due to improved conductivity, intermediate stabilization, and increased urea molecules adsorption rate. These studies will apply to renewable energy generation technology with long-term energy sustainability and great potential for reducing water pollution.

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CP-200-EIHE 2023



Porphyrin-Based Conducting Polymer Hydrogel for Supercapacitor Application



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Abstract:

Supercapacitors are energy storage devices that can be viable alternatives to replace batteries when high power and extended cycling stability are required. Biocompatible, economically viable, and innocuous nature of organic materials opens up the possibility of developing organic electrodes for energy storage devices. Organic electrode materials such as porphyrins have very fast redox kinetics due to the small HOMO– LUMO gaps.¹ Herein, the electrochemical properties and energy storage capability of a flexible, all-solid-state supercapacitor based on the supramolecular assembly of polypyrrole (PPy) and the anion of 5,10,15,20-tetrakis(4-sulfonatophenyl)-21H, 23H-porphine manganese (III) chloride (MnTSPP) are reported. The electrode material consists of a conductive polymer hydrogel formed through the gelation



initiated by cross-linking of the dopant MnTSPP anion in the PPy chains. The morphology of the cross-linked polymer hydrogel is that of a particledecorated nanofiber, which can perform as a flexible supercapacitor electrode material with a specific capacitance of 300 Fg⁻¹ and capacitance retention of 78% up to 10 000 cycles. The anion of MnTSPP plays a pivotal role in enhancing the charge storage capability by facilitating the electron

transfer between the polymer interchains. In addition, the steric hindrance due to the large size of the dopant counter ions of MnTSPP reduces the counterion drain effect and structural pulverization of PPy, thereby improving the capacitive retention.

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<u>CP-201-EIHE 2023</u>



Hydrothermal synthesis of NiO-CuO Nanocomposite Supported Pd NPs as Potential Electrocatalyst for Ethanol Sensing Application



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Abstract:

Fine dispersion of Pd nanostructures supported on hydrothermally synthesized bimetal oxides on Ni foam substrate was successfully achieved by simple electrochemical approach. The incorporated metal oxides provide excellent support and active surface area which enhance the electro-catalytic performance of the fabricated sensor towards ethanol sensing application. The synthesized nanocomposite material was characterized by XRD, FE-SEM HR-TEM and EIS techniques. The electrochemical behaviour of the synthesized catalyst was investigated using cyclic voltammetry and chronoamperometry techniques. The proposed sensor demonstrated excellent catalytic activity for ethanol electro-oxidation. The fabricated sensor displayed excellent sensitivity 1277 μ A.mM-1.cm-2, in the concentration range of 0.1 to 2.1 mM with limit of detection 0.7 μ M.



Scheme 2. Schematic representation of synthesis, fabrication and electrochemical sensing application of Pd@NiO-CuO@Ni foam electrode.

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Electrooxidation of urea using cerium promoted NiFe-LDH materials



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Abstract

Urea-based energy technology has attracted more and more attention such as the direct urea fuel cell as well as hydrogen production via urea electrolysis [1]. The electrochemical urea oxidation reaction (UOR) is crucial for various industrial and commercial applications that are employing urea-based energy conversion devices. For this purpose, layered double hydroxides (LDH) containing transition metals can be used to design and synthesize highly active, low-cost, and stable electrocatalysts for UOR [2]. The Ni-based electrocatalyst is considered to be the best nonprecious catalyst, and has demonstrated promising activity toward urea electro-oxidation in alkaline medium [3]. The effect of Ce on Ni_xFe_y-LDH structure and subsequent enhancement of the performance of electrooxidation of urea in terms of current density and electrode stability is reported recently [4]. However, optimization of cerium content and identifying the



active sites in Ni_xFe_y-LDH materials is lacking. We have prepared Ni_xFe_yCe_z-LDH materials $(Ni_3Fe_{0.8}Ce_{0.2},$ Ni₃Fe and $Ni_{2.4}Fe_{0.6}Ce$) to the increase electrochemical surface area, and also identify the exact composition and active sites. The LDH materials are characterized by XRD, SEM, TEM, Raman, XPS, and electrochemical methods. The Ni₃Fe_{0.8}Ce_{0.2} shows much higher catalytic activity, lower

overpotential, better stability and superior electrocatalytic performance towards urea electrooxidation compared to Ni₃Fe and Ni_{2.4}Fe_{0.6}Ce catalysts. The Ni₃Fe_{0.8}Ce_{0.2} shows current density of 8.4 mAcm⁻²mg⁻¹ at 0.36 V (vs. SCE) in 1 M KOH containing 0.33 M urea.

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<u>CP-203-EIHE 2023</u>



Effects of Li-content of Copper Oxide on the Electrochemical Reduction of Carbon Dioxide Catalysed by Oxide-derived Copper



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Abstract:

We present here the development of CuO-based electrocatalysts possessing different Li-contents (in lieu of Cu), and the influences of the same towards the electrochemical CO_2 reduction (eCO₂RR) process. The Li-content was found to influence the Cu-content (*i.e.*, Cu:CuO ratio) of the electrochemically pre-reduced lithiated CuOs, which are also known as 'oxide-derived lithiated Cu', with the greater Cu:CuO ratio primarily helping with the eCO₂RR process, in terms of the resultant current densities and faradaic efficiencies of the products formed. One of the practically significant results is that Li-incorporation in CuO up to solubility limit (*viz.*, ~30 mol%; as established here) progressively enhances the current density and faradaic efficiencies of the products (yielding CO, HCOO⁻, CH₃COO⁻, C₂H₄, ethanol), but with the performances getting degraded beyond 30 mol% Li-content. By contrast, undoped CuO could not yield ethanol and resulted in lower FEs. Accordingly, the present work reveals the relative roles of Li-content and Cu/CuO-content of 'CuO-derived lithiated Cu' electrocatalysts on the current densities, product formation and associated faradaic efficiencies on eCO₂RR, including the beneficial role of Li-incorporation towards enhancing the efficacy of CuO as electrocatalyst for eCO₂RR in significant terms.

Keywords: Electrochemical CO₂ reduction, Cu/CuO ratio, Lithiated CuO, structure, electrocatalysis, multi-products.



Eco-friendly method of preparing sulfur cathode for Li-S battery



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Abstract:

For relatively newer developments such as Li-S battery; polysulphide shuttle effect, volume expansion and low conductivity of sulphur have been the main hurdles in the path towards its commercialisation. To get rid of the notorious shuttle effect, we looked at the binder material of the cathode component. An attempt at keeping up with the capacity while making components sustainable led us to explore a protein-based biopolymer, Zein. Combined with an activated carbon obtained using another natural source (chitosan), a capacity decay of merely 10% over 100 cycles at 0.2 C rate and 12% at 0.5 C rate were observed. The carbonyl rich binder helped to glue the components together while the long chain of amino acids aided to preserve the performance. An impressive extent of adsorption of polysulphides by zein was verified by UV-Visible spectroscopy technique. The carbon host used for this study possessed a high surface area of around 1900 m^2/g (BET) which helped to load higher amounts of sulphur as revealed by thermogravimetric analysis. Owing to a porous host, the volume expansion effect could also be diverted to maintain the performance which was observed through stability studies.

<u>CP-205-EIHE 2023</u>



Hybrid Fe₂O₃-MXene Nanocomposite for Supercapacitor Applications



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Abstract:

Recently, MXene (Ti₃C₂X_n) has become a trending topic in the field of energy storage, due to its high performance, flexibility and ease at which it can form composites with polymers, CNT's, metal oxides and more. Herein, we have synthesized bi-composite of MXene and Fe₂O₃, to enhance its electrical conductivity, stability and capacitance. First MXene was prepared using its MAX(TiAlC) phase, subsequently Fe₂O₃-MXene composite was prepared. Structural analysis of the prepared materials was performed using characterization techniques such as XRD, FTIR, BET, Raman, SEM (EDAX) and TEM. Further to understand its electrochemical properties, Chronopotentiometry, Cyclic voltammetry and Electrochemical impedance spectra were carried out using CH-Electrochemical work station. The specific capacitance of MXene was found to be 205 F/g at 10 mV/s which is enhanced after the addition of Fe₂O₃ with improved retention capacity. Chrono potentiometric studies exhibited an improvement in discharge time too.



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<u>CP-206-EIHE 2023</u>



Defect and valence engineering in CeO₂ through aliovalent ion doping for enhanced activity towards ORR catalysis



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Abstract:

Engineering of the defect architecture is pivotal in the design of rare earth and transition metal oxide based heterogeneous catalysts with superior performance. Here in this work, we employed Positron Annihilation Lifetime Spectroscopy (PALS) along with other complementary techniques like X-Ray photoelectron

spectroscopy (XPS), Photoluminescence (PL) and Electrochemical Impedance Spectroscopy (EIS) to understand defect evolution in CeO₂ nanoparticles doped with distinct sized trivalent rare-earth ions, namely, Y³⁺, Eu³⁺ and La³⁺ of varying concentration and correlated the same with their activity towards Oxygen Reduction Reaction (ORR) catalysis. The ceria nanocatalysts were synthesized via gelcombustion technique and characterized by powder XRD followed by





Rietveld refinement analysis. The combined results showed enhanced defect density with doping in general and higher concentration of oxygen vacancies, weaker vacancy-dopant association and greater Ce^{3+} fraction in larger sized ion La^{3+} doped ceria as compared to Y^{3+} and Eu^{3+} counterparts. Improved ORR activity with higher current density, lower overpotential and reduced electron transfer resistance was also observed in case of La^{3+} doped

ceria. The studies are expected to help in further tuning of the catalysts in terms of dopant type and concentrations.

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CP-207-EIHE 2023



Enhancing lithium storage capacity of bismuth sulfide via addition of bismuth oxide



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Abstract:

Bismuth sulfide has attracted much attention as a Li-storage material due to its high theoretical gravimetric and volumetric capacities. However, poor cyclability and large volume change during Li insertion and de-insertion results in low capacity and degradation of this material. In this work, Bi_2S_3 , and its composite with Bi_2O_3 has been explored to improve its electrochemical performance. Anode materials with high capacity are urgently required to substitute graphite. In this regard, conversion type materials like metal sulfides (M_xS_y) have gained prominence as it generally has higher capacity compared to graphite [1]. Though the theoretical gravimetric and volumetric capacities of Bi_2S_3 are much higher than those of graphite, the cycling performance of Bi_2S_3 is poor due to its large volumetric expansion. In this work, Bi_2S_3/Bi_2O_3 composites were synthesized and their properties as anode materials compared to Bi_2S_3 have been analysed. The active material has been characterized using powder XRD (Fig. 1). The cathodic peaks



at 1.85 and 1.69 V is owing to the reduction of Bi_2O_3/Bi_2S_3 to metallic Bi and Li_2S , another two peaks located at 0.76 and 0.69 V are described as further alloying process with Li ions to form LiBi and Li_3Bi , respectively. In the reverse process, the anodic peak at around 1.0 V corresponds to the Li_3Bi dealloying to Bi, while the peaks at 2.1, 2.3 and 2.6 V represent the regeneration of Bi_2O_3/Bi_2S_3 particles. A high capacity of ~ 495mAh g⁻¹ and 258mAh g⁻¹ were obtained from $Bi_2(O,S)_3$ and $Bi_2S_3@Bi_2O_3$ composite, respectively, compared to 33mAh g⁻¹ for pristine Bi_2S_3 after a run of 350 cycles. Electrochemical studies confirm the superior performance of the synthesized anode materials.

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CP-208-EIHE 2023



An Effective and Stable Electrocatalyst for Oxygen Evolution Reactions is a Nickel-Ferrous Derived Spherical Nanoalloy



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Abstract:

An important issue in environmental management and energy generation is the development of extremely effective electrocatalysts for treating urea-rich wastewater. Here, spherical ferrous nickel nanoalloys (FeNi-

1 alloy NCs) have been created utilizing the common precipitation method at ambient temperature. Fe-Ni alloy NCs were found to have a spherical shape as the synthesized nanoalloy was characterized by X-ray diffraction, FE-SEM, HR-TEM, and XPS. These methods also revealed the Fe, Ni, C, and O components in the Fe-Ni-1 alloy NCs chemical composition and valence states. Additionally, the electrochemical oxygen evolution reaction (OER) has been demonstrated using synthesized Ni, Fe, FeNi, and FeNi-1 alloy NCs with various Ni:Fe ratios in alkaline electrolytes. These



NCs were investigated using a linear sweep voltammetry (LSV) test, overpotential to obtain a 10 mA cm⁻² current density and potential of 1.36 V vs. RHE, showing a higher electrochemical activity on FeNi-1 alloy faster electron transfer was seen in electrochemical impedance spectroscopic (EIS) tests as a result of better conductivity, intermediate stability, and higher urea molecule adsorption rates. These studies will be used to develop renewable energy generation technology that is both highly capable of minimizing water pollution and has a long history of energy sustainability.

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<u>CP-209-EIHE 2023</u>



Ethanol formation via CO₂ electroreduction at low overvoltage over exposed (111) plane of CuO thin film



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Abstract:

The depletion of fossil fuels leads to the production of massive volumes of carbon dioxide, which contributes significantly to climate change. Hence, CO_2 conversion to valuable chemicals is of great significance. We report the fabrication of CuO thin films using the sol-gel spin coating method, for electrocatalytic reduction of CO_2 (CO_2ER). Thin film provides a large surface area and a more exposed

(111) crystal plane for ethanol selectivity. It is further verified by comparing it with bulk powdered material which does not give such activity. CO₂ER over thin film electrode specifically forms CO(g) and Ethanol, 2 and 12 electron reduction products, and eliminates the possibility of unwanted HER as a side reaction in the CO₂ saturated NaHCO₃ electrolyte. Significant product selectivity and faradaic efficiency, utilizing the very low potential for



both CO and ethanol is reported. DFT calculations also suggest that CuO (111) and CuO (-111) surfaces promote CO_2 adsorption and subsequent formation of CO. However, a direct CO-dimerization is observed only on the CuO (111) surface that facilitates the formation of C2 product. This comparative study of bulk and thin-film opens new insight and highlights the importance of catalyst fabrication for the specific product formation utilizing significantly less energy.

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Defect engineering of BaSnO₃ photoanodes for efficient photoelectrochemical water splitting



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Abstract:

Barium stannate (BaSnO₃) crystallizes in the cubic perovskite-type structure and typically exhibits a wide band gap of >3.0 eV; thus, it is often considered unsuitable as a photo-absorber material for solar energy conversion.¹⁻² We present a spray-pyrolysis method for the fabrication of BaSnO₃ photoanodes, with a smaller optical gap of ~2.2 eV. By annealing the photoanodes in 5% hydrogen sulfide (H₂S) gas, the optical gap is further reduced to ~1.7 eV, with an ~20-fold increase in photocurrent density and an improved onset potential of ~0 V_{RHE}. To understand the reasons behind this performance enhancement, we utilize a combination of spectroscopy techniques, including photoluminescence, wavelength-dependent time-resolved surface photovoltage analysis, and photoconductivity measurements. We find that H₂S annealing of BaSnO₃ generates a set of filled defect states associated with oxygen vacancies ($V_0^{\bullet\bullet}$), Sn²⁺ centres (Sn"), and sulfur substitutions (S_0^{\times}), which are situated ~1.4 to 1.9 eV below the conduction band minimum and exhibit a degree of orbital overlap with the valence band maximum.³ Increasing the density of these defects shifts the optical onset of photocurrent generation to ~1.7 eV and enables holes to transport via a hopping mechanism. Resultantly, the charge carrier mobility is shown to increase by 20-fold, reaching ~0.04 cm² V⁻¹ s⁻¹.

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Synthesis of Cathode Material for SIB: NASICON based NVP through wet-chemical route with ultrasound assistance



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Abstract:

Sodium-ion batteries (SIBs) are considered to be the most promising electrochemical energy storage devices for large-scale grid and electric vehicle applications due to the advantages of resource abundance and cost-effectiveness. The electrochemical performance of SIBs largely relies on the intrinsic chemical properties of the cathodic materials. Among the various cathodes, rhombohedral $Na_3V_2(PO_4)_3$ (NVP), a typical sodium super ionic conductor (NASICON) compound, is very popular owing to its high Na^+ mobility and firm structural stability. However, the relatively low electronic conductivity makes the theoretical capacity of NVP cathodes unviable even at low rates. Fe-substituted $Na_3V_{2-x}Fe_x(PO_4)_3$



compounds with a sodium superionic conductor structure are attempted to synthesize by a single and easily scalable sol-gel route. Iron substitution enhances ionic diffusivity and lowers a bandgap, and, thus, improves sodium storage performance. Sodium Vanadium

Phosphate (NVP) is prepared in a single-phase form via wet-chemical route with assistance from high power (100 W) ultrasound. We were able to achieve single-phase $Na_3V_2(PO_4)_3$ with some impurities by calcinating sonicated solution at 650°C for 6 h under Argon atmosphere. The use of these accelerated synthesis techniques could accelerate the nucleation rate, and thus could result in reduction of phase formation temperature/time. Powder X ray Diffraction (PXRD) was used for the primary characterization of the materials. Simultaneously, solid state synthesis of NVP was carried out to get information about the role played by mechanical assistance in phase formation through analysis of XRD after gradual heating in inert atmosphere.

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Electrochemical and Catalytic Conversion CO₂ into Formic Acid on Cu-InO₂ Nano alloy Decorated on Reduced Graphene Oxide



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Abstract:

The catalytic and electrochemical hydrogenation of CO_2 delivers a substitute for a carbon-neutral cycle for sustainable energy and value-added chemicals. This section reveals the *in-situ* decoration of Cu-InO₂ nanoalloy on reduced graphene oxide (Cu-InO₂@rGO) nanocomposite. The synthesized Cu-InO₂@rGO has been characterized by various techniques such as scanning electron microscopy (SEM) confirms the spherical shape Cu-InO₂ nanoalloy decorated on reduced graphene oxide, the average size calculated by HR-TEM shown Cu-InO₂ alloy is ~4 nm on rGO surface (~100 nm). More importantly, the XRD pattern



confirms FCC crystal structure and FT-IR analyses Cu-O and Cu-In-O existing in nanocomposites. The linear sweep voltammetry (LSV) demonstrates an ultra-low potential of -0.9 V vs SCE. Furthermore, we have performed the bulk electrolysis on Cu-InO₂@rGO electrocatalyst at a potential of -1.1 V vs SCE to reach HCOOH with a Faradic yield of 76.10 %. The alloying of Cu and InO₂ with rGO is responsible for the variation of adsorption assets of

intermediates. This indicates an enhanced selectivity and inhibited the formation of H_2 and CO. In catalytic hydrogenation used as the same catalyst and was found to, an excellent yield towards HCOOH is of 5.5 mmol. Current studies highlighted the enhancement in activity along with selectivity towards product formation could be due to having a capable active interface from electrocatalysts for low-cost and proficient production of fuels.¹⁻³

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Electrochemical and Spectroscopic Investigation of HER2-Targeting Peptide



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Abstract

Elevated expression of HER2 receptors in breast cancer and associated metastatic sites entails development of specific radiopeptides for molecular imaging and therapy. Towards this HER2-specific A9 peptide was synthesized manually by solid phase peptide synthesis. Electrochemical investigations of the peptide were carried out with and without the presence of reduced graphene oxide (rGO). Shifting of the cyclic voltammetry peak of peptide indicated the formation of rGO-peptide conjugate. The UV-VIS spectra of the peptide in presence of different concentrations of rGO were also recorded. The absorbance of peptide enhanced with the addition of rGO present in the phosphate buffer solution, indicating enhancement in the electron density at the chromophore center, the plots are shown in Fig.1. Based on the peak position and relative shifting of peaks in the differential pulse voltammetry and UV-VIS spectral measurements the



conjugation sites are being evaluated. The peptide was further conjugated with chelator DOTA at N-terminus for radiolabeling with

¹⁷⁷LuCl₃ and characterized by mass spectrometry. Radiolabeling yield of ¹⁷⁷Lu-DOTA-A9 was >98% as determined by RP-HPLC. Radiotracer ¹⁷⁷Lu-DOTA-A9 was hydrophilic in nature with log P value -3.29 ± 0.1. In vitro stability of radiopeptide (100 μL, 3.7 MBq) was investigated by incubation with human serum (400 μL, pH 7.4) at 37°C. Aliquots (100 μL) withdrawn at different time points (6, 24 and 48 h) were precipitated with acetonitrile (100 μL), centrifuged and analysed by RP-HPLC. To determine the percentage of intact radiopeptide peak areas were quantified. ¹⁷⁷Lu-DOTA-A9 was observed to be stable in human serum with 92.3% intact radiopeptide after 48 h incubation.

Fig.1 (a) The differential pulse voltametric plot of the peptide at different concentrations of rGO (b) The UV-VIS spectra of the peptide with subsequent addition of rGO.

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rGO, CNT and Carbon nano sphere inclusion PEDOT for the Sensitive Determination of Dopamine and Uric Acid and ascorbic acid



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Abstract:

Development of suitable modified electrode in generating the electrochemical signals from dopamine (DA), uric acid (UA) and ascorbic acid (AA) has remained challenging issue even after decades of research in the related field. Under the present investigation EDOT is electrochemically polymerized over the glassy carbon electrode substrate to generate PEDOT. The polymer has been included with rGO, CNT and Carbon nano sphere after different levels of functionalization. The inclusion carbon in its different forms and functionalization has improved the sensitivity of the electrochemical oxidation of UA, DA and AA. The composite electrode system could separate the three peaks, well suited for their analytical determination. The response from the carbon nano sphere included polymer electrode has provided better sensitivity, however the peak separation is better with the CNT modifications. The analytical method has been developed with the detection limit (S/N=3) of 5 nM, 2 μ M and 10 μ M for DA, UA and AA respectively.

The interference test was carried out using the commonly occurring interfering agents. The analytical method has been applied for the detection of analytical signals of DA and UA in synthetic samples.



Fig. 1. The electrochemical response of PEDOT-CNT composite electrode for UA, DA and AA.



Electrical Characterization of Doped/Co-doped LaScO₃



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Abstract:

Solid oxide electrolyte fuel cells are energy conversion devices with high efficiency and environmental friendly. Recently, SOFCs using oxide proton conductors as a solid electrolyte has attracted more interests as compared to the traditional SOFC with oxide ion conduction due to its possible low



temperature operation i.e. between 400°C to 700°C. Perovskite materials such as substituted LaScO₃ are considered as better candidates as electrolyte because of their high proton as well as oxide ion conductivity. Proton conductivity of such electrolytes is dependent on the concentration of oxygen vacancies in the lattice. The oxygen vacancies in these oxides can be considerably increased by acceptor doping i.e. doping on the B-site by lower valent elements typically, alkali or alkaline earth metals. Here we

report the details of preparation and electrical properties of Mg and Ba doped LaScO₃. The doped and co-doped samples were synthesized by gel-combustion route using glycine as fuel and characterized by X-ray diffraction technique. The maximum solubilities of Mg and Ba in the lattice of LaScO₃ are: 10 and 40 mol % respectively. The electrical measurements were carried out in dry and wet N₂ atmosphere in between 200-800°C. All these materials exhibit enhanced



proton and oxide ion conductivities. Comparison of the electrical properties of the studied materials revealed an increasing trend in the ionic conductivity with increase in Ba⁺² concentration. The analyses of the grain and grain boundary conductivities revealed a steady increase in the grain conductivity with the increase in barium content. Further the impedance measurements under different partial pressure of water vapor suggested proton conduction behaviour via thermally activated hopping mechanism.

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Electrochemical degradation of Polymethylmethacrylate (PMMA) microplastic by photochemical route



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Abstract:

Microplastics (MPs) pollution in wastewater has become a global environmental concern due to their threat to environment and human being. Since the size of microplastic is small compared to large plastic items, so conventional water treatment plants are unable to remove this MPs from water. Photochemical oxidation is being used for decomposition of polymers into smaller molecules such as CO₂ and H₂O. On a large scale, this process is inefficient as well as costly. However, combining electrochemical oxidation with UV irradiation can solve the above problem more effectively due to electrochemical oxidation's strong controllability, ease of operation, and lower secondary pollution. The goal of this paper is to degrade Polymethylmethacrylate (PMMA) MP in water using electrochemical oxidation in the presence of UV light. Both homogeneous and heterogeneous irradiation protocols are adopted to irradiate the microplastics. TiO₂ treated iron oxide over FTO plate has been used as the photoelectrode for the degradation process, while for homogeneous treatments, suspended Fe-oxides are used. The suspended catalyst showed better degradation efficiency, however considering the regeneration and continued operation in a device level the catalysts coated over the FTO substrate performed better. The results show that after 2 hours of photoelectrochemical the particle concentrations of the microplastics has been reduced by about 50%.

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