Transition Metal - Oxygen Bond Covalency Driven Phase Control in 'Layered' Transition Metal Oxides for Sodium - Ion Battery Cathodes

Brijesh Yadav[1,2,3], Parama Chakraborty Banerjee[4], Mainak Majumder[3], Amartya Mukhopadhyay[2]*

[1]IITB-Monash Research Academy, Indian Institute of Technology Bombay, Mumbai 400076, India
[2] Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India
[3]Nanoscale Science and Engineering Laboratory (NSEL), Department of Mechanical and Aerospace Engineering, Monash University, Clayton, Victoria, 3168 Australia
[4]Department of Chemical and Biological Engineering, Monash University, Clayton, Victoria, 3800 Australia
*Email: amartya_mukhopadhyay@iitb.ac.in

Abstract

This work introduces a universal strategy towards facilitating and controlling the formation of biphasic P2/O3 structures, along with other preferred structural types (P-type and O-type), in 'layered' Na- transition metal (T_M) oxides. Building on our previous study[1], where we revealed that it is the overall degree of covalency of the cation-oxygen bonds in the T_MO_2-'slab', as governed by the overall average charge:size ratio (C:S) of the cation-combination in the T_M-layer (*viz.*, electronegativity), that tilts the balance between P2 vs. O3 phase formation for a given Na-content, we reveal here the possibility of facilitating and controlling the P2 + O3 (*i.e.*, bi-phasic/single phase) content in 'layered' Na-T_M-oxide based on the same concept. Using a predominantly Ni-Mn-based composition, we systematically modulated the overall covalency of the T_M–O by substituting a low-electronegativity cation (Ti^{4+}, having a lower "charge:size" ratio ~6.5 Å^{-1}) into the transition metal (T_M) layer for Mn^{4+} (having a higher "charge:size" ratio of ~7.5 Å^{-1}). This reduction in covalency enhanced the relative stability of the O3 phase over that of the P2 phase for the original composition, enabling a controlled phase formation/content for the mixed phase (*i.e.*, O3 + P2) and then eventually in phase pure O3. The effects of the phase assemblage on the electrochemical behaviour have also been studied in Na 'half' cells. These findings offer insights into the design of mixed-phase (O3/P2) cathode materials by precisely tuning the covalency of the T_M-O bond and following the map reported in our previously published work[1] (*viz.*, the C:S corresponding to the T_M-layer relative to the stoichiometric Na content), enabling optimized structural stability and improved electrochemical performance as cathodes for sodium-ion batteries.

Keywords: layered Na- transition metal oxide, phase evolution, cathode, Na-ion battery

References

1. **Kumar, B. S.; Kumar, R.; Pradeep, A.; Amardeep, A.; Srihari, V.; Poswal, H. K.; Chatterjee, A.; Mukhopadhyay, A.** Fundamental Principles toward Designing High Na-Containing P2-Structured "Layered" Na-Transition Metal Oxides as High-Performance Cathode Materials for Na-Ion Batteries. *Chem. Mater.* **2022**, *34* (23), 10470–10483. https://doi.org/10.1021/acs.chemmater.2c02150

From Active to Inactive: Quantifying Lithium Degradation in Practical Li-CO_2 Battery

Rikta Salui[1], Debalina Deb[2], Aninda J. Bhattacharyya [1,2]*

[1] *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru*

[2] *Interdisciplinary Center for Energy Research, Indian Institute of Science, Bengaluru*

*Email: anindajb@iisc.ac.in[1]

Rechargeable aprotic lithium-carbon dioxide (Li-CO_2) batteries have attracted significant interest for its potential as a carbon capture technology and sustainable energy storage. The Li-CO_2 battery, with a theoretical energy density of 1876 Wh/kg, features a CO_2-fed cathode, a lithium metal anode, and an organic electrolyte. Li_2CO_3 forms as the main discharge product and dissociates back into Li and CO_2 during charging. However, its practical viability is hindered by several fundamental challenges. Primarily, the high kinetic barrier between gaseous CO_2 and the solid Li_2CO_3 product[1]. The irreversible formation of insulating Li_2CO_3 results in a low operating voltage (<2.5 V) and poor energy efficiency. Moreover, although Li-metal serves as a high energy density anode, its instability and continuous degradation during cycling severely impact long-term performance, ultimately contributing to battery failure.

Differentiating and quantifying inactive lithium species is crucial for understanding the battery failure mechanisms, as this provides essential insights into the underlying challenges. Therefore, a systematic examination of the dynamic evolution of inactive Li and its fundamental relationship with lithium loss, electrolyte decomposition, and solid electrolyte interphase (SEI) formation is necessary.[2, 3] To accomplish this, we employed a comprehensive set of analytical techniques, including electrochemical, spectroscopic characterization, and chromatographic techniques. This integrated approach allows us to quantify the evolution of dead lithium metal and SEI components separately, providing a deeper understanding of degradation pathways in Li-CO_2 batteries.

As the degradation mechanisms of Li-CO_2 batteries remain largely unexplored, this study offers a detailed investigation using various quantification techniques. Due to the inherent instability of Li-metal in organic solvents, our findings reveal that repeated cycling leads to progressive passivation of the anode. This degradation is primarily driven by electrolyte decomposition, which forms LiOH deposits, and CO_2 crossover effects, which lead to Li_2CO_3 accumulation. These combined processes accelerate surface passivation, increase dead lithium formation, and ultimately contribute to capacity loss and battery failure. Our quantitative analysis provides critical insights into these degradation mechanisms, paving the way for future advancements aimed at mitigating capacity loss and enhancing the long-term stability of Li-CO_2 batteries.

Keywords: *Li-CO_2 battery, Dead Li quantification, SEI components*

References:

1. Jinshuo Zou, *et. al.* Revisiting the Role of Discharge Products in Li–CO2 Batteries*, Adv. Mater.*, **2023**, 2210671.
2. Jun Liu, *et al.* Pathways for practical high-energy long-cycling lithium metal batteries. *Nat Energy*, **2019**, 4, 180–186.
3. Abhishek Bharti *et.al.* CO_2 Crossover to the Li Anode and Its Implications on the Solid Electrolyte Interphase Composition in a Rechargeable Li–CO_2 Battery, *J. Phys. Chem. C* **2024**, 128, 28, 11543–11551.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Conducting Li_xPO_y Interface Generated from Insulating Residual Lithium Compounds on $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ Surface Improves Cycle Life and Assists in Fast Cycling

Jyotirekha Dutta[1], Shuvajit Ghosh [1], Kiran Kumar Garlapati [2], and Surendra K. Martha*[, 1]

[1] *Chemistry Department, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, 502284, Telangana, India*

[2] *Center for Interdisciplinary Programs, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, 502284, Telangana, India*

* Corresponding author, Email: martha@chy.iith.ac.in

Abstract

$LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) is a leading cathode candidate for next-generation lithium-ion batteries (LIBs) due to its high energy density. However, the commercialization of NMC811 is hindered by its structural instability and surface reactivity. Surface chemical instability towards exposure to ambient moisture induces residual lithium compounds (RLCs: Li_2CO_3, LiOH), which form resistive layers and trigger parasitic electrolyte reactions. To address this issue, we propose an "Adverse-to-Beneficial" approach to eliminate RLCs by chemically transforming them into a Li_xPO_y (Li_3PO_4 and $LiPO_3$) interface. [1] The interface protects the NMC811 surface from moisture attack and unwanted side reactions with electrolytes.

The key achievements in the work include enhanced cycling stability, improved kinetics, and reduced interfacial resistance. The protective Li_xPO_y interface enhances the cycle life of NMC811 by retaining 70 % of the initial capacity after 300 cycles at a 0.5C rate and 60 % after 500 cycles, even at a 5C rate in the voltage window of 3.0 – 4.3 V *vs.* Li^+/Li. The coexistence of two Li-conducting phases lowers the voltage polarization of the kinetically sluggish H1 → M phase transition, which enhances fast cycling, reduces cationic disorder, improves coulombic efficiency, improves ion diffusion kinetics, and minimizes particle crack formation after long-term cycling. [1] This approach leverages RLCs, typically detrimental, to construct a stabilized interface, demonstrating a viable pathway for deploying NMC811 in commercial batteries without complex coating infrastructure.

Keywords: NMC811 cathode, residual lithium compounds, Li_xPO_y interface, fast-charging, Li-ion batteries

References

(1) Dutta, J.; Ghosh, S.; Garlapati, K. K.; Martha, S. K. Conducting Li_x PO_y Interface Generated From Insulating Residual Lithium Compounds on $LiNi_{0.8}$ $Mn_{0.1}$ $Co_{0.1}$ O_2 Surface Improves Cycle Life and Assists in Fast Cycling. *Small* **2024**, 2405432. https://doi.org/10.1002/smll.202405432.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Hierarchical Pore Engineering of Biomass-Derived Carbon Cathodes for Rechargeable Aluminium Batteries

Sruthy E S[1, 2], Menestreau Paul[3], Gopinathan Manavalan[2], Nicolas Boulanger[4], Palanivel Molaiyan5, Tao Hu[5], Ulla Lassi[5], Mikael Thyrel[2], Shaikshavali Petnikota[2], Christie Thomas Cherian[1*]

1School of Electronic Systems and Automation, Digital University Kerala, Thiruvananthapuram, India

2Biomass Technology Centre, Department of Forest Biomaterials and Technology, Swedish University of Agricultural Sciences, SE-90183 Umeå

3Public Research University Engineering School, IMT Mines Albi, Albi 81000, France

4Department of Physics, Umeå University, SE-90187 Umeå, Sweden

5Research Unit of Sustainable Chemistry, University of Oulu, P.O. Box 3000, FI-90014 Oulu, Finland

* christie.cherian@duk.ac.in

Abstract

Aluminium batteries (ABs) are promising candidates for next-generation energy storage due to aluminium's abundance, low cost, and high theoretical capacity. In this work, birch wood-derived carbons were synthesised via carbonisation followed by KOH activation at biochar-to-KOH ratios of 1:4 (CBW14) and 1:6 (CBW16). Material characterisation reveals that activation conditions play a critical role in governing pore evolution, allowing for the controlled tuning of micro- and mesoporosity. Micropores enhance accessible surface area and charge storage sites, while mesopores facilitate ion transport and electrolyte penetration. An optimised activation ratio yields a hierarchical pore architecture with a balanced micro/mesopore distribution, whereas under- or over-activation leads to inferior pore connectivity. Galvanostatic charge-discharge measurements confirm that the optimised carbon delivers superior capacity, rate capability, and energy density. These findings highlight that rational pore hierarchy engineering, rather than maximising surface area alone, is key to improving the electrochemical performance of biomass-derived carbon cathodes.

Keywords **:** Aluminium batteries, Biomass, Activated carbon, Porosity, Electrochemical performance

References

[1]O. Oginni, K. Singh, G. Oporto, B. Dawson-Andoh, L. McDonald, and E. Sabolsky, "Influence of one-step and two-step KOH activation on activated carbon characteristics," *Bioresour Technol Rep*, vol. 7, Sep. 2019, doi: 10.1016/j.biteb.2019.100266.

[2]Y. Ji, T. Li, L. Zhu, X. Wang, and Q. Lin, "Preparation of activated carbons by microwave heating KOH activation," *Appl Surf Sci*, vol. 254, no. 2, pp. 506–512, Nov. 2007, doi: 10.1016/j.apsusc.2007.06.034.

[3]F. A. Kayakool *et al.*, "Mesoporous carbon derived from lignin sulfonate as a sustainable cathode for high-performance aluminium batteries," *Carbon Resources Conversion*, vol. 8, no. 1, Mar. 2025, doi: 10.1016/j.crcon.2024.100301.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Mg/Cu Co-Doping Strategy for High-Voltage Stable and Long-Life O3-Type Layered Cathodes in Sodium-Ion Batteries.

***Shreya Jose*[a,b], *K Ramesha*[a,b*]**

[a]*Council of Scientific and Industrial Research, Central Electrochemical Research Institute-Chennai Unit, CSIR Madras Complex, Chennai 600113, India*

[b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad -201002, India*

**Corresponding author*

Email address: ramesha.cecri@gmail.com , ramesha@cecri.res.in

Abstract

O3-type layered oxides are considered promising cathode materials for sodium-ion batteries (SIBs) due to their high specific capacity and energy density. However, their practical application is often limited by rapid capacity fading, which arises from severe structural degradation and complex phase transitions during cycling. In this work, we develop a Mg/Cu co-doped O3-type layered oxide, $Na[Mg_{0.03}(Ni_{0.25}Cu_{0.05}Fe_{0.2}Mn_{0.5})_{0.97}]O_2$ (NFM-MC), as a high-performance cathode for SIBs. The co-doping strategy effectively widens Na^+ diffusion channels and enhances electronic conductivity, resulting in significantly improved rate capability. In-situ XRD analysis reveals that Mg/Cu co-doping suppresses irreversible phase transitions and minimizes volume strain during cycling, thereby enhancing structural stability. The NFM-MC cathode demonstrates outstanding long-term cycling performance, delivering 95% capacity retention over 500 cycles at a 2C rate in the 2.0–4.0 V range, far surpassing the 40% retention observed in the undoped counterpart. Additionally, the co-doped cathode exhibits improved high-voltage stability, maintaining 90% capacity after 300 cycles at 1C in the 2.0–4.2 V range. These findings highlight the effectiveness of Mg/Cu co-doping in stabilizing O3-type layered structures for high-performance sodium-ion batteries.

Keywords: Sodium ion batteries, O3-type layered oxide, co-doping

References

(1) Li, Y., Lei, L., Hou, J., Wang, G., Ren, Q., Shi, Q., Wang, J., Chen, L., Zu, G., Li, S. and Wu, J. Manipulating local electronic and interfacial structure of O3-type layered oxides for high-rate sodium-ion battery cathodes. *Journal of Energy Chemistry*, 2025, *105*, 224-232.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Tuning Fe Content in O3-Type Layered Cathodes: Opportunities and Challenges for Sodium-Ion Batteries

Vasantha A. Gangadharappa[1,2] and Annigere S. Prakash[1,2*]

1CSIR–Central Electrochemical Research Institute-Chennai Unit, Taramani 600113 Chennai, India;

2Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India;

**E-mail : prakash@cecri.res.in ; prakash.as@gmail.com*

Abstract

Layered sodium transition metal oxides ($NaTMO_2$, TM = 3d metals) have emerged as promising cathode materials for sodium-ion batteries (SIBs) due to their structural versatility and cost advantages. Among these, Fe-based layered oxides attract significant attention for their unique ability to incorporate high Fe content into the transition metal layer—an advantage not seen in their lithium counterparts. Here we have approached a different strategies varying Fe content in the O3 type Cathode material, This capability enables activation of the Fe^{3+}/Fe^{4+} redox couple, providing high capacity and low-cost alternatives for SIBs. However, increased Fe content introduces challenges such as Fe ion migration, structural instability, and oxygen release during electrochemical cycling. These effects lead to capacity fading, voltage decay, and irreversible phase transitions. Strategies such as Cu-Ni/Fe substitution have shown promise in suppressing Fe migration and stabilizing the structure. This review discusses the structural evolution, redox behavior, and electrochemical performance of Fe-rich $NaTMO_2$ systems, highlighting both the opportunities and limitations of Fe incorporation, and outlines future directions for optimizing Fe-based layered cathodes for practical SIB applications.

Keywords (max 5): SIBs, Cathode, phase transition, Iron based cathode, electrochemical cycling

References

1.Xu Gao; Huanqing;Liu,Wentao Deng; Ye Tian; Guoqiang Zou; Hongshuai Hou; Xiaobo Ji ; Iron-Based Layered Cathodes for Sodium-Ion Batteries *Batteries & Supercaps* ***2021****, 4, 1–24*

2. Xi Chen;Sooyeon Hwang; Robin Chisnell; Yichao Wang;Fan Wu; Sooran Kim; Jeffrey W. Lynn; Dong Su; Xin Li; Reversible Flat to Rippling Phase Transition in Fe Containing Layered Battery Electrode Materials, *Adv. Funct. Mater.* ***2018,*** *28, 1803896*

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhanced Mg^{2+} diffusion and cycling stability in $Mo_{5.5}W_{0.5}S_8$ cathode for rechargeable magnesium batteries

Gazal Gupta[1,2], Amit Gupta[2], Deepak Kumar[1,*]

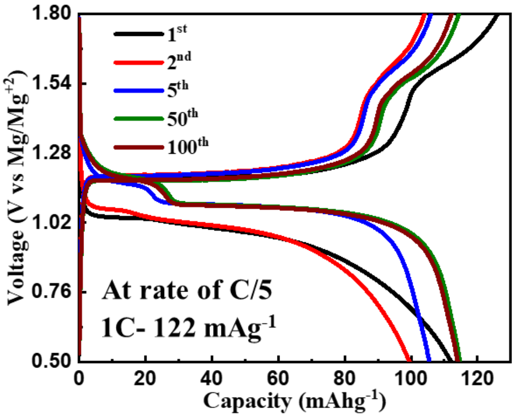
[1] *Centre for Automotive Research and Tribology (CART), Indian Institute of Technology, Hauz Khas, New Delhi, India 110016*

[2] *Department of Mechanical engineering, Indian Institute of Technology, Hauz Khas, New Delhi, India 110016*

*Email- dkumar@iitd.ac.in

Abstract

Rechargeable magnesium batteries (RMBs) are gaining attention as a potential next-generation energy storage technology due to magnesium's high theoretical volumetric capacity, low cost, and widespread availability. Despite these advantages, their practical application remains limited by key challenges, such as the lack of cathode materials capable of reversible magnesium intercalation and the scarcity of stable electrolytes compatible with magnesium metal anodes. In this study, $Mo_{5.5}W_{0.5}S_8$ cathode material is synthesized for the first time using a high-energy ball milling method. Structural and morphological analysis performed via X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and energy-dispersive X-ray spectroscopy (EDS), Inductively coupled plasma mass spectroscopy (ICPMS) confirms the formation of a rhombohedral crystal structure and the successful substitution of W into the Mo_6S_8 lattice with a distinct cuboidal morphology. The W-doped material also demonstrates improved electronic conductivity compared to pristine Mo_6S_8. Electrochemical testing of a $Mo_{5.5}W_{0.5}S_8$||Mg coin cell at room temperature shows a first discharge capacity of 116 $mAhg^{-1}$ at a C/5 rate. Also, a specific capacity of 112 $mAhg^{-1}$ achieved at a C/3 rate, with 97% capacity retention over 400 cycles. Additionally, the study investigates the magnesium ion diffusion behaviour within the $Mo_{5.5}W_{0.5}S_8$ structure. Diffusion coefficients, derived from electrochemical impedance spectroscopy (EIS), and galvanostatic intermittent titration technique (GITT), span a range from 10^{-8} to 10^{-14} cm^2/s. Furthermore, post-mortem analysis using ex-situ XRD and FESEM, confirms the structural integrity of the electrode after extended cycling.



GCD curves for different cycles at C/5 rate

Keywords: Diffusion kinetics, Conductivity, Post-mortem analysis.

References

(1) Gupta, G.; Gupta, R.; Gupta, A.; Kumar, D. Electrochemical Studies and Diffusion Kinetics in the Chevrel Phase (Mo_6S_8) for Rechargeable Mg Batteries. *J. Phys. D: Appl. Phys*. **2024**, 57, 485503-485514.

Influence of Disorder in Titania Oxyhydroxides on High-Rate Sodium ion Storage

Dnyanesh Vernekar,[1] Soumyajit Gupta,[1] Gi-Hyeok Lee,[2] Reshma Devi,[3] Mohamed Ruwaid Rafiuddin,[4] Gopalakrishnan Sai Gautam,[3] Wanli Yang,[2] Srinivasan Ramakrishnan[1*]

[1] Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai-400076, India

[2] Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

[3] Department of Materials, Indian Institute of Science Bengaluru 560012, India

[4] School of Computing and Engineering, University of Huddersfield, Huddersfield, United Kingdom

* sriniramk@iitb.ac.in

Abstract

The inability of graphite to efficiently store Na^+ ions at low potentials necessitates the exploration of alternate materials as viable anodes for Na-ion batteries. The current work primarily focuses on comprehending how material disorder induced via synthesis enhances high-rate sodium ion storage in a series of anatase titania analogs prepared through a sol-gel protocol. The degree of disorder in titanium oxyhydroxide materials is systematically tuned by modulating the post-synthesis annealing temperature.The variable disorder in these class of materials arises from residual Ti^{3+}, nitrogen dopants, and oxygen vacancies, as suggested by several spectroscopic techniues.Electrochemically, we observe a distinct, non-monotonic relation between Na^+ storage capacity and the degree of disorder which is in contrast with the typical size dependence as observed for fully crystalline anatase. The disorder in these titanium oxyhroxides facilitates bulk Na^+ storage modes alongside surface-confined modes, as evidenced by scan-rate-dependent cyclic voltammetry. These findings correlated with first principles simulations, suggesting higher Na^+ occupation sites at moderate disorder levels. In summary, our work aims to understand the role of material disorder in advancing the development of high-rate battery storage systems with a goal to mitigate climate change and promote sustainability .

Keywords : Sodium ion battery, fast charging, sol gel, oxyhydroxides, tunable disorder

References

(1) Wei, Q.; Chang, X.; Butts, D.; DeBlock, R.; Lan, K.; Li, J.; Chao, D.; Peng, D. L.; Dunn, B. Surface-Redox Sodium-Ion Storage in Anatase Titanium Oxide. *Nat. Commun.* **2023**, *14* (1), 1–9.

(2) Li, W.; Fukunishi, M.; Morgan, B. J.; Borkiewicz, O. J.; Chapman, K. W.; Pralong, V.; Maignan, A.; Lebedev, O. I.; Ma, J.; Groult, H.; Komaba, S.; Dambournet, D. A Reversible Phase Transition for Sodium Insertion in Anatase TiO2. *Chem. Mater.* **2017**, *29* (4), 1836–1844.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Improving Mn-Rich NASICON Cathodes via Mo-Doping for Stable and Efficient Sodium-Ion Storage

Madhav Sharma[1], and Rajendra Singh Dhaka[1,*]

[1] *Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India*

* rsdhaka@physics.iitd.ac.in

Abstract

We report the electrochemical performance and diffusion kinetics of a newly designed NASICON-type $Na_{3.3}Mn_{1.2}Ti_{0.75}Mo_{0.05}(PO_4)_3/C$ composite cathode for cost-effective sodium-ion batteries. The undoped $Na_{3.4}Mn_{1.2}Ti_{0.8}(PO_4)_3$ shows secondary phases, indicating phase separation due to high Mn content [Fig. 1(a1)]. In contrast, the Mo-doped composition exhibits a single-phase solid solution [Fig. 1(a2)], suggesting improved structural stability. The Mo-doped sample delivers a higher discharge capacity of 124 mAh/g at 0.1C, compared to 100 mAh/g for the undoped one [Fig. 1(b)]. Mo substitution not only enhances structural integrity but also improves high-rate performance, with a capacity of 99 mAh/g at 2C versus 49 mAh/g for the undoped. Moreover, it demonstrates excellent reversibility and cycling stability, retaining 77% capacity after 300 cycles and 70% after 400 cycles at 2C. Sodium-ion diffusion coefficients, estimated via GITT and CV, range from 10^{-9} to 10^{-11} cm^2/s. Bond-valence site energy (BVSE) mapping indicates a Na^+ migration energy barrier of 0.76 eV. Additionally, distribution of relaxation times (DRT) analysis effectively deconvolutes impedance spectra, identifying solid-state sodium-ion diffusion as a key process with a characteristic relaxation time of ~50 s, consistent with the trend derived from GITT and Warburg-based evaluations across various states of charge.

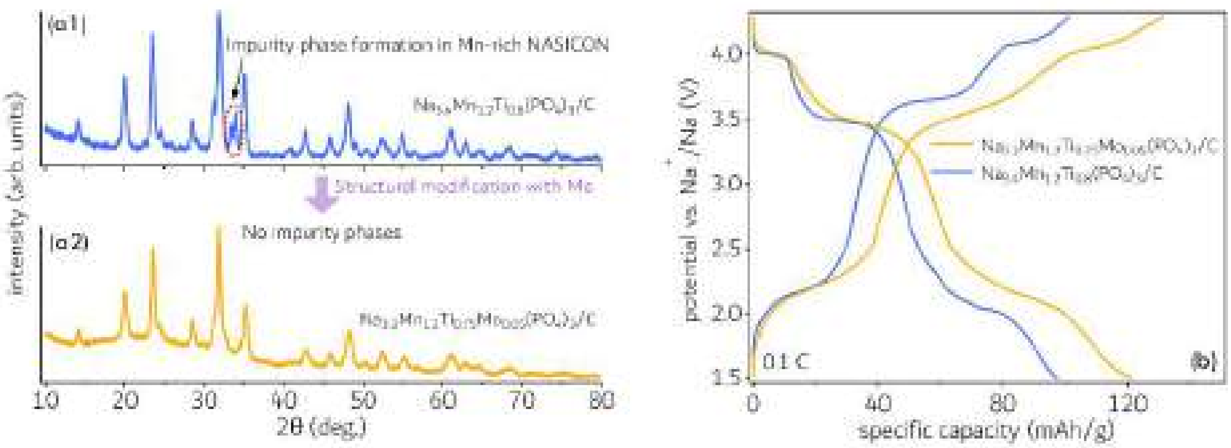


Figure 1 (a1, a2) XRD pattern of $Na_{3.4}Mn_{1.2}Ti_{0.8}(PO_4)_3/C$ and $Na_{3.3}Mn_{1.2}Ti_{0.75}Mo_{0.05}(PO_4)_3/C$ cathode materials. (b) The second cycle of galvanostatic charge discharge at 0.1 C.

Keywords: High Mn-content, Mo-assisted phase stabilization, BVSE mapping, DRT, sodium-ion batteries.

References

(1) Sharma, M.; Dhaka, R. S. Electrochemical Performance and Diffusion Kinetics of a NASICON Type $Na_{3.3}Mn_{1.2}Ti_{0.75}Mo_{0.05}(PO_4)_3/C$ Cathode for Low-Cost Sodium-Ion Batteries. arXiv May 13, 2025. https://doi.org/10.48550/arXiv.2505.10572.

(2) Sharma, M.; Gulati, R.; Dhaka, R. S. Synergistic Role of Transition Metals and Polyanionic Frameworks in Phosphate-Based Cathode Materials for Sodium-Ion Batteries. *Coordination Chemistry Reviews* **2025**, *543*, 216912. https://doi.org/10.1016/j.ccr.2025.216912.

ACEPS-13, January 11-14, 2026, Bengaluru, India

SiO_2-Templated Polyaniline-Derived Nitrogen-Rich Hollow Carbon Nanospheres as a High-Performance Anode for Sodium-Ion Batteries

Kirti Chhabra[1,2], **Gazal Gupta**[3], **Deepak Kumar**[3], **Om P. Khatri**[1,2,*]

[1]*CSIR-Indian Institute of Petroleum, Dehradun 248005, India*

[2]*Academy of Scientific and Innovative Research, Ghaziabad 201002, India*

[3]*Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India*

Email: om.khatri@csir.res.in

Abstract

In light of escalating environmental concerns and energy demand, exploring cleaner and efficient electrochemical energy conversion technologies is run of the mill. The shift from non-renewable to renewable sources minimizes greenhouse gas emissions and promotes resource sustainability.[1–3] Lithium-ion batteries (LIBs) have gained a significant market for energy storage devices in pursuit of cleaner energy drives. However, the limited lithium reserves paved the way for the era of sodium-ion batteries (SIBs), which is attributed to the similar electrochemistry of sodium.[3] The carbon-based materials of controlled textural and structural features have been used as anode materials for SIBs. The low initial coulombic efficiency (ICE) and poor rate capability have been the major issues with SIBs.

Polyaniline (PANI) has been a promising precursor for synthesizing nitrogen-rich carbon materials for various applications.[4] Herein, we synthesized the mesoporous nitrogen-rich interconnected carbon nanospheres by thermal activation of SiO_2-templated polyaniline (PANI) at different temperatures, i.e., 800, 1000, and 1200°C under an inert atmosphere. The average interlayer spacing (d_{002}) for N-rich carbon is estimated between 0.38 and 0.40 nm, ideal for the intercalation/deintercalation of Na^+ ions. The porous hollow nanospherical structure facilitates utilizing multiple active adsorption sites and a capacitive-dominated Na+ storage. Furthermore, the high micropore volume (0.11 cm^3/g) promotes the Na^+ insertion into micropores and improves the charge storage capabilities through enhanced transportation and kinetics. A discharge capacity of 174 mAh/g is obtained for the N-rich carbon after the SEI formation cycling. Moreover, ~100% coulombic efficiency is obtained when the cell attains its reversibility. The pseudocapacitive mechanism of SIBs will be discussed during the presentation.

Keywords: Nitrogen-rich carbon, Polyaniline, Sodium-ion batteries, Anode materials, Electrochemical performance

References

(1) Dahbi, M.; Kiso, M.; Kubota, K.; Horiba, T.; Chafik, T.; Hida, K.; Matsuyama, T.; Komaba, S. Synthesis of Hard Carbon from Argan Shells for Na-Ion Batteries. *J. Mater. Chem. A* **2017**, *5* (20), 9917–9928. https://doi.org/10.1039/C7TA01394A.

(2) Nita, C.; Zhang, B.; Dentzer, J.; Ghimbeu, C. M. Hard Carbon Derived from Coconut Shells, Walnut Shells, and Corn Silk Biomass Waste Exhibiting High Capacity for Na-Ion Batteries. *Journal of Energy Chemistry* **2021**, *58*, 207–218. https://doi.org/10.1016/j.jechem.2020.08.065.

(3) Zhang, M.; Li, Y.; Wu, F.; Bai, Y.; Wu, C. Boost Sodium-Ion Batteries to Commercialization: Strategies to Enhance Initial Coulombic Efficiency of Hard Carbon Anode. *Nano Energy* **2021**, *82*, 105738. https://doi.org/10.1016/j.nanoen.2020.105738.

(4) Wang, H.; Lin, J.; Shen, Z. X. Polyaniline (PANi) Based Electrode Materials for Energy Storage and Conversion. *Journal of Science: Advanced Materials and Devices* **2016**, *1* (3), 225–255. https://doi.org/10.1016/j.jsamd.2016.08.001.

Functional Interface Engineering of MOF-Modified Separators for High-Energy Lithium–Sulfur Batteries

Anwar Hussain[1] , Rahul R. Salunkhe[1]*

[1]Material Research Laboratory, Department of Physics, Indian Institute of Technology Jammu, NH-44, Jammu, J&K, India, 181221.

* rahul.salunkhe@iitjammu.ac.in

Abstract

Lithium-sulfur (Li-S) batteries are promising for future energy storage due to their high energy density, low cost, and sulfur abundance. However, challenges like the shuttle effect caused by the dissolution and migration of polysulfides (Li_2S_8–Li_2S_6) impede their commercialization. To tackle these issues, separator modification has emerged as an effective strategy. Metal-organic frameworks (MOFs), such as the thermally stable Zr-based UiO-66, can immobilize lithium polysulfides through strong chemical interactions, reducing the shuttle effect. UiO-66 has been functionalized with $-NO_2$ (electron-withdrawing) and $-NH_2$ (electron-donating) groups and coated onto a polypropylene separator. The $-NH_2$ group enhances interactions with polysulfides, while the $-NO_2$ group increases the framework's polarity, promoting better electrostatic interactions. The Li-S battery with this modified separator shows impressive performance, achieving a capacity of 1398 mAh g^{-1} and 1226 mAh g^{-1} at 0.1 C under lean electrolyte conditions. It also maintains a specific capacity of 736 mAh g^{-1} over 350 cycles at a 1 C rate.

Keywords: Lithium sulfide, metal-organic framework, separator, polysulfides

References

(1) Li, S.; Lin, J.; Ding, Y.; Xu, P.; Guo, X.; Xiong, W.; Wu, D.-Y.; Dong, Q.; Chen, J.; Zhang, L. Defects Engineering of Lightweight Metal–Organic Frameworks-Based Electrocatalytic Membrane for High-Loading Lithium–Sulfur Batteries. ACS Nano 2021, 15 (8), 13803–13813. https://doi.org/10.1021/acsnano.1c05585.

(2) Zhou, Y.; Chen, J.; Sun, J.; Zhao, T. Engineering the D-Orbital Energy of Metal–Organic Frameworks-Based Solid-State Electrolytes for Lithium–Metal Batteries. Nano Lett. 2024, 24 (6), 2033–2040. https://doi.org/10.1021/acs.nanolett.3c04654.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Engineering $MnCo_2O_4$ for Dual-Functionality: Oxygen Evolution Catalysis and Application in Primary Aluminum–Air Batteries

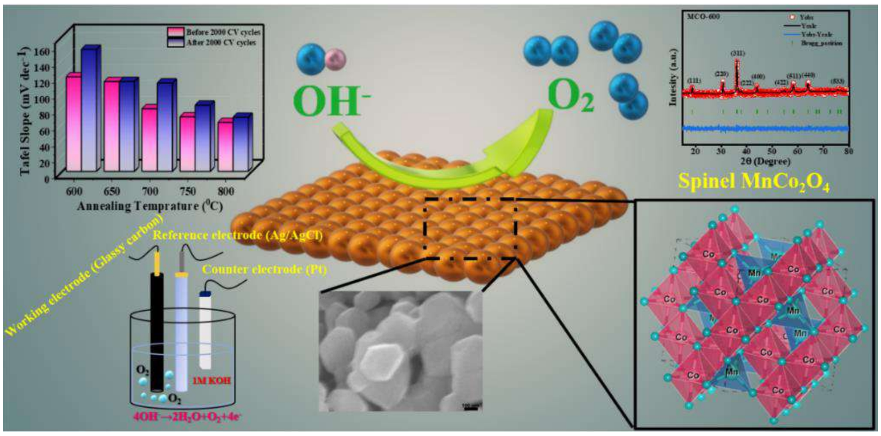
Shraddha M. Rajore[1], Parasharam M. Shirage*[1]

[1] *Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Simrol-453552. India.*

*Corresponding author: pmshirage@iiti.ac.in; paras.shirage@gmail.com

A detailed investigation was conducted to understand the effect of calcination temperature on the structure-property-performance relationship of $MnCo_2O_4$ (MCO) electrocatalysts for oxygen evolution reaction (OER) and aluminum-air battery (AAB) applications[1]. Thermal treatment significantly influenced the crystallinity, surface morphology, particle size, and electronic structure of MCO. The sample calcined at 700 °C (MCO-700) exhibited optimal structural features, retaining its spinel phase while showing enhanced electrochemical performance. It demonstrated excellent OER durability, with only a 7 mV increase in overpotential after 2000 cyclic voltammetry cycles, and maintained stable current during 20 hr of chronoamperometric testing. Additionally, MCO-700 exhibited superior bifunctional behavior, showing high oxygen reduction reaction (ORR) activity with minimal shifts in onset and half-wave potentials after extended cycling. When used as an air cathode in primary AABs, MCO-700 enabled a stable discharge voltage and high rate capability, even under elevated current densities. These findings highlight the pivotal role of calcination temperature in tailoring the physicochemical properties of spinel oxides and demonstrate the potential of MCO-700 as a robust bifunctional electrocatalyst for advanced energy storage and conversion technologies.

$MnCo_2O_4$; Effect of calcination; Oxygen Evaluation Reaction; Oxygen Reduction Reaction; Aluminum-air batteries.



Spinel-structured $MnCo_2O_4$ as a highly efficient and stable bifunctional electrocatalyst for the oxygen evolution and reduction reactions and its application in aluminum-air systems.

References: (1) S.M.Rajore, P. M. Shirage, *et al.* Journal of Poewer Sources, 616, 2024, 235101, 0378-7753.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Synergistic Effects of Halloysite Nanotubes in Electrospun PVDF-HFP Separator for advanced Sodium-Ion Battery

Akash Kankane[1], Dhirendra Kumar Rai[2], *S Janakiraman[1]

[1]Department of Mechanical Engineering, Indian Institute of Technology Indore, INDIA

[2]Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, INDIA

*janakiramans@iiti.ac.in

Abstract

Sodium-ion batteries (SIBs) are emerging as a sustainable option for energy storage, standing out as a cost-effective and resource-abundant substitute to lithium-ion batteries (LIBs). However, the development of sustainable SIBs necessitates the innovation of separator materials capable of enhancing battery efficiency and safety. This research highlights the fabrication and characterization of a novel separator made up of polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) filled with halloysite nanotubes (HNTs) via the electrospinning technique for SIBs application. The electrospun composite separator was systematically fabricated and comprehensively characterized to investigate its morphological, electrochemical, mechanical and thermal properties. Field emission scanning electron microscopy (FESEM) analysis revealed a well-dispersed HNTs network within the PVDF-HFP matrix, resulting in a fibrous structure with enhanced mechanical strength (23.6 MPa). Electrochemical performance was evaluated through electrochemical impedance spectroscopy (EIS) and galvanostatic charge-discharge (GCD) cycling. The halloysite filled PVDF-HFP separator demonstrated higher ion conductivity (2.11 mS cm-1) and electrochemical stability at ambient temperature, leading to enhanced battery performance, including higher specific capacity (171 mA h g-1) at 0.1 C-rate. Thermal stability studies confirmed the improved thermal resistance of the composite separator, crucial for maintaining structural integrity under high temperatures. The incorporation of HNTs into the structure of PVDF-HFP contribute to the development of robust and efficient separators for SIBs, facilitating the development of sustainable and scalable energy storage technologies.

Keywords: Polymer, Electrospinning, Halloysite, Composite separator, Sodium Ion Battery

ACEPS-13, January 11-14, 2026, Bengaluru, India

Entropy-Engineered Cobalt-Free Cathodes for Ultra-Durable Sodium-Ion Batteries

Kavya Prakash Agrim[1], Prakash Kumar Pathak[1], Rahul R. Salunkhe[1,*],

[1] *Materials Research Laboratory, Department of Physics, Indian Institute of Technology Jammu, NH-44, Jammu 181221, Jammu and Kashmir, India*

* rahul.salunkhe@iitjammu.ac.in

Abstract

Prussian blue analogue (PBA) has emerged as a potential candidate for SIB cathodes due to its numerous advantages, such as low cost, easy synthesis, and an open framework with sufficiently large three-dimensional pathways to facilitate a highly reversible de/intercalation of ions.[1] However, with all these benefits, PBA suffers from poor cycling and rate performance, which is mainly caused by $[Fe\ (CN)6]^{4-}$ vacancies and coordinated water coming while synthesis, the structural collapse while charging and discharging. Different attempts have been made to overcome the issues, such as modifications in synthesis techniques, such as the utilization of surfactants and chelating agents, structural control, composite material construction, metal substitution, etc. Recently, the high-entropy approach has gained attention in energy storage, where one element is replaced by five or more in equal ratios to increase configurational entropy and stabilize the crystal structure.[2] In our work, we have utilised the high entropy approach and synthesised the PBA by replacing Fe in its structure with five equimolar elements, named as HE-PBA, in a controlled inert atmosphere to reduce the coordinating water and vacancies in the structure. The HE-PBA cathode demonstrated excellent electrochemical performance, benefiting from the structural stabilization due to the increased entropy, cocktail effect of multiple elements, and low water content in the structure. The cell demonstrated an ultralong cycling life of 5,000 cycles with 75% capacity retention at 10C and 76% retention after 1,500 cycles at 1C rate.

Keywords: High entropy, Prussian blue analogue, Sodium-ion battery, Cathode

References

(1) Yi, H.; Qin, R.; Ding, S.; Wang, Y.; Li, S.; Zhao, Q.; Pan, F. Structure and Properties of Prussian Blue Analogues in Energy Storage and Conversion Applications. *Adv. Funct. Mater.* **2021**, *31* (6). https://doi.org/10.1002/adfm.202006970.

(2) Ma, Y.; Ma, Y.; Dreyer, S. L.; Wang, Q.; Wang, K.; Goonetilleke, D.; Omar, A.; Mikhailova, D.; Hahn, H.; Breitung, B.; Brezesinski, T. High-Entropy Metal–Organic Frameworks for Highly Reversible Sodium Storage. *Adv. Mater.* **2021**, *33* (34). https://doi.org/10.1002/adma.202101342.

ACEPS-13, January 11-14, 2026, Bengaluru, India

In-Situ Amino-Aldehyde Condensation Derived Nitrogen-Doped Hard Carbon from Bagasse for High-Performance Sodium-Ion Batteries

Nagmani[1,2*], Priyanka Pal[2] and Raju Kumar Gupta[1,2,3,4,5*]

[1] *Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, 208016, Uttar Pradesh, India*

[2] *Department of Sustainable Energy Engineering, Indian Institute of Technology Kanpur, Kanpur, 208016, Uttar Pradesh, India*

[3]*Chandrakanta Kesavan Centre for Energy Policy and Climate Solutions, Indian Institute of Technology Kanpur, Kanpur, 208016, India*

[4]*Kotak School of Sustainability, Indian Institute of Technology Kanpur, Kanpur, 208016, India*

[5]*Center for Environmental Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, 208016, India*

* nagmani@iitk.ac.in, guptark@iitk.ac.in

Abstract

Hard carbon materials have emerged as promising anodes for sodium-ion batteries (SIBs), owing to their low cost, structural tunability, and compatibility with sodium storage mechanisms. This study presents a novel synthetic strategy for producing nitrogen-doped hard carbon derived from sugarcane bagasse via an *in-situ* amino-aldehyde condensation reaction, employing a facile polymerization and carbonization route.

The *in-situ* condensation reaction between amino and aldehyde precursors leads to the formation of a robust polymeric network that, upon controlled pyrolysis, transforms into a porous hard carbon matrix rich in closed pores. These closed pores play a critical role in facilitating sodium ion adsorption and reversible intercalation while simultaneously limiting electrolyte penetration, thereby stabilizing the solid electrolyte interphase (SEI) and reducing irreversible capacity loss. Moreover, the in-situ nitrogen doping, primarily in the form of pyridinic and pyrrolic species, enhances the electronic conductivity and provides additional active sites for sodium storage.

Electrochemical evaluation reveals that the nitrogen-doped hard carbon delivers a high reversible capacity exceeding 372 mAh/g with an improved initial Coulombic efficiency (ICE) of over 75%, outperforming conventional hard carbon counterparts. The optimized material also exhibits excellent rate performance (232 mAh/g at 1C) and excellent cycling stability, attributable to the synergistic effects of pore structure regulation and heteroatom doping. This work not only introduces a cost-effective and scalable route for synthesizing high-performance hard carbon anodes but also provides insights into the structure–performance relationship in sodium storage systems, paving the way for the practical implementation of SIBs in large-scale energy storage applications.

Keywords: Sodium-ion batteries, Hard carbon, Amino-aldehyde condensation, Engineered pores

ACEPS-13, January 11-14, 2026, Bengaluru, India

Iron-based Prussian White material for sodium ion batteries: navigating its intrinsic material properties for improved electrochemical performance

Nirmal Shreyam[1], Priyanka Gupta[1], Suddhasatwa Basu[1*]

[1] *Department of Chemical Engineering, IIT-Delhi, India*

* E-mail: sbasu@chemical.iitd.ac.in

Abstract

A sustainable electrochemical energy storage solution with the help of sodium chemistry, owing to its abundance, is integral to our efforts towards a climate-conscious future. As such, the development of positive electrode materials for sodium-ion batteries (SIB) is crucial. These need to be sustainable, economical and their production scalable. Regarding this, Prussian blue or cyanometallate materials have garnered significant attention.

In this work, we show that Sodium Iron(II) hexacyanoferrate, or Prussian White (PW) with a theoretical charge capacity of 170.8 mAh/g and average working voltage of 3.1 V vs. Na^+/Na, large interstitial space and high sodium content (Na:Fe ratio ≥1) possess multiple advantages as a battery material for SIB, However, despite much published literature on this, some technical challenges persist. Hence, understanding the factors behind its electrochemical performance is key, i.e., synthesis conditions, particle morphology, type and form of H_2O content, vacancies, and sodium content. This requires a robust understanding to be developed to proceed towards effective electrode fabrication, and to extract its lucrative electrochemical performance. Specifically, development of synthesis to cell fabrication protocols.

In this work, we have attempted to develop an understanding to address these key material challenges through (SEM-EDS, HR-XRD, FTIR, and Raman) for an improved electrochemical performance. Development of PW as an effective positive electrode material has been explored through material synthesis advancement and a higher electrode loading (~10mg/cm^2) approach.

Keywords: Energy storage, sodium ion battery, positive electrode material, Prussian blue. Iron-based electrodes

References

(1) Sada, K.; Greene, S. M.; Kmiec, S.; Siegel, D. J.; Arumugam Manthiram. Unveiling the Influence of Water Molecules on the Structural Dynamics of Prussian Blue Analogues. *Small* **2024**. https://doi.org/10.1002/smll.202406853

(2) Brant, W. O.; Mogensen, R.; Colbin, S.; Ojwang, D. O.; Schmid, S.; Lennart Häggström; Ericsson, T.; Jaworski, A.; Pell, A. J.; Reza Younesi. Selective Control of Composition in Prussian White for Enhanced Material Properties. **2019**, *31* (18), 7203–7211. https://doi.org/10.1021/acs.chemmater.9b01494

ACEPS-13, January 11-14, 2026, Bengaluru, India

A Facile Pre-sodiation Strategy Enabling First-Charge Capability of Organic Cathode for Sodium-ion Batteries.

Keerthivasan Pulia Venkatachalapathy, Shantikumar Nair, Dhamodaran Santhanagopalan*

Nano Energy Division, Amrita School of Nanoscience and Molecualar Medicine, Amrtita Vishwa Vidyapeetham, Kochi, 682041, India.

* Corresponding author's email address – dsgopalan20710@aims.amrita.edu.

Abstract

Organic Sodium-ion Batteries (OSIBs) are the emerging energy storage systems focused as sustainable technologies. Variety of organic electrodes with diverse storage mechanism have been exploited recently. Out of which, n-type organic cathode materials have been largely focused owing from its redox-based reversible sodium storage and high theoretical capacity based on number of active functional groups present in an organic molecule. Despite, most of the n-type organic cathode is electrochemically sodiated in initial discharge due to absence of retrievable sodium-ions at initial charging[1]. This will limit in fabricating full-cell sodium-ion batteries since no sodium source present at cathode side. Tetrahydroxy-1,4-benzoquinone disodium salt (TBQ)[2] as a moderate voltage n-type organic cathode. Herein, we demonstrate a facile chemical presodiation strategy using sodium biphenyl solution on TBQ electrodes, fabricate half-cells and charge first. The pristine TBQ does not provides any initial charge capacity contribution, whereas, the sodium biphenyl-based chemically presodiated TBQ delivered a initial charging capacity of 145 mAh g^{-1} at 25 mA g^{-1} and a good rate capability. The redox behavior and mechanism was thoroughly analysed by electrochemical studies, ex-situ FT-IR and ex-situ XPS reveals that the instant sodiation at carbonyl (-C=O-) functional group in TBQ structure and direct phase transition. This study demonstrates a viable approach to enable the first charge capability in n-type cathode for organic sodium-ion batteries.

Keywords: Organic Sodium-ion Batteries (OSIBs), n-type cathode, Chemical presodiation, First-charge capability.

References

(1) Lee, M.; Hong, J.; Lopez, J.; Sun, Y.; Feng, D.; Lim, K.; Chueh, W. C.; Toney, M. F.; Cui, Y.; Bao, Z. High-Performance Sodium-Organic Battery by Realizing Four-Sodium Storage in Disodium Rhodizonate. *Nat. Energy* **2017**, *2* (11), 861–868. https://doi.org/10.1038/s41560-017-0014-y.

(2) Huang, J.; Li, S.; Kim, E. Y.; Cheng, L.; Xu, G.-L.; Amine, K.; Wang, C.; Luo, C. A Self-Healing Chemistry-Enabled Organic Cathode for Sustainable and Stable Sodium-Ion Batteries. *Small Struct.* **2023**, *4* (12), 2300211. https://doi.org/10.1002/sstr.202300211.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Unveiling the Crosstalk Effect of Ni Single-Atom Catalysts in Li–S Batteries: NiPc vs. Ni–NC SACs

Ashok vallal Saravanan[1,2], Keseven Lakshmanan[1], Wei-Nien Su [1,*], Chun-Chen Yang [2,*], Bing Joe Hwang [1,3,*]

[1] *Sustainable Electrochemical Energy Development Center, National Taiwan University of Science and Technology, Taipei City 106, Taiwan*

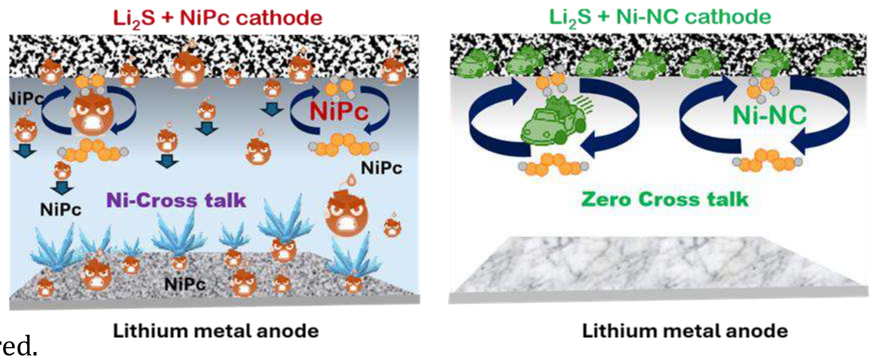
[2] *Battery Research Center of Green Energy, Ming Chi University of Technology, New Taipei City, 24301, Taiwan*

[3] *National Synchrotron Radiation Research Center (NSRRC), Hsinchu, 30076, Taiwan*

* Wei-Nien Su, wsu@mail.ntust.edu.tw, Chun-Chen Yang, ccyang@mail.mcut.edu.tw, Bing Joe Hwang, bjh@mail.ntust.edu.tw

Abstract

Lithium-sulfur (Li-S) batteries are among the most promising candidates for high energy density storage systems; however, their commercialization is hindered by sluggish redox kinetics and the polysulfide shuttling effect.[1] To address these challenges, single-atom catalysts (SACs) have emerged as effective electrocatalysts for promoting polysulfide conversion and enhancing sulfur utilization. Nevertheless, their structural stability remains underexplored.



Herein, we report the first comprehensive study of the catalyst crosstalk effect in lithium-sulfur batteries, focusing on the degradation of nickel phthalocyanine (NiPc) SAC during electrochemical cycling. To overcome this limitation, NiPc is thermally anchored onto pyridinic nitrogen-rich doped carbon (Ni–NC) SAC, forming atomically dispersed and electrochemically stable Ni–N_4 active sites. The Ni–NC catalyst exhibits superior catalytic activity for polysulfide redox reactions, mitigates catalyst poisoning, and suppresses catalyst crosstalk. Compared to molecular NiPc, the Ni–NC carbon-supported nanostructured catalyst delivers enhanced reaction kinetics and significantly improves the electrochemical performance of Li–S batteries.

Keywords: Single-atom catalyst; Crosstalk effect; Solubility of catalyst; Polysulfides shuttling; Electrolyte contamination

References

(1) Weret, M. A.; Jiang, S.-K.; Shitaw, K. N.; Chang, C.-Y.; Tekaligne, T. M.; Chiou, J.-C.; Yang, S.-C.; Temesgen, N. T.; Nikodimos, Y.; Wu, S.-H. Reviving Inactive Lithium and Stabilizing Lithium Deposition for Improving the Performance of Anode-Free Lithium–Sulfur Batteries. *ACS Energy Letters* **2023**, *8* (6), 2817-2823.

Role of Template-free monodisperse carbon sphere on the electrochemical performance of Li-S batteries

Debayan Chatterjee[1], Subhasish Basu Majumder [2]

[1] *Affication-1, Materials science centre, Indian Institute of Technology, Kharagpur*

[2] *Affication-2, Materials science centre, Indian Institute of Technology, Kharagpur*

* Corresponding author's email address: - subhasish@matsc.iitkgp.ac.in

Lithium-sulfur cells are receiving significant attention as alternative power source for zero-emission vehicles, unmanned aerial vehicles and advanced electronic devices due to high theoretical capacity (1675 mAh/g), high gravimetric energy density (2600 Wh/Kg), low cost and low environmental impact(1). However, the insulating nature of sulfur and the migration of soluble polysulfides during the cycling process limits their practical application. Additionally, the volume change (~80%) of active sulfur molecules during charge-discharge cycle further adds to woes, leading to pulverization of electrode upon prolonged cycling. Although plethora of efforts has been devoted to mitigate these drawbacks, most of them involves usage of carbon host prepared from expensive precursors or involves intricate processing techniques with treatment of sulfur particles by expensive conducting polymer materials (i.e., PEDOT, PSS etc.)(2). Keeping all this points in consideration we are proposing an efficient, cost-effective measure to prepare CTAB (a cationic surfactant)-assisted submicrometer-sized sulfur-carbon composite. This carbon is prepared using emulsion polymerization and carbonization-activation process. The as synthesized sulfur@carbon composite was in-situ grown via wet-chemical synthesis. Here the composite powder is prepared via a more facile hand-mixing process, potentially making the melt impregnation process redundant. This makes the process more energy efficient. The S-C composite was mixed with a zwitterionic aqueous binder to form a slurry. This slurry is coated on an aluminium foil to prepare the electrode. Here the role of CTAB is dual functional. On one side it helps to modify the morphology of sulfur which have hollow spherical structure in order to buffer the volume change and on another side the polar ionic tale of CTAB helps to physically confine the polysulfides (Li_2S_n, $4 \le n \le 8$) which improves the cyclability, rate performance, above all helps to extinguish the polysulfide shuttle effect. Additionally, polysulfides can also be physically anchored at the pores of carbon host which further Here we have used a sulfur cathode with a sulfur content of ~70% with electrolyte to sulfur ratio ~10-12 µl/mg which could deliver a specific capacity ~1000 mAh/g with a capacity fading of ~75% after 200 cycles at 0.5C. This effort could be seen a potential step forward towards practical Li-S batteries with facile synthesis process using low-cost, easily available ingredients and keeping all other essential parameters (high sulfur loading, low E/S ratio etc.) under consideration.

Keywords: - sulfur, Li-S battery, S/C composite, E/S ratio, porous carbon

(1) Bruce, P. G.; Freunberger, S. A.; Hardwick, L. J.; Tarascon, J.-M. Li-O2 and Li-S Batteries with High Energy Storage. *Nat. Mater.* **2011**, *11* (1), 19–29. https://doi.org/10.1038/nmat3191.

(2) Anilkumar, K. M.; Jinisha, B.; Manoj, M.; Pradeep, V. S.; Jayalekshmi, S. Layered Sulfur/PEDOT:PSS Nano Composite Electrodes for Lithium Sulfur Cell Applications. Appl. Surf. Sci. 2018, 442, 556–564. https://doi.org/10.1016/j.apsusc.2018.02.178.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Powering India's EV Mission: A Cobalt-Free, High-Voltage (~5 V) Lithium Manganese Oxysulfide Cathode

Swarnima Mukherjee and Mir Wasim Raja*

Energy Materials and Devices Division (EMDD)
CSIR-Central Glass & Ceramic Research Institute
196 Raja S C Mullick Road, Kolkata 700032, West Bengal
Corresponding author Email: mwraja@cgcri.res.in/mwraja.cgcri@csir.res.in

India is strongly motivated to develop cobalt-free lithium-ion battery cathodes due to concerns about supply chain security, cost, and environmental impact [1]. Lithium Manganese Oxide (LMO) emerges as a promising alternative, offering advantages like abundant raw materials, lower cost, good safety, and high power capability. However, LMO faces significant challenges including structural instability with considerable volume changes, rapid capacity and voltage degradation, manganese dissolution, and poor long-term cycling stability [2]. To overcome these limitations, researchers are actively pursuing strategies such as cationic doping (e.g., with Ni, Co, Cr), surface coating (e.g., with Al_2O_3, TiO_2), and advanced synthesis methods. Recent research highlights anionic doping as a particularly effective approach to mitigate the problematic Jahn-Teller distortion in LMO, thereby enhances its structural stability, cycling performance, and overall lifespan by improving electronic structure, strengthening bonds, and reducing manganese dissolution [3].

Here we explored the "dual therapy" approach of simultaneously doping manganese (Mn) sites with nickel (Ni) and oxygen (O) sites with sulfur (S^{2-}) in spinel $LiMn_2O_4$ cathodes to improve their performance. The synthesis of $LiNi_xMn_{2-x}O_{4-\delta}S_\delta$ (x=0.4, δ=0.1-0.4) was carried out via a soft chemical combustion method. X-Ray diffractogram showed characteristic peaks of spinel with slight shifts as sulfur content increased. FESEM micrographs revealed well-defined octahedral particles with exposed, thermodynamically stable [111] crystallographic facets. Such facets are less prone to manganese dissolution and contribute to enhanced structural stability, improved lithium-ion diffusion, and reduced polarization. The uniform octahedral shapes also minimize reactive sites where Mn^{3+} disproportionation occurs. XPS study confirmed sulfur doping through S2p doublets at 168.9 eV and 170.08 eV indicating sulfur substitution and formation of M-O-S bond, consequently a change in stable oxygen environment. Cyclic voltammetry indicated a high voltage peak attributed to the Ni^{3+}/Ni^{4+} redox couple at 4.7 V/4.6 V. Fabricated 2032 coin cells using these oxysulfide cathodes delivered significantly higher capacities of 160-170 mAh/g, a substantial improvement over pure spinel (80-100 mAh/g). Further detailed cell data will be presented at the conference.

Keywords: Lithium Manganese Oxide, Cobalt-free Lithium Batteries, JT distortion, Octahedral geometry, Phase Stability

Reference:

[1] Report on R&D Plan for technology Platform on Electric Mobility: Prepared by TIFAC, DST; https://www.tifac.org.in/images/pdf/pub/Electric%20Mobility%20Report.pdf
[2] Z. I. Radzi [a], K. H. Arifin [b c], M. Z. Kufian [d], V. Balakrishnan [a], S. R. S. Raihan [a], N. Abd Rahim [a], R. Subramaniam, Journal of Electroanalytical Chemistry, 2022 (920) 116623; doi.org/10.1016/j.jelechem.2022.116623
[3] U. Pal, B. Roy, M.Hasanpoor, H. Ilbeygi, T. Mendes, R. Kerr, L. Vazhapully, C. Song, D. Wang, M. Boot-Handford, M. G. Sceats, M. Forsyth, D. Al-Masri, P. C. Howlett, Batteriers & Supercaps, 2024 (Vol.7, Iss.6) e202400072;doi.org/10.1002/batt.202400072

ACEPS-13, January 11-14, 2026, Bengaluru, India

Transition Metal Fluorides as an efficient cathode material for Room Temperature working Fluoride ion batteries (FIBs)

Sumol V Gopinadh[1,2*], Peddinti VRL Phanendra[1], Bibin John[1], Mercy TD[1]

[1]*Energy Systems Development Division (ESDD), Vikram Sarabhai Space Centre (VSSC/ISRO), Thiruvananthapuram, Kerala, India*

[2]*Faculty of Science, Cochin University of Science and Technology (CUSAT), Cochin, Kerala, India*

* sumolvg@gmail.com / sumol_vg@vssc.gov.in

Abstract

Fluoride ion batteries (FIBs) are a promising post-lithium-ion battery technology that utilizes fluoride ions (F^-) for charge transfer, offering potential advantages in energy density, cost, and safety. Unlike lithium-ion batteries, FIBs rely on the movement of fluoride ions between electrodes, enabling higher theoretical energy densities and potentially lower manufacturing costs due to the abundance of fluorine resources [1]. Among various transition metal fluorides, FeF_3 is a promising candidate for the cathode material of fluoride batteries because of its high specific capacity. In this report, the reversibility of FeF_3 cathode is investigated in conjunction with KF and CeF_3 based liquid electrolyte and lithium metal as the counter-electrode material. For the first time, the discharge–charge performance of a fluoride battery using FeF_3 cathode in liquid electrolyte is investigated. The cell showed a stabilised discharge capacity of greater than 200 mAh g^{-1} for 100 cycles and discharge midvoltage of 1.5 V. The reversible conversion reaction mechanism of FeF_3 with its reversible morphological changes was clarified by X-ray diffraction (XRD) and scanning electron microscopy (SEM). In addition, the above observations were further confirmed by Electrochemical Impedance Spectroscopy (EIS) studies of the cell in the discharged and charged state. The results of our findings will pave the way for development of room temperature working Fluoride ion batteries.

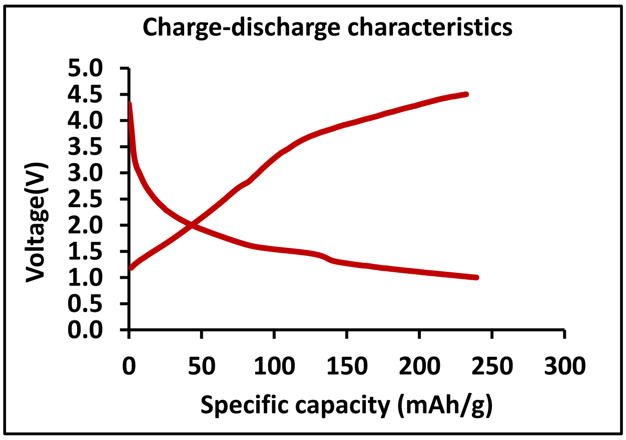


Figure 1: Electrochemical performance of Room temperature working Fluoride ion cell using FeF_3 cathode in liquid electrolyte

Keywords: Fluoride ion batteries, Transition metal cathode, electrolyte, Cycle life

References

[1] Zou, P.; Wang, C.; He, Y.; Xin, H. L.; Lin, R. A water-in-salt electrolyte for room-temperature fluoride-ion batteries based on a hydrophobic-hydrophilic salt. *Nano Lett.* **2024**, 24, 5429–5435.

ACEPS-13, January 11-14, 2026, Bengaluru, India

TiO2 coated silicon nanoparticles: A strategy to boost graphite anode performance in lithium-ion batteries

Rudraksh Chander Gupta[1,*], Gazal Gupta[1], Deepak Kumar[1], Husain Kanchwala[1]

[1] *Centre for Automotive Research and Tribology (CART), Indian Institute of Technology, Hauz Khas, New Delhi, India 110016*

* rudrakshgupta07@gmail.com

Abstract

This work investigates a high-performance lithium-ion full cell (CR2032) composed of anode of graphite blended with TiO_2 coated Si nanoparticles (Si@TiO_2) and commercially used $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA). The use of highly abundant silicon, known for its exceptionally high theoretical capacity of ~3579 $mAh^{-1}g$, significantly boosts the overall energy density. Detailed characterizations were carried out to validate the elemental composition and the structural integrity of the in-house synthesized Gr/Si@TiO_2. Transmission electron microscopy (TEM) and field emission scanning electron microscopy (FESEM) confirmed the formation of a well-defined Si@TiO_2 core-shell structure while elemental mapping validated the uniform TiO_2 coating on silicon nanoparticles. The electrode architecture incorporated optimized thin layers (cathode: ~50 μm, anode: 23 μm) along with suitable mass loadings (cathode: 3.04 $mg.cm^2$, anode: 1.80 $mg.cm^2$), promoting effective lithium-ion transport and ensuring structural integrity. Although NCA cathodes deliver a practical and stable capacity of ~200 $mAh^{-1}g$, the pairing with Gr/Si@TiO_2 anodes enables a more effective lithiation/delithiation mechanism. The full cell achieved a specific capacity of 100 $mAh^{-1}g$ at a 5C rate with a capacity retention rate of about 90% of its initial value over 200 charge/discharge cycles. The findings support the viability of Gr/Si@TiO_2-NCA configuration for real world applications demanding high energy density without sacrificing cycle life. This study highlights the practical potential of silicon-based anodes and lays the foundation for future advancements involving silicon content optimization and innovative electrolyte systems to improve electrochemical stability and cycle performance.

Keywords: Core-shell nanoparticles, Gr/Si@TiO_2 composite, NCA cathode, energy density

References

(1) Vats, B.N.; Kumar, A.; Singh, R. *J. Electrochem. Soc.* 2024, *171,* 010523.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Synergistic P and K Co-Engineering in MnO_2 Spheres: A New Horizon for Durable High-Rate Zinc-Ion Battery Cathodes

Sudhakaran M.S.P[1], Arya Chandran[1], Dibyasha Panda[1], Manorajan Behera[1,2], Saravanakumar Balasubaramaniam[1*]

[1] Materials Development Group, School for Advanced Research in Petrochemicals (SARP) – Laboratory for Advanced Research in Polymeric Materials (LARPM), Central Institute of Petrochemicals Engineering & Technology (CIPET), Bhubaneswar-751024, Odisha, India

[2] Department of Physics, Ravenshaw University, Cuttack, Odisha-753003, India

*Corresponding author's email: kumar@cipet.gov.in; kumar@larpm.in

Abstract

Zinc-ion batteries promise safe, low-cost, large-scale energy storage but are plagued by tunnel collapse, manganese dissolution, and sluggish kinetics in MnO_2 cathodes.[1] Here, we report a series of phosphorus-doped, potassium-stabilized tunnel MnO_2 (P-K@MnO_2) materials synthesized by tuning the K-MnO_2/P precursor ratio from 1:0.5 to 1:2, harnessing the synergistic benefits of P and K co-modification. In the optimal sample, the introduction of P forms strong P–O bonds that fortify and subtly expand the one-dimensional MnO_2 tunnels, while intercalated K^+ ions act as pillars to lock in the widened channels.[2] This dual modification not only lowers Zn^{2+} diffusion barriers by stabilizing and enlarging the tunnels, introduces lattice vacancies and defect states to enhance ionic and electronic conductivity, and suppresses Mn dissolution via a reinforced P–O network and buffered overpotentials. As a result, the optimal P-K@MnO_2 electrode delivers remarkable capacity at 0.1 C, which is 2 fold times higher than undoped K@MnO_2 and retains outstanding cyclic stability with excellent Coulombic efficiency (~99%) . By forging a robust, fast-charging tunnel architecture through tailored P + K co-doping, this work charts a scalable pathway toward high-capacity, durable aqueous ZIBs.

Keywords : Zinc-ion batteries (ZIBs), Phosphorus-doped MnO_2, Potassium intercalation, Monodispersed spherical morphology, Chemical vapor deposition

References

(1) Zhang, N.; Ji, Y.-R.; Wang, J.-C.; Wang, P.-F.; Zhu, Y.-R.; Yi, T.-F. Understanding of the Charge Storage Mechanism of MnO2-Based Aqueous Zinc-Ion Batteries: Reaction Processes and Regulation Strategies. *J. Energy Chem.* **2023**, *82*, 423–463. https://doi.org/https://doi.org/10.1016/j.jechem.2023.03.052.

(2) Li, T.; Zhang, N.; Liu, B.; Wang, P.; Liu, Z.; Wang, Y.; Xu, D.; Tian, H.; Zhang, Q.; Yi, T.-F. Unlocking the Critical Role of Cations Doping in MnO2 Cathode with Enhanced Reaction Kinetics for Aqueous Zinc Ion Batteries. *Adv. Funct. Mater.* **2025**, *35* (20), 2423755. https://doi.org/https://doi.org/10.1002/adfm.202423755.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Reinventing Battery Safety: Advanced Nanofiber Separator with Thermal Stability for Lithium Ion Battery

Arya Chandran, Sudhakaran M.S.P. , Saravanakumar Balasubramaniam*

SARP: Laboratory for Advanced Research in Polymeric Materials (LARPM), Central Institute of Petrochemicals Engineering and Technology (CIPET),

B/25, CNI Complex, Patia, Bhubaneswar-751024, Odisha, India.

*Corresponding Email: kumar@larpm.in ; kumar@cipet.gov.in

Abstract

With the growing demand for high-safety, high-performance lithium-ion batteries (LIB), separator is a vital component in determining the performance and safety of the battery[1]. In this work, we present a functional non-woven PAN/PVDF core-shell structured nanofiber separator[2] and biopolymer modified PAN/PVDF core-shell nanofiber separator fabricated via coaxial electrospinning. Modification in the PVDF shell of the core-shell nanofiber enhance the performance of LIB. This composite separator exhibits high porosity(<40%), robust thermal dimensional stability(<200°C), superior electrolyte uptake and high ionic conductivity, outperforming conventional polyolefin separators. LIB cell incorporating this membrane maintained stable cycling performance with high coulombic efficiency. The findings of this study offer valuable insights into the design of high-performance separators for next-generation LIBs. The detailed methodology and the outcomes will be presented at the conference.

Keywords : Lithium ion battery, Separator, PAN/PVDF nanofibrous separator, coaxial electrospinning.

References

(1) Trinh, H. N.; Eesaee, M.; Shahgaldi, S.; Singh, J.; Hoang, T. L. G.; Nguyen-Tri, P. Advancements and Challenges in Polymer-Based Separators for Lithium-Ion Batteries. *Energy Storage Mater.* **2025**, *77*, 104153. https://doi.org/10.1016/j.ensm.2025.104153.

(2) Gao, X.; Sheng, L.; Yang, L.; Xie, X.; Li, D.; Gong, Y.; Cao, M.; Bai, Y.; Dong, H.; Liu, G.; Wang, T.; Huang, X.; He, J. High-Stability Core–Shell Structured PAN/PVDF Nanofiber Separator with Excellent Lithium-Ion Transport Property for Lithium-Based Battery. *J. Colloid Interface Sci.* **2023**, *636*, 317–327. https://doi.org/10.1016/j.jcis.2023.01.033.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Electrospun NVP@C Nanofiber Networks for High-Performance Binder-Free Sodium-Ion Cathodes

Asha Chaudhary[1], Yogesh Sharma[1,2,*]

[1] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*

[2] *Centre for Sustainable Energy , Indian Institute of Technology Roorkee, Roorkee 247667, India*

* yogesh.sharma@ph.iitr.ac.in

Abstract

Electrospun nanostructured cathodes are increasingly being explored to enhance the electrochemical performance of sodium-ion batteries (SIBs), owing to their high surface area, interconnected porous architecture, and efficient ion/electron transport pathways[1]. In this work, we report the synthesis of one-dimensional, porous $Na_3V_2(PO_4)_3$@C (NVP@C) nanofibers via electrospinning, followed by controlled calcination at 800 °C under an argon atmosphere. The fibrous morphology not only offers a continuous electronic percolation network through the embedded carbon matrix but also facilitates rapid Na^+ diffusion and mitigates volume changes during cycling. Structural, morphological, and compositional analyses confirm the successful formation of phase-pure NVP uniformly encapsulated within conductive carbon. The electrochemical performance of these NVP@C fibers is evaluated in a half-cell configuration against sodium metal, employing both doctor blade casting and electrophoretic deposition (EPD) techniques to fabricate binder-free cathodes. Among the tested electrodes, the EPD-fabricated NVP@C cathodes demonstrate superior rate capability, cyclic stability, and reversible capacity, owing to enhanced interparticle connectivity and uniform deposition. These results highlight the potential of electrospinning-assisted nanostructuring and binder-free electrode processing routes for developing high-performance cathodes for next-generation SIBs. Additional electrochemical data and characterization insights will be presented at the conference.

Keywords: Sodium-ion batteries, $Na_3V_2(PO_4)_3$@C cathode, Electrospinning, Binder-free electrodes, Electrophoretic deposition (EPD)

References

(1) Lu, X.; Li, S.; Li, Y.; Wu, F.; Wu, C.; Bai, Y. From Lab to Application: Challenges and Opportunities in Achieving Fast Charging with Polyanionic Cathodes for Sodium-Ion Batteries. *Advanced Materials* **2024**, *36* (36), 2407359. https://doi.org/10.1002/adma.202407359.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Thermally stable cathode active material for lithium-ion batteries

Vinoth Kumar Jayaraman[1], Vasantha A Gangadharappa[1,3], P. Devi [2,3], Anil Kumar U[1,3], P. Murugan[2,3], Annigere S. Prakash[1,2*]

[1]*Council of Scientific and Industrial Research, Central Electrochemical Research Institute-Chennai Unit, CSIR Madras Complex, Taramani, Chennai, 600113, India.*

[2]*Council of Scientific and Industrial Research, Central Electrochemical Research Institute, Karaikudi, Tamil, Chennai, 600113, India.*

[3]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India.*

* prakash.as@gmail.com

Abstract

Lithium-ion batteries (LIBs) are widely used across industries like automotive and consumer electronics due to their high energy density and efficiency. However, safety concerns, particularly regarding thermal runaway, caused by factors such as internal short circuits, overcharging, or physical damage are an ongoing challenge. To address this, a focus on design optimization, strict safety protocols, and careful material selection is crucial. The cathode material is particularly impactful in enhancing battery stability and safety. In response to this need, a thermally stable NMC-based cathode material has been developed, with a comprehensive analysis of its structural, morphological, electrochemical, and thermal properties. Structural and morphological studies reveal a well-ordered, layered composition that contributes to improved performance and stability. Furthermore, thermal and electrochemical assessments indicate the cathode material can endure temperatures up to 280°C without compromising capacity, and shows better performance than commercially available NMC cathodes. Additionally, the enhanced thermal stability has been validated through first-principles theoretical studies. The obtained results demonstrate the material's potential to significantly reduce thermal runaway risks in LIBs from a material perspective.

Keywords (max 5): Lithium-ion batteries, cathodes, NMC622, thermal stability

Effect of d^0 element substitution in disordered Li-excess manganese oxyfluorides for reversible anion redox

Sayandeep Guin[1], Urmimala Maitra[1]

[1]*Indian Association for the Cultivation of Science, Jadavpur, India*

Li-rich cation-disordered rock salt (DRS) cathodes are being widely investigated due to their high capacity & high energy density obtained from activating anion redox. However, they undergo rapid capacity decay with irreversible anion redox originating from activation of oxygen redox at high voltages. O-redox is known to have poor kinetics and leads to large voltage hysteresis. We synthesised $Li_{1.2}Mn_{0.6}Ti_{0.2}O_{1.8}F_{0.2}$ (LMTOF) systems and substituted Ti^{4+} with Mn^{4+} and obtained greatly improved reversible anion redox at high voltage. The Mn^{4+} substituted compound (LMOF) shows voltage profile with plateaus at 3V and 4V over multiple cycles, indicative of spinel-like local structure formation, as observed by Ceder et. al.[1]

The dQ/dV plots of the samples cycled at C/10 rate are shown in Fig. b, c. Two peaks are observed, first around 3.5V which is related to Mn^{3+} to Mn^{4+} redox and the second around 4.5V related to O-redox. A new reversible peak at 4.1V arises for the Mn^{4+} substituted sample. This 4.1V peak and its corresponding plateau in the Ecell vs Li^+ (de)intercalated data (Fig. a) increases with cycling from the 2nd cycle to the 50th cycle. This 4V plateau arises because of the occupation of the spinel-like 8a sites with Li^+ ion and Li-Li repulsions of the adjacent 8a sites. This peak is absent in the Ti^{4+} substituted sample. Instead we see a continuous decrease in the anion redox peak with cycling. On discharge a weak irreversible 4V hump is observed. This suggests that while phase transition to a spinel like phase is observed for both cases, the spinel-like 16c sites in LMTOF may be filled with immobile Ti^{4+} cation preventing the reversible occupation of 8a sites by Li^+ ion.

RIXS spectra were collected for both the samples at different states-of-charge (SOC) during 1st & 20th galvanostatic cycling. A hump was observed at between -6.0 eV and -10.0 eV energy loss region which is related to the formation of trapped molecular O_2 for samples in the charged state. Vibration peaks corresponding to molecular O_2 vibration were observed in the energy loss region of -0.1 eV to -2.0 eV for 1st charge of both samples.[2] But 20th charge of LMOF sample does not show this molecular O_2 vibration, while that for LMTOF sample shows similar intensity as in the 1st charge. This indicates the spinel-like phase formed on cycling suppresses the formation of molecular O_2 in LMOF sample.

Keywords: Disordered rocksalt, anion redox

References.

1. Ceder et.al., Nature Energy, 2024, **9**, 27–36
2. Tarascon et. al., Nature Materials, 2025, **24**, 743-752

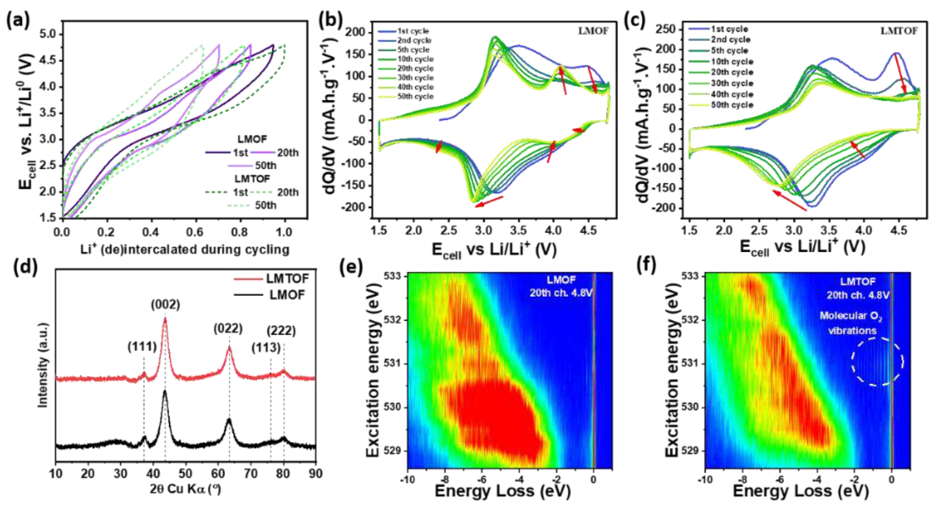


Fig. a) Ecell vs Li^+ (de) intercalated during galvanostatic cycling. dQ/dV curves of (b) LMOF, (c) LMTOF. (d) Powder XRD data. RIXS map collected at 20th charge for (e) LMOF and (f) LMTOF.

ACEPS-13, January 11-14, 2026, Bengaluru, India

High performance lithium-ion battery using carbon aerogel as anode

Sarathchandran C[1,*], Job M Skaria[1], Sweta Prakash[1], Ajeesh K. S[2], Bibin J[2], Damodharan Santhanagoplan[3]

[1]*Materials Chemistry Research Lab, Amrita School of Engineering, Amrita Vishwa Vidyapeetham, Chennai, Tamil Nadu, India.*

[2]*Vikram Sarabhai Space Centre, Indian Space Research Organization (ISRO), Trivandrum, Kerala, India.*

[3]*Amrita Center for Nanosciences and Molecular Medicine, AIMS Kochi, India.*

*c_sarathchandran@ch.amrita.edu , sarathchandranc1@gmail.com

Abstract

Lithium-ion batteries have a prominent place in the field of electronics owing to their high discharge voltage, environmental benignity, low self-discharge rate and good cycling stability[1]. But their increased utilization necessitates more economic viability. Employing carbon materials as anode could play a significant role towards achieving this goal. The properties like high structural stability, specific surface area, electronic conductivity, and pore volume makes porous carbon efficient for energy storage functions. Among different types of porous carbon, carbon aerogels with 3-D porous network gained more attention due to the easy synthesis method, pore tuning features etc[2]. Herein, doped carbon aerogel samples were applied as anode materials in lithium-ion batteries and its electrochemical performance were evaluated. BET and X-ray diffraction were done to analyse the pore features and crystalline behaviour of the synthesized material. The electrochemical performance was evaluated by GCD, CV and EIS measurements. The optimal sample CA-10 exhibited an initial reversible capacity of 523.82 mAh/g at 100 mA/g, which is much better than that of bare CA and CA-5. The combined effects of the nanoporous network skeleton of CA and the evenly dispersed doped nanoparticles are primarily responsible for CA-10's increased cycle performance, specific capacity, and rate capability.

Keywords: Lithium-ion battery, carbon aerogel, nanoporous network, reversible capacity, high performance material.

References

(1) Kim, T.; Song, W.; Son, D.-Y.; Ono, L. K.; Qi, Y. Lithium-Ion Batteries: Outlook on Present, Future, and Hybridized Technologies. *J. Mater. Chem. A* **2019**, *7* (7), 2942–2964. https://doi.org/10.1039/C8TA10513H.

(2) *Highly Porous Carbon Aerogels for High-Performance Supercapacitor Electrodes*. https://www.mdpi.com/2079-4991/13/5/817 (accessed 2025-07-06).

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhancing Fe^{2+}/Fe^{3+} Redox Stability via a Dual-Approach in a Novel Potassium-Rich Iron Fluorophosphate Cathode for K-Ion Batteries

Dipannita Saha[1] and Amartya Mukhopadhyay*

[1]*Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai 400076, India*

*Corresponding Author *Email*: amartya.28nov@gmail.com

Potassium-ion (K-ion) batteries are emerging as a promising alternative to lithium-ion (Li-ion) and sodium-ion (Na-ion) batteries due to their sustainability, cost-effectiveness, and the abundance of potassium. However, a critical challenge in advancing K-ion technology is the development of a high-capacity, stable, and cost-effective cathode material[1,2]. In this study, we present a novel Fe-based Potassium (K) rich polyanionic cathode-active material synthesized through a facile low-temperature method, which exhibits promising electrochemical and structural stability for K-ion batteries.

The synthesized material demonstrates an initial reversible discharge capacity of approximately 102 mAh g^{-1} at a current density of C/15 in K-ion half-cells, and 70 mAh g^{-1} in full cells. This performance is accompanied by excellent air stability, which is essential for the material's long-term use in real-world applications. Importantly, the cathode material maintains good electrochemical stability over extended charge/discharge cycles, demonstrating its potential for high-performance K-ion battery systems. To further enhance the material's electrochemical performance, we optimized a Pre-potassiation technique which significantly improves the material's electrochemical properties, overcoming the initial in-efficiencies in potassium intercalation without relying on the electrochemical Potassiation process. Our findings offer a promising step towards the commercialization of K-ion batteries, with a focus on providing cost-effective, high-capacity, and stable cathodes suitable for large-scale energy storage applications. These advancements pave the way for the development of next-generation sustainable energy storage technologies.

Keywords: Energy storage, Polyanionic cathode material, Air-stable, K-ion battery, Economical.

References

[1] Kim, H.; Seo, D. H.; Bianchini, M.; Clément, R. J.; Kim, H.; Kim, J. C.; Tian, Y.; Shi, T.; Yoon, W. S.; Ceder, G. A New Strategy for High-Voltage Cathodes for K-Ion Batteries: Stoichiometric KVPO4F. *Advanced Energy Materials* **2018**, *8* (26). DOI:10.1002/aenm.201801591.

[2] Sauvage, F.; Quarez, E.; Tarascon, J. M.; Baudrin, E. Crystal Structure and Electrochemical Properties vs. Na+ of the Sodium Fluorophosphate Na1.5VOPO4F0.5. *Solid State Sciences* **2006**, *8* (10), 1215–1221. DOI:10.1016/j.solidstatesciences.2006.05.009.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Optimizing Gelatin-Citric Acid blend as crosslinked high performance binders for anode applications in Lithium Ion Batteries

Sylvester Avijit Gomes [1*], Aaron Abraham Athiyalil[1], Devanand Raj M[1], Swapnabit Das[1], Benson K Money[1]

[1] *Centre of Excellence in Frontier Materials Research, School of Engineering and Technology, CHRIST University, Kanminike, Kumbalgodu, Bangaluru - 560074, India*

* sylvesteravijitgomes@gmail.com

Abstract

In this article, cross-linked binder systems comprising gelatin (G) and citric acid (CA) were studied for its application as high performance binders in anode for Lithium Ion Batteries (LIB). Gelatin, a bio-derived macromolecule, is reportedly being researched as a suitable anode binder due to its viable properties [1]. Citric acid, a highly water-soluble, weak organic polyfunctional monomer, is of particular interest due to its ability to cross-link through amide and ester bonds with gelatin [2]. Cross-linking the binders enhances their electrochemical performance, mechanical strength, and thermal stability. The binder systems, in this study, consisted of various ratios of Gelatin and Citric Acid (G:CA), were prepared systematically. The G:CA ratio also influenced the phase behaviour of the prepared compositions, which in turn determined their viscosity and suitability for LIB anode applications. Electrical conductivity studies as a function of the compositions, were conducted to analyse the electrochemical properties of G:CA compositions to determine the optimum ratio for use as binders in anodes. The initial conductivity measurements showed a decrease in ionic conductivity with the reduction of the CA concentration in the G:CA compositions. Fourier Transform Infrared (FTIR) and Raman spectroscopy were also deployed to analyse the variation of the chemical bonds and intermolecular interactions in the G:CA systems. Differential Scanning Calorimetry (DSC) studies were carried out to observe the phase transitions in the various compositions. These characterization techniques provided deeper insight into the gelatin-citric acid systems, demonstrating their potential as an effective binder for LIB anodes.

Keywords: Gelatin, Citric Acid, Cross-linked Binder, Anode, LIB

References

(1) Dai, S.; Huang, F.; Yan, J.; Sun, Y. Y.; Chen, C.; Li, H. **Construction of Protein-like Helical-Entangled Structure in Lithium-Ion Silicon Anode Binders via Helical Recombination and Hofmeister Effect.** *Adv. Sci. (Weinh.)* **2025**, *12* (20), e2412769. https://doi.org/10.1002/advs.202412769.

(2) Salehabadi, M.; Medhi, K.; Werner-Zwanziger, U.; Obrovac, M. N. **Citric Acid as a Small Molecule Binder for Si-Based Li-Ion Battery Anode Materials.** *J.Electrochem.Soc.* **2025**. https://doi.org/10.1149/1945-7111/adb185.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Sn@CNFs Composite as a Robust Anode Material for Advanced Sodium-Ion Batteries

Kuldeep Sharma[1], Abhinav Tandon[2],Yogesh Sharma[1,*]

[1] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

[2] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

* Corresponding author's email address: yogesh.sharma@ph.iitr.ac.in

Sodium-ion batteries (SIBs) are a proper substitute for Lithium-ion batteries (LIBs), but because of low energy density, these are not commercialized for high-end applications. So, this drawback can be improved by designing an anode with a huge capacity and low cost. Various studies conclude that Tin (Sn) is one of the good anode materials based on an alloying mechanism that provides a high theoretical capacity of 847mAh/g and good cyclability. Using the simple and inexpensive electrospinning method, we created Sn@carbon nanofibers (Sn@CNFs). Carbon nanofibers (CNFs) serve as phenomenal support materials due to their one-dimensional structure, which offers a robust foundation for the flow of ions and electrons and adeptly adapts to accommodate changes in volume during the charging and discharging processes. The Sn@CNFs composite was extensively characterized through FE-SEM, XRD, TGA, and EDS to investigate its structural, morphological, and thermal properties. In its pristine form, the Sn@CNFs nanocomposite demonstrates impressive electrochemical performance, delivering a high reversible capacity of 610 mAh g^{-1}, excellent cycling stability over 50 cycles, and a strong ability to operate effectively at various current rates. These results highlight its strong potential as a promising anode material for next-generation sodium-ion batteries.

Keywords: SIB, Carbon nanofiber (CNF), electrospinning.

References

(1) Bresser, Dominic, et al. "Embedding tin nanoparticles in micron-sized disordered carbon for lithium-and sodium-ion anodes." Electrochimica Acta 128 (2014): 163-171.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Molybdate and Tungstate Alluaudite-type Anode Materials for Sodium-Ion Batteries

Megha Karn[1,*], Pubali Barman[1], Prabeer Barpanda[1]

[1] *Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India.*
* meghakarn@iisc.ac.in

Abstract

Alluaudite mineral type frameworks can be employed as electrode materials for secondary batteries.[1] These three-dimensional frameworks with large one-dimensional hexagonal channels enables easy movement of alkali ions, making them suitable for secondary batteries. Their general formula, $A(1)A(2)M(1)M(2)_2(XO_4)_3$, accommodates alkali (A) and transition metal (M) ions, with X = S, B, Si, P, As, Mo, W and V.[2] The polyanionic moieties (XO_4) provide structural stability and high-operational voltage via the inductive effect. X being more electronegative forms stronger covalent bond with O, thereby making the TM-O bonding more ionic and delivering a higher (M^{n+1}/M^{n+}) redox potential.[3] Recent studies on sulfate-and orthophosphate-based alluaudites reveal their potential as cathode materials for Li-ion and Na-ion batteries.[4] Extending the alluaudite family, molybdate-based alluaudite $Na_{2.67}Mn_{1.67}(MoO_4)_3$ has also been reported as a 3.45 V cathode leveraging both Mn and Mo redox centres.[5]

In this study, we investigated Cu-based molybdate analogue $Na_{2+2x}Cu_{2-x}(MoO_4)_3$ as potential anode materials for secondary Na-ion batteries. We synthesized this compound for the first time using the solution combustion route. This Mo alluaudite exhibited electrochemical activity at lower voltage levels, utilizing Cu and Mo as redox centers. The structure, mechanism, electrochemical and magnetic properties of these MoO_4-based alluaudites will be detailed using a range of analytical techniques. Subsequently, $Na_{2+2x}Mn_{2-x}(WO_4)_3$ will be presented as a novel tungstate alluaudite functioning as an anode for Na-ion batteries. This research highlights the adaptability of alluaudite frameworks in developing new battery electrode materials.

References

(1) Fisher, D. J. Alluaudite. *Am. Mineral.* **1955**, 40 (11–12), 1100–1109.
(2) Dwibedi, D.; Barpanda, P.; Yamada, A. Alluaudite Battery Cathodes. *Small Methods* **2020**, 4(7), 2000051. https://doi.org/10.1002/smtd.202000051
(3) Barpanda, P.; Lander, L.; Nishimura, S.; Yamada, A. Polyanionic Insertion Materials for Sodium-Ion Batteries. *Adv. Energy Mater.* **2018**, 8(17), 1703055. https://doi.org/10.1002/aenm.201703055
(4) Barpanda, P.; Oyama, G.; Nishimura, S.; Chung, S.-C.; Yamada, A. A 3.8-V Earth-Abundant Sodium Battery Electrode. *Nat. Commun.* **2014**, 5(1), 4358. https://doi.org/10.1038/ncomms5358
(5) Gao, J.; Zhao, P.; Feng, K. $Na_{2.67}Mn_{1.67}(MoO_4)_3$: A 3.45 V Alluaudite-Type Cathode Candidate for Sodium-Ion Batteries. *Chem. Mater.* **2017**, 29(3), 940–944. https://doi.org/10.1021/acs.chemmater.6b05308

ACEPS-13, January 11-14, 2026, Bengaluru, India

Layered Oxide Materials for Potassium-Ion Batteries

Mata Prasad Sharma[1,*], Pawan Kumar Jha[1] , Prabeer Barpanda[1]

[1] *Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India.*

* matasharma@iisc.ac.in

Abstract

The increasing demand for Li-ion batteries in energy storage applications along with their growing cost have accelerated the search for cost-effective alternatives. Potassium-ion batteries (KIBs) form one such option, offering comparable energy density, cycling stability, and power density.[1] Among various cathode materials, we have explored P3- and P2-type layered oxide materials for KIB, in which P2-type layered materials exhibit greater ionic diffusivity. However, synthesizing P2-type compounds poses challenges due to their metastable nature, as indicated by density functional theory (DFT) calculations. While electrochemical synthesis methods have been explored in previous studies, these approaches are often complex and unsuitable for producing bulk materials. To address these challenges, we employed a soft chemistry approach via the ion-exchange method (*Chimie Douce*) to produce three P2-type structured compounds for KIBs.[2] Various characterization techniques used, including X-ray diffraction (XRD), inductively coupled plasma (ICP) analysis, Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy, were utilized to investigate the local coordination environment and crystal structure of the synthesized materials. The materials were then tested in half-cell configurations, demonstrating decent capacity and stable electrochemical performance. Our work offers insights into P3-type and the synthesis of metastable P2-type of layered oxide for potassium-ion batteries, which are challenging to obtain through direct calcination methods.[3] These findings highlight the potential of soft chemistry routes for developing next-generation cathode materials for potassium-ion batteries.

Keywords: Potassium-ion batteries, Cathodes, Layered oxides, *Chime Douce*, Ion exchange

References

(1) Hosaka, T.; Kubota, K.; Hameed, A. S.; Komaba, S. Research Development on K-Ion Batteries. *Chem. Rev*. **2020**, *120* (14), 6358-6466. https://doi/10.1021/acs.chemrev.9b00463.
(2) Jha, P. K.; Golubnichiy, A.; Sachdeva, D.; Banerjee, A.; Sai Gautam, G.; Fichtner, M.; Abakumov, A. M.; Barpanda, P. Chimie Douce Derived Novel P2-Type Layered Oxide for Potassium-Ion Batteries. *Adv. Funct. Mater.* **2024**, *34* (41), 2410665. https://doi.org/10.1002/adfm.202410665.
(3) Figlarz, M. Soft Chemistry: Thermodynamic and Structural Aspects. *Mater. Sci. Forum.* **1994**, *152–153*, 55–68. https://doi.org/10.4028/www.scientific.net/MSF.152-153.55.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enabling Fast Charging and Long-lasting Sodium-ion Batteries with a High-Performance NASICON Anode

Biplab Patra[1], Swathy Narayanan[1], Suraj Halder[2], Mayank Sharma[3], Dorothy Sachdeva[4], Narayanan Ravishankar[4], Swapan K. Pati[3], Sheetal K. Jain[2], and Premkumar Senguttuvan[1],*

[1]*New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research; Jakkur, Bangalore-560064, India.*

[2]*Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science, Bengaluru-560012, India.*

[3]*Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore-560064, India.*

[4]*Materials Research Centre (MRC), Indian Institute of Science, Bengaluru-560012, India.*

**Email:* prem@jncasr.ac.in

Abstract

Developing low-cost, safe, and durable rechargeable batteries is vital for future sustainable energy storage. While lithium-ion batteries (LIBs) dominate the market, concerns over resource availability and cost motivate research into sodium-ion batteries (SIBs) as a promising alternative. Although many cathode chemistries are well studied for SIBs, hard carbon remains the commercial anode, yet suffers from low volumetric energy density, poor initial coulombic efficiency, and the risk of sodium plating during fast charging. These challenges highlight the need for advanced intercalation-type anodes that combine high-rate performance with long cycle life.

NASICON (Natrium Super-Ionic CONductor) frameworks, known for their structural robustness and high ionic conductivity, offer a compelling alternative but have been underexplored as anodes. Here, we developed an "empty" Nb-based $Nb_2(PO_4)_3$ anode utilizing multi-redox activity ($Nb^{5+}/Nb^{4+}/Nb^{3+}$), achieving high capacity (~150 mAh g^{-1}) and moderate voltage (~1.2 V), but with rapid capacity fading due to framework instability.[1] To overcome this, extra sodium was introduced to stabilize the structure, significantly improving capacity retention to 89% after 500 cycles at 5C rate.[2] To further meet practical fast-charging demands, we applied carbon coating and particle downsizing along with aliovalent doping (Al^{3+}), enhancing conductivity and creating disordered Na-ion pathways.[3] This engineered anode demonstrated excellent rate performance (80 mAh g^{-1} at 20C) and exceptional cycling stability (95.2% retention after 5000 cycles). A full SIB pairing this anode with a polyanionic cathode reached a high power density of 6493 W kg^{-1} and long cycle life. Finally, we explored the role of electrochemically active and inactive dopants to clarify structure–property relationships. Results indicate that carefully designed substitutions at the Nb site promote fast Na^+ transport, structural stability, and ultra-fast rechargeability, while poorly chosen dopants cause severe structural distortions and capacity loss. This work establishes a clear pathway to develop high-rate, long-lasting SIB anodes through crystal engineering, doping, nanoscaling, and carbon coating, advancing the practical realization of sodium-ion batteries.

Keywords: Na-ion batteries, NASICON anode, fast charging, multi-redox, structural stabilization.

References

[1] B. Patra, K. Kumar, D. Deb, S. Ghosh, G. S. Gautam, P. Senguttuvan, *J. Mater. Chem. A* **2023**, *11*, 8173.

[2] B. Patra, R. Hegde, A. Natarajan, D. Deb, D. Sachdeva, N. Ravishankar, K. Kumar, G. S. Gautam, P. Senguttuvan, *Adv. Energy Mater.* **2024**, *14*, 2304091.

[3] B. Patra, S. Narayanan, S. Halder, M. Sharma, D. Sachdeva, N. Ravishankar, S. K. Pati, S. K. Jain, P. Senguttuvan, *Adv. Mater.* **2025**, 2419417.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Optimization of PVA-PEG Based Blended Solid Polymer Electrolytes for Enhanced Lithium-ion Dynamics

MOHAN.B.N[1], TEONA JOBY[2,*], RIYA S[2], SUNITHA.V.R[2], BENSON K MONEY[2]

[1] *Christ PU College Residential, Bengaluru-74, Karnataka, India*

[2] *Center of Excellence in Frontier Material Research, School of Engineering & Technology Christ (Deemed to be university) Bengaluru-74, Karnataka, India*

**teona.joby@btech.christuniversity.in*

Abstract

Solid polymer electrolytes (SPEs) are progressively essential for next-generation energy storage systems due to their safety, flexibility and electrochemical stability. The present study focuses on a blended SPE film which was synthesized through solution casting of a polymer blend comprising polyvinyl alcohol (PVA) and polyethylene glycol (PEG) in a particular mass ratio, dissolved in deionized water and followed by the incorporation of lithium perchlorate (LiClO4) as an ion-conducting salt. The incorporation of PVA and PEG draws upon their complementary properties, with PVA providing structural integrity and PEG enhancing chain flexibility, while $LiClO_4$ contributes to ionic conductivity. This blending technique, a well-established approach, facilitates ion hopping and enhances the amorphous phase, thereby optimizing lithium-ion diffusion within the polymer matrix. Conductivity and dielectric properties were investigated under varying thermal conditions on these systems by changing the weight percentages (wt%) of PVA and PEG. Electrical characterization was performed using impedance spectroscopy. The optimized composition formed a stable, flexible film maintaining precise control over the polymer ratio. The resulting film is expected to exhibit ionic conductivity in the range of 10^{-6} to 10^{-5} S/cm, suitable for applications in batteries and supercapacitors.

Keywords: Blended Solid polymer electrolytes (BSPE), polyvinyl alcohol (PVA), polyethylene glycol (PEG), lithium perchlorate ($LiClO_4$), solution casting.

References

(1) GUL, R.; MAHMOOD, W. A. K. Studies of the Properties of New Electrospun Based on PVA-PEG Polymer Systems Electrolytes for Energy Storage Devices. *Journal of the Turkish Chemical Society Section A: Chemistry* **2024**, *11* (1), 313–320. https://doi.org/10.18596/jotcsa.1262560.

(2) Paul Sharma, J.; Kumar, P.; Sharma, K.; Kumar, M.; Arora, A.; Kumar Singh, P. Optical and Structural Properties of Drop-Cast PVA/PEG. Polyblends. Materials Today: Proceedings **2020**. https://doi.org/10.1016/j.matpr.2020.03.801.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Building NASICON-Based Sodium-ion Full Cells through Capacity Balance and Electrolyte Modulation

Ayon Phukan[1], Biplab Patra[1], Premkumar Senguttuvan[1]

[1]*New Chemistry Unit (NCU), Jawaharlal Nehru Centre for Advanced Scientific Research(JNCASR), Jakkuru, Bengaluru, Karnataka-560064, India*

Email ID: prem@jncasr.ac.in

Abstract

Achieving an optimal capacity balance between the cathode and anode, commonly referred to as the N/P ratio, is vital for enhancing the overall performance of sodium-ion batteries. This balance ensures that both electrodes operate efficiently, ultimately leading to improved energy density, longer cycle life, and greater efficiency in energy storage and release. While extensive research has been conducted on lithium-ion batteries[1–4], leading to significant advancements in their performance and longevity, there remains a limited body of studies focused specifically on sodium-ion batteries[5]. This investigation examines a NASICON-based sodium-ion battery with varying N/P ratios. The materials utilized include NASICON based $Na_3V_2(PO_4)_3$ (NVP) as the cathode and VAlMgNb as the anode. Electrochemical testing demonstrates that an N/P ratio of 1.0 yields optimal performance, characterized by a higher intercalation voltage and minimal capacity fading. Full cells based on the NASICON framework are evaluated using different electrolytes, including ether and carbonate-based. Among them, the ether-based electrolyte exhibits superior performance due to its stable solid electrolyte interface (SEI), higher conductivity and reduced bulk resistance. The NVP||VAlMgNb full cell provides a reversible capacity of approximately 100 mAh g^{-1}, with an average operating voltage of 1.92 V. Furthermore, the cell achieves an energy density of 100 Wh kg^{-1} when considering the total weight of both the cathode and anode. The results of this study establish a robust framework for the design of sodium-ion batteries that effectively balance energy density and operational lifespan.

Keywords: NASICON, SEI, Capacity Balance, Electrolyte Modulation, Sodium ion Batteries

References

(1) Chen, Z.; Zhang, L.; Wu, X.; Song, K.; Ren, B.; Li, T.; Zhang, S. Effect of N/P Ratios on the Performance of LiNi0.8Co0.15Al0.05O2||SiOx/Graphite Lithium-Ion Batteries. *J. Power Sources* **2019**, *439*. https://doi.org/10.1016/j.jpowsour.2019.227056.

(2) Baasner, A.; Reuter, F.; Seidel, M.; Krause, A.; Pflug, E.; Härtel, P.; Dörfler, S.; Abendroth, T.; Althues, H.; Kaskel, S. The Role of Balancing Nanostructured Silicon Anodes and NMC Cathodes in Lithium-Ion Full-Cells with High Volumetric Energy Density. *J. Electrochem. Soc.* **2020**, *167* (2), 020516. https://doi.org/10.1149/1945-7111/ab68d7.

(3) Yourey, W.; Fu, Y.; Li, N.; Battaglia, V.; Tong, W. Design Considerations for Fast Charging Lithium

Ion Cells for NMC/MCMB Electrode Pairs. **2021**. https://doi.org/10.3390/batteries70.

(4) Kasnatscheew, J.; Placke, T.; Streipert, B.; Rothermel, S.; Wagner, R.; Meister, P.; Laskovic, I. C.; Winter, M. A Tutorial into Practical Capacity and Mass Balancing of Lithium Ion Batteries. *J. Electrochem. Soc.* **2017**, *164* (12), A2479–A2486. https://doi.org/10.1149/2.0961712jes.

(5) Song, T.; Chen, Y.; Chen, L.; Kendrick, E. Areal Capacity Balance to Maximize the Lifetime of Layered Oxide/Hard Carbon Sodium-Ion Batteries. *J. Power Sources* **2024**, *624*. https://doi.org/10.1016/j.jpowsour.2024.235599.

Title: Layered V_2O_5 as a Bifunctional Host for Na^+ and Al^{3+}: Advanced Cathode Material for Realizing Low-Cost Energy Storage Technology

Omkar Sharma[1], Parul Goel[2] Abhigna HG[1], Gajanan V Honnavar[1*]

[1]Quantum and Nano Devices Lab, Dept of Science and Humanities, PES University EC Campus, Hosur Road, Near Electronic City, Bengaluru - 560100, India

[2] St. Joseph's University, Department of Physics, Langford Road, Bengaluru - 560027, India

Abstract

Abstract:

The advancement of high-performance, cost-effective, and sustainable energy storage devices has generated heightened interest in sodium-ion and multivalent-ion chemistries. This study offers a thorough structural and electrochemical analysis of a Na-Al-V_2O_5 (Na-Al-VO) dual-ion system, aimed at effectively using the mobility of Na^+ ions alongside the high charge density of Al^{3+}. X-ray diffraction (XRD) validates the successful incorporation of both cations into the V_2O_5 lattice, with crystallite dimensions ranging from 15 to 25 nm as ascertained by Debye-Scherrer analysis. X-ray photoelectron spectroscopy (XPS) demonstrates stable oxidation states of vanadium and the presence of sodium and aluminum, confirming efficient dual-ion intercalation.

Direct current (DC) conductivity tests reveal a significant enhancement in electronic conductivity with the addition of aluminum, which is ascribed to enhanced charge percolation and electron hopping pathways within the host matrix. Cyclic voltammetry (CV) electrochemical measurements reveal distinct redox peaks, validating the effective and reversible insertion/extraction of Na^+ and Al^{3+}. Galvanostatic charge-discharge (GCD) testing demonstrates stable cycling and elevated specific capacitance.

The dual-ion mechanism increases charge storage and adds complementary transport channels, providing a strategic advantage over traditional single-ion systems. This study emphasizes the function of V_2O_5 as a multifaceted host for dual-ion storage and identifies the Na-Al-VO system as a formidable contender for advanced sodium-based energy storage technologies, characterized by improved conductivity and cycling stability.

Keywords: Mixed-ion intercalation ,Layered cathode materials, Na^+/Al^{3+} transport mechanism

References

[1] Vedpathak A, Shinde T, Desai MA, Thombare BR, Humane R, Raut SA, Kalubarme R, Sartale SD, Bhagwat S. One-dimensional layered sodium vanadate nanobelts: a potential aspirant for high-performance supercapacitor applications. ACS Applied Energy Materials. 2023 Apr 17;6(9):4693-703.

[2] De, P., Halder, J., Priya, S., Srivastava, A.K. and Chandra, A., 2023. Two-dimensional V2O5 nanosheets as an advanced cathode material for realizing low-cost aqueous aluminum-ion batteries. *ACS Applied Energy Materials*, *6*(2), pp.753-762.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Linking Carbon-Network Architecture and Local Atomic Structure to High-Performance $Na_4VMn(PO_4)_3/C$ Cathodes

Songyoot Kaewmala[1, 2*], Natthapong Kamma[3], Sujeera Pleuksachat[1], Pornjira Phuenhinlad[4], Wanwisa Limphirat[3], Natthawan Prasongthum[1, 2], Jeffrey Nash[1], and Nonglak Meethong[1, 2]

[1] *Institute of Nanomaterials Research and Innovation for Energy (IN-RIE), Khon Kaen University, Khon Kaen 40002, Thailand*

[2] *Battery and New Energy Science Program, Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

[3] *Synchrotron Light Research Institute, 111 University Avenue, Suranaree, Muang, Nakhon Ratchasima, Thailand*

[4] *Department of Mechanical and Materials Engineering, Worcester Polytechnic Institute, Worcester, MA, 01609 USA*

*Email:songka@kku.ac.th

Abstract

$Na_4VMn(PO_4)_3$ is a promising NASICON-type cathode for sodium-ion batteries, yet its practical performance is restricted by low intrinsic electronic conductivity and structural instability associated with MnO_6 and VO_6 octahedral distortion. In this work, $Na_4VMn(PO_4)_3/C$ composites were synthesized via scalable sol–gel and solid-state reaction methods to elucidate the coupled roles of carbon-network architecture and local atomic structure in governing electrochemical behavior. Multiscale characterization using XRD, TEM, Raman spectroscopy, and X-ray absorption spectroscopy reveals that the solid-state route produces a continuous, tightly bonded carbon coating and reduced MnO_6/VO_6 distortion, whereas the sol–gel method yields loosely attached carbon sheets and greater local structural disorder. The improved structural integrity and carbon connectivity in the solid-state–derived material result in higher electronic conductivity, enhanced Na^+ diffusion coefficients (10^{-13}–10^{-14} cm^2 s^{-1}), and superior cycling and rate performance compared with the sol–gel counterpart. After 300 cycles, the solid-state sample maintains higher crystallinity and lower charge-transfer resistance, while the sol–gel material exhibits significant local structural degradation. These findings establish the critical interplay between carbon-network engineering and local atomic stability in optimizing polyanionic-based cathodes, offering practical design guidelines for high-performance sodium-ion batteries.

Keywords: NASICON-Type Cathode, Carbon-Network Engineering, Local Structural Stability

ACEPS-13, January 11-14, 2026, Bengaluru, India

Stabilizing Oxygen Redox in Layered Oxide Cathodes via Site Engineering for High-Energy Sodium-Ion Batteries

Panya Thanwisai[1,2,*], Songge Yang[2], Zeyi Yao[2], Zifei Meng[2], Jiahui Hou[2], Panawan Vanaphuti[3], Maksim Sultanov[4,5], Jianguo Wen[4], Zhenzhen Yang[6], Yu Zhong[2], Nonglak Meethong[1] and Yan Wang[2]

[1]*Battery and New Energy Science Program, Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.*

[2]*Department of Mechanical and Materials Engineering, Worcester Polytechnic Institute, Worcester, MA 01609, USA*

[3]*Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

[4]*Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439, USA*

[5]*Department of Physics, Northern Illinois University, Dekalb, IL 60115, USA*

[6]*Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA*

*E-mail: panyth@kku.ac.th

Abstract

The recent development of sodium-ion batteries (SIBs) aims not only to reduce reliance on critical Ni/Co elements but also to increase energy density to satisfy both sustainability and high-performance demand. Layered oxide cathodes based on Mn-rich and oxygen redox chemistries have gained escalating interest in recent years since they promise high energy density with no such critical metals used. Nevertheless, the cathodes are still challenged by high-voltage lattice oxygen loss and Mn^{3+}-induced Jahn-Teller structural distortion that trigger undesired phase transformation and microstructural damage, ultimately leading to poor cycling stability. To cope with the challenges, we herein propose a site engineering strategy by selectively substituting Zn^{2+} into Na sites and Al^{3+} into transition-metal (TM) sites, innovating a novel cathode chemistry of $[Na_{0.73}Zn_{0.03}]$ $[Li_{0.25}Mn_{0.76}Al_{0.01}O_2]$ (AlZn). Comprehensive experimental and computational investigations reveal that the synergy between robust Al–O in TM layers and O–Zn–O pillar effects in Na layers effectively suppresses severe inactive spinel/rock-salt phase transformations and intragranular cracks in the AlZn cathode. As a result, the modified cathode exhibits greatly enhanced electrochemical performance in both half- and full-cell systems. Altogether, this work provides mechanistic insight into improving electrochemical properties of oxygen-redox-based layered oxides by Al/Zn co-substitution towards high-energy SIB cathodes.

Keywords: Oxygen Redox Chemistry, Sodium-Ion Batteries, Structural Stability Enhancement

References

Thanwisai, P., Yang, S., Yao, Z., Meng, Z., Hou, J., Vanaphuti, P., ... & Wang, Y. (2025). Anionic-Based Layered Oxide Cathodes with High Electrochemical Performance through Dual-Site Substitutions for Sodium-Ion Batteries. *Small*, *21*(11), 2411928.

Microwave-Engineered $TiO_2/Ti_3C_2T_x$ Heterostructures from Electrochemically Etched MXene for Sodium-Ion Battery Anodes

Kaifee Sayeed[1], , Aditya Sadhanala[2], Kavita Pandey[1*]

[1] *Centre for Nano and Soft Matter Sciences (CeNS), India*

[2] *Centre for Nano Science and Engineering (CeNSE), IISc, India*

* kavitapandey@cens.res.in

Abstract

Sodium-ion batteries (SIBs) have emerged as a sustainable and cost-effective alternative to lithium-ion technology, particularly for large-scale energy storage applications. In this study, we developed a high-performance $Ti_3C_2T_x$ MXene-based anode material through an innovative low-HF electrochemical etching approach. This synthesis strategy yielded high-quality MXene with exceptionally large lateral flake sizes of 11-12 µm while maintaining excellent electrochemical performance. To further enhance the electrochemical performance, we engineered a $TiO_2/Ti_3C_2T_x$ nanohybrid through a precisely controlled microwave-assisted synthesis method, which enabled the optimal growth of TiO_2 nanoparticles on the MXene matrix. When evaluated as an anode for SIBs, this unique hybrid architecture demonstrated remarkable electrochemical properties, delivering a high reversible capacity of 286 mAh/g at 100 mA/g current density. More importantly, the material exhibited exceptional cycling stability, maintaining its performance over 500 charge-discharge cycles, along with significantly improved charge transfer kinetics and sodium-ion diffusion characteristics.

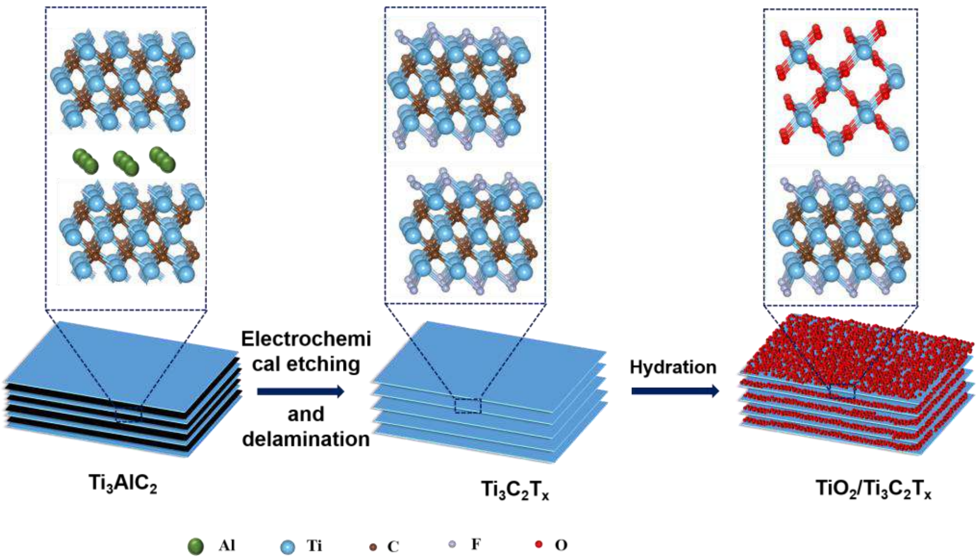


Figure: Schematic representation of MXene electrochemical etching and subsequent hydration.

Keywords: MXene, Electrochemical etching, Sodium-ion battery, Anode, Energy storage

Title: Enhanced Electrochemical Properties of V_2O_5-SrO-Li_2O based glass ceramic cathodes for Li-ion Batteries

Parul Goel[1*], Omkar Sharma[2], Abhigna HG[2]

[1]St Joseph's University, Department of Physics, 36 Lalbagh Road, Bengaluru - 560027, India
[2]Quantum and Nano Devices Lab, Dept of Science and Humanities, PES University, EC Campus, Bengaluru - 560100, India

Abstract

This study elucidates the effect of ball milling and heat treatment temperature on the structural and electrochemical properties of lithium-doped vanadium strontium glasses. Though the effect of heat treatment in the devitrification of glasses has been studied by researchers earlier, its effect on electrochemical properties has not been studied much.

The studied glasses were prepared using the conventional melt-quench technique. They were then ball milled and further subjected to suitable heat treatment for in vitro nanocrystallization. Structural characterization was done using XRD, FTIR, and SEM. The electrochemical properties of these base glasses and the nanocrystallized glass-ceramics were analyzed using cyclic voltammetry and galvanostatic charge-discharge (GCD).

The formation of nanocrystallized phases within the amorphous glass structure increases the surface area and provides interfaces for faster ion transport and higher charge storage capacity. Some of the glass ceramics thus showed significantly improved specific capacitance and capacity retention. The effect of appropriate heat treatment and its role in enhancing the electrochemical properties of glasses were analyzed in this study. This study will play a significant role in improving the glass cathodes for Li-ion batteries.

Keywords: Glass, glass ceramic, nanocrystallisation, cyclic voltammetry, galvanostatic charge-discharge (GCD).

References:

[1] Takayuki Komatsu, Design and control of crystallization in oxide glasses, Journal of Non-Crystalline Solids 428 (2015) 156–175
[2] Michael Kindle, Steven Kmiec, Igor d'Anciaes Almeida Silva, Hellmut Eckert, Steve W. Martin, Min-Kyu Song, John S. McCloy, Structural properties of alumina-doped lithium borovanadate glasses and glass-ceramics, Journal of Non-Crystalline Solids 521 (2019) 119551

ACEPS-13, January 11-14, 2026, Bengaluru, India

Investigating the Effect of Fluorination on Acrylonitrile Polymer-based Gel Electrolytes for the Application in Sodium-ion/metal batteries

Sanhita Pal[1], Debalina Deb[2], Aninda Jiban Bhattacharyya[1,2] *

[1]*Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru, India*

[2]*Interdiciplinary Center for Energy Research, Indian Institute of Science, Bengaluru, India*

*Email: anindajb@iisc.ac.in

Abstract

Rechargeable batteries, especially state-of-the-art lithium-ion batteries (LIBs), are crucial in modern-day society for diverse applications. Sodium-ion/sodium-metal batteries (SIBs/SMBs) are emerging as the most viable alternative to complement the LIBs and LMBs because of the high natural abundance and homogenous distribution of Sodium (Na) compared to Lithium (Li). Unstable Solid Electrolyte Interface (SEI) on the Na metal and carbonaceous anode materials are one of the key challenges in Liquid electrolyte (LE) based SIBs/SMBs. Dendrite formation and anode volume change over repeated cycling are other issues that lead to SEI breakdown, electrolyte consumption, and, in severe cases, short-circuiting of the battery. Moreover, the flammable commercial LEs pose fire hazards, creating a need for a safer and better alternative.[1]

Solid or solid-like electrolytes, for instance Gel Polymer Electrolyte (GPEs) can address some of the key challenges. GPEs are prepared by entrapping LEs into a polymer matrix, leveraging the ion conduction by LEs and mechanical stability of the polymer matrix, being a potential stand-alone alternative to both liquid and ceramic-based electrolytes. As electrolyte additives, fluorinated liquid electrolytes and monomers have been widely used in Li-based systems to enhance cell stability, but their effects on Na-based systems remain underexplored. This gap creates an opportunity for further research to enhance the performance and longevity of SIBs/SMBs. [2,3,4]

In this work, we discuss the effect of incorporating various fractions of a fluorinated monomer into the polymer matrix. The polymerization was done via UV-initiated free radical polymerization to obtain a self-standing GPE film. The fluorinated GPEs show high ionic conductivity (> 1 mS/cm) at room temperature, high electrochemical stability window (~4.8 V) and excellent cycling stability, enabling the striping and plating of sodium for over 1000 cycles. The GPEs, when paired with well reported cathodes, show enhanced cycling stability. These results show the potential of fluorinated GPEs for developing safer and better SIBs/SMBs technology for widespread applications.

Keywords: Sodium-ion batteries, Gel polymer electrolytes, Fluorinated monomers, Solid electrolyte interphase, Energy storage

References:

[1] Hwang, J.-Y., Myung, S.-T., & Sun, Y.-K. (2017). Sodium-ion batteries: present and future. *Chem. Soc. Rev., 46*(12), 3529–3614.

[2] George, S. M.; Sampath, S.; Bhattacharyya, A. J. A Self-Standing Flexible Gel Polymer Electrolyte for Dendrite-Free Lithium-Metal Batteries. *Batteries & Supercaps* **2022**, *5* (11)

[3] Pan, J.; Wang, N.; Fan, H. J. Gel Polymer Electrolytes Design for Na-Ion Batteries. *Small Methods* **2022**, *6* (11), 2201032.

[4] Jia, M.; Wen, P.; Wang, Z.; Zhao, Y.; Liu, Y.; Lin, J.; Chen, M.; Lin, X. Fluorinated Bifunctional Solid Polymer Electrolyte Synthesized under Visible Light for Stable Lithium Deposition and Dendrite-Free All-Solid-State Batteries. *Adv. Funct. Mater.***2021, 31 (27).**

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhanced Na-Ion Transport in Filler-Rich Composite Polymer Electrolytes

Teja Vardhana Reddy Kunnam[1], Sanhita Pal[1], Aninda Jiban Bhattacharyya [1,2*]

[1] *Solid-State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru*

[2] *Interdisciplinary Center for Energy research, Indian Institute of Science, Bengaluru*

*E-mail: anindajb@iisc.ac.in

Abstract

Electrochemical energy storage devices are becoming increasingly important for large scale applications e.g., conventional electric grids and electric motor vehicles. The current state-of-the-art lithium-ion batteries use graphite anode and LFP/NMC cathode and have shown exemplary cyclability and rate capability. Despite their widespread usage in portable electronic devices, their energy density is limited to 250 Wh/kg which can be surpassed by using bare metal anodes[1]. The limited earth's abundance of lithium metal (20 ppm) provides space to explore various alternatives to it and sodium metal is one of the best alternatives which has low reduction potential (-2.71V) , high specific capacity(1166 mAh/g) , high abundance (23,600 ppm) and economically cheap[2]. The detrimental effects of liquid electrolytes can be nullified by employing solid state electrolytes such as Inorganic solid electrolytes, solid polymer electrolytes and composite polymer electrolytes.

Inorganic solid-state electrolytes like NASICON offer high ionic conductivity (>10^{-4} S/cm) and transport number (~1), but suffer from surface inhomogeneities and poor interfacial contact, leading to failure at low current densities. Polymers, though flexible, have limited ionic conductivity and mechanical strength at room temperature. Composite polymer electrolytes combine the advantages of both, enabling flexible, high-transport films. While previous studies[3,4] limited filler content (<30 wt%) to preserve film integrity, we fabricated flexible composite films with 10–60 wt% NASICON via electrospinning, followed by in-situ UV polymerization of glycol-based precursors. The resulting films show 0.3 mS/cm conductivity and 30–50 mV overpotential at 0.05 mA/cm^2, demonstrating the promise of active-filler-rich flexible electrolytes for electrochemical applications.

Keywords: Na-ion batteries, Solid-polymer electrolytes, flexible electrolytes, composite electrolytes

References:

1) Manthiram, A. An Outlook on Lithium Ion Battery Technology. *ACS Cent Sci* **2017**, *3* (10), 1063– 1069.
2) Yabuuchi, N.; Kubota, K.; Dahbi, M.; Komaba, S. Research Development on Sodium-Ion Batteries. *Chem. Rev.* **2014**.
3) Yu, X.; Xue, L.; Goodenough, J. B.; Manthiram, A. All-Solid-State Sodium Batteries with a Polyethylene Glycol Diacrylate–Na3Zr2Si2PO12 Composite Electrolyte. *Advanced Energy and Sustainability Research* **2021**, *2* (1), 2000061.
4) Li, F.; Ren, K.; Hou, M.; Lin, M.; Yang, X.; Zhou, Y.; Xiong, S.; Liang, F. Ultrafast UV Curing Enabling A Stable Interphase and Interface for Solid-State Sodium−Metal Batteries. *ACS Energy Lett.* **2024**, *37*, 35.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Electrochemical Passivation of Reactive Interphases for Stable Anodeless Solid-state Batteries

Piyali Pahari[1,], Srinivasan Ramakrishnan[1*],

[1] *Department of Chemistry, IIT Bombay, Mumbai-400076, India*

* Sriniramk@iitb.ac.in

Abstract

Solid-state Li batteries are considered as a promising alternative to commercial Li ion batteries due to their superior energy and power density and safety. Moreover, their anodeless configuration is even more attractive as it can further boost volumetric energy density by eliminating any dead volume in the cell. The application of NASICON type ceramics (LATP ($Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$/ LAGP($Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$) as solid electrolyte (SE), is preferred as compared to oxide-based ceramics such as LLZO due to their higher ionic conductivity at ambient conditions and higher air stability. However, their practical implementation in SSBs is still challenging due to the anodic instability against reduction, as well as their high cost of manufacturing. Herein, we pre-engineered the Cu current collector surface by introducing a porous reactive layer via controlled corrosion reaction involving the hydrolytic instability of $LiPF_6$ in EC-DEC. Subsequently, through a series of conversion reaction in an anodeless solid-state half-cell with Li metal and LATP solid electrolyte, the reactive layer was transformed to Li_2O and LiF rich passivating interphases in between Cu current collector and solid electrolyte. Morphologically this layer was dense and well-adhered on the Cu current collector which helped to achieve ~90% Coulombic efficiency at ambient temperature and pressure.

Keywords : Anodeless solid-state batteries, current collector modification, corrosion, Interfacial passivation, anode-Solid electrolyte interphase

References

(1) Hartmann, P.; Leichtweiss, T.; Busche, M. R.; Schneider, M.; Reich, M.; Sann, J.; Adelhelm, P.; Janek, J. Degradation of NASICON-Type Materials in Contact with Lithium Metal: Formation of Mixed Conducting Interphases (MCI) on Solid Electrolytes. *J. Phys. Chem. C* **2013**, *117* (41), 21064–21074.

(2) Ding, D.; Ma, H.; Tao, H.; Yang, X.; Fan, L.-Z. Stabilizing a Li 1.3 Al 0.3 Ti 1.7 (PO 4) 3 /Li Metal Anode Interface in Solid-State Batteries with a LiF/Cu-Rich Multifunctional Interlayer. *Chem. Sci.* **2024**, *15* (10), 3730–3740.

(3) Hobold, G. M.; Wang, C.; Steinberg, K.; Li, Y.; Gallant, B. M. High Lithium Oxide Prevalence in the Lithium Solid–Electrolyte Interphase for High Coulombic Efficiency. *Nat. Energy* **2024**, *9* (5), 580–591.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Loading of LATP in PEO as composite polymer Solid-State Electrolyte in Solid-State Lithium-ion batteries (SSLIBs)

Tandrima Saha, Dr. Karan Pal Singh, Dr. Sudarshan Narayanan

Department of Sustainable Energy Engineering, IIT Kanpur, India

tandrimas24@iitk.ac.in

ABSTRACT

In this experiment we are designing a composite solid-state electrolyte with optimal loading and distribution of LATP into a polymer of PEO. The PEO is found most compatible as a polymer matrix among few probable candidates. The symmetric cell and full cell assembly is seen and the electrochemical performance have been studied. LATP a NASICON based solid-state electrolyte has been prepared using solid-state synthesis. The ceramic material is calcined into two-step and sintered by making pellet at 1000°C. These pellets are crushed and kept for later use. This solid-state electrolyte is stirred in acetonitrile and distributed into polymer matrix of PEO over a weight % of (30,40,50,70,80,90) by vacuum mixing along with lithium salt(LiTFSI). After the mixing the ceramic into polymer matrix mixture is coated using doctors blade over a teflon sheet and dried at 35°C overnight in a vacuum oven. The dried electrolyte is peeled off from the Teflon sheet and kept into glove box for 24hours to remove any moisture present in the sample. Later 12mm diameter disc were puched out from the sheet for ionic conductivity studies of the sample in a Swagelok cell. The ionic conductivity at room temperature was ~10^{-4} S/cm and studied over a temperature upto 70°C for all the weight% of LATP in PEO. The symmetric cell study using Lithium foil on both the sides packed in a CR2032 coin cell inside an argon-based glove box and a plating-stripping was studied over a current density of 0.05mA/cm^2 ,0.1mA/cm^2 and so on. Characterization studies of the pristine ceramic powder was done through XRD, FESEM, EDX, Raman and FTIR. Characterization of the polymer film was done as well by XRD, FESEM, EDX. Electrochemical studies like EIS, Plating-stripping was done. Planning to do a full cell study with the best performed LATP+PEO film and to do a charge discharge of the full cell. The full cell will be assembled using hot-pressing technique inside a glove box. Postmortem study of the best performed symmetric cell and full cell will be done using XPS, XRD and FESEM.

Keywords: *NASICON, solid-state electrolyte, LATP, composite polymer electrolyte*

ACEPS-13, January 11-14, 2026, Bengaluru, India

Scalable Asymmetric Single-Layer Composite Electrolyte with Engineered Interfacial Layers for Dendrite-Free and High-Performance Solid-State Lithium Metal Batteries

Pratiksha Gami, Asish Kumar, Sunil Kumar*

Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Simrol, 453552, India.

*Corresponding author, E-mail: sunil@iiti.ac.in

Abstract

Conventional lithium-ion batteries (LIBs) are approaching their theoretical energy density limits, prompting growing interest in lithium metal batteries (LMBs) for next-generation energy storage. However, LMBs using liquid electrolytes face critical safety challenges due to lithium dendrite formation. All-solid-state lithium metal batteries are emerging as promising candidates for next-generation energy storage due to their enhanced safety and high energy density. However, challenges such as low ionic conductivity and high interfacial resistance hinder their practical deployment. In this work, we address these issues through two complementary approaches. First, Al-substituted $LiHf_2(PO_4)_3$ (LAHP) inorganic electrolytes were synthesized via a solid-state reaction route. Rietveld refinement confirmed a rhombohedral phase, with the highest ionic conductivity (7.09×10^{-5} S cm^{-1}) achieved at 25% Al substitution. Stable lithium plating/stripping over 170 h and excellent performance in Li||$LiFePO_4$ cells underscore its potential. Building on this, we developed an asymmetric single-layer electrolyte (ASE) integrating a soft polymer-rich (PVDF-HFP/PVP/LiTFSI) side for improved cathode contact and a LAHP-rich side for robust lithium metal protection. The ASE demonstrates high ionic conductivity (6.05×10^{-5} S cm^{-1} at 35 °C), long-term cycling in symmetric Li cells (2500 h at 0.2 mA cm^{-2}), and outstanding performance in Li||$LiFePO_4$ full cells (85% capacity retention over 500 cycles at 2C). This innovative single-layer asymmetric design effectively embeds ceramic reinforcement within the polymer matrix on one side, offering improved interfacial compatibility, simplified fabrication, and optimal compositional asymmetry, together enabling a practical pathway toward high-performance solid-state lithium metal batteries.

Keywords: Solid-state lithium-metal batteries, Asymmetric single-layer electrolyte, Dendrite suppression, Interfacial compatibility.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Fabrication and characterization of all-solid-state Li-S batteries using argyrodite-based composite as the cathode active material

Satoshi Yamamoto[1], Dai Namba[1], Toshinari Koketsu[1], Naohiro Horiuchi[1] and Norihiko Miyashita[1,*]

[1] *Mitsui Mining & Smelting Co., Ltd., 1333-2 Haraichi, Ageo, Saitama 362-0021, Japan*

* n_miyashita@mitsui-kinzoku.com

Abstract

Li-S batteries are the promising candidate for the next generation batteries with their high energy density. In particular, all-solid-state Li-S batteries, which employ the solid-state electrolyte instead of organic solvents, are very attractive systems. They improve not only safety but also cyclability due to the suppression of dissolution of lithium polysulfide from the cathode active material generated upon charge-discharge cycling.

We focused on the Argyrodite-type sulfide (Li_6PS_5Cl) with high ionic conductivity, as both cathode materials and electrolyte for new high-performing Li-S batteries. In order to unlock the stable redox activity of Argyrodite-type sulfide as the cathode, its electronic and ionic conductivity was enhanced by mixing with a carbon material and additional Argyrodite-type sulfide. We carried out a mechanistic analysis and revealed charge/discharge mechanisms, leading to optimized compositions with superior performance. In addition to the cathode, we also improved Argyrodite solid-state electrolyte to stabilize the cathode/electrolyte interface by improving chemical and electrochemical stability as well as mechanical properties.

Using the developed argyrodite-based composite cathode and the argyrodite-type sulfide electrolyte, and Li metal anode, we fabricated a dry-pressed powder type all-solid-state battery. It demonstrated reversible capacity with high energy density of ~400 Wh/kg, based on battery components without casing. In this presentation, we will report on the effects of current collectors and binders in cathode on battery cycling performance. Besides, coat-type cathode and pouch cells, as well as issues to be addressed for practical application will be discussed.

Keywords: All-solid-state battery, Li-S battery, Argyrodite, Cathode

ACEPS-13, January 11-14, 2026, Bengaluru, India

Room temperature Fluoride-ion Battery with substitutional doping of K^+ in $BaSnF_4$ solid electrolyte

Meena M[1], Amrtha Bhide[1,*]

[1] *National Institute of Technology Puducherry, India*

* amrthabhide@nitpy.ac.in

Abstract

Fluoride ion batteries are prominent next-generation energy storage systems due to their high theoretical energy density of 5000 Wh/L, thermal safety, and wide electrochemical stability window owing to high redox stability. Still, the feasibility of FIB faces challenges due to the inadequate ionic conductivity of solid electrolytes at room temperature. $BaSnF_4$ is a solid electrolyte with high ionic conductivity, next to $PbSnF_4$, making it suitable for fabricating fluoride ion batteries at room temperature. In this work, $Ba_{1-x}K_xSnF_{4-x}$ ($0 \leq x \leq 0.15$) is synthesized through a hydrothermal strategy. $Ba_{1-x}K_xSnF_{4-x}$ (x=0.1) has shown comparatively high ionic conductivity of 1.46×10^{-4} S/cm with activation energy of 0.18 eV for its implementation in cell fabrication. The ionic transference number of the solid electrolyte Ba_{1-x} K_xSnF_{4-x} (x=0.1) investigated through the combined ac-dc technique is measured to be 0.94. The constructed room temperature Fluoride ion cell Sn(anode)/$Ba_{1-x}K_xSnF_{4-x}$ (x=0.1)/PbF_2.rGO(Composite cathode) is demonstrated with an electrochemical stability window of 1.5 V (in the range 0.3-1.8 V). The cell performance with an initial discharge capacity of 212 mAh/g is demonstrated at room temperature. Therefore, the substitutional doping of K^+ into the $BaSnF_4$ framework synthesized through the hydrothermal route has improved the ionic conductivity and enabled electrochemical performance at room temperature.

Keywords: Ionic conductivity, Cycling stability, Electrochemical stability window, Fluoride shuttle batteries, Solid electrolytes.

References

(1) Meena, M.; Bhide, A. Development of All-Solid-State Fluoride Ion Battery with Enhanced Electrochemical Stability. *J. Alloys Compd.* **2025**, *1016*, 178963. https://doi.org/10.1016/j.jallcom.2025.178963.

Fluorination Versus High-Entropy Cation Strategies in LLZO for Enhanced Ionic Conductivity and Stability

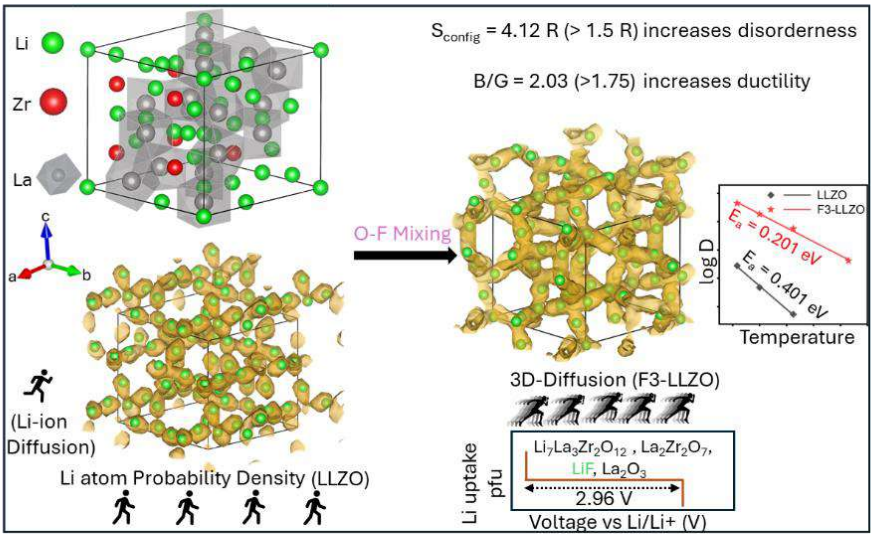
Saumya Ranjan Mahanta[1,*], Swastika Banerjee[1]

[a]*Computational Laboratory for Energy Application, Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand, 247667*

***E-mail:** sbanejee@cy.iitr.ac.in

Abstract

Solid-state electrolytes (SSEs) are critical to the development of next-generation lithium-ion batteries, offering enhanced safety, broad electrochemical stability, and the potential for high energy density. Among them, LLZO garnets have emerged as promising candidates due to their excellent chemical stability, reasonable lithium-ion conductivity, and robust mechanical properties. However, key challenges remain particularly at the electrode-electrolyte interface and in achieving ionic conductivities comparable to those of liquid electrolytes.[1,2]



The relationship between lithium vacancies and ionic transport in garnets is non-trivial; while vacancies facilitate Li-ion movement, excessive concentrations can induce (electro)chemical instability. In this study, we explore both cationic and anionic substitution strategies, including high-entropy (HE) cation mixing and anion doping, to overcome these limitations. Our findings reveal that the garnet structure inherently accommodates high compositional diversity, enabling tuning without compromising stability. Specifically, fluorine substitution in the oxygen sublattice (optimal F-doping) enhances Li-ion conductivity while maintaining low vacancy concentrations, simultaneously improving ductility and interfacial compatibility. These results underscore the potential of co-engineering both cation and anion chemistry to unlock high-performance, chemically stable garnet SSEs.

References

(1) Grey, C. P. Prospects for Lithium-Ion Batteries and Beyond — A 2030 Vision. *Nat. Commun.* **2020**, *11*, 6279.

(2) Frith, J. T.A Non-Academic Perspective on the Future of Lithium-Based Batteries. *Nat. Commun.* **2023**, *14*, 420.

(3) Mahanta, S. R.; Banerjee, S. Manuscript submitted, **2025**.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Composite Polymer Interface Design for High-Performance Na-ion Solid-State Batteries

Ravi P. Srivastava[$,1,2], Saurabh Sharma[$,1,*], Sandipan Bhattacharyya[1], Pratap Sharma[1], Mohd. Aman[1], Shobit Omar[1]

[1]*Department of Materials Science & Engineering, Indian Institute of Technology, Kanpur-208016, India*

[2]*Department of Metallurgical & Materials Engineering, Indian Institute of Technology Jodhpur, Karwar-342030, India*

[*] *saurabhs21@iitk.ac.in (Presenting author)*

[$] *contributed equally to the work*

Abstract

Solid-state sodium-ion batteries (SSSBs) have emerged as a promising alternative to lithium-ion batteries, offering enhanced safety, thermal stability, and cost-effectiveness. Despite their potential, the practical performance of SSSBs is often hindered by poor interfacial compatibility between the rigid ceramic solid electrolyte (SE) and the cathode, particularly under ambient conditions and high current operations. To address this limitation, this study introduces a simple and effective strategy involving a composite polymer interface modifier (CPIM) to enhance the cathode-SE interface.

The incorporation of CPIM significantly enhances ionic transport and interfacial contact, resulting in stable and efficient electrochemical performance. The modified SSSBs deliver near-theoretical discharge capacity with minimal degradation over extended cycling, even under high current rates. The improved performance is primarily attributed to the CPIM's high ionic conductivity and its ability to establish a more conformal and conductive interface between the cathode and the solid electrolyte. This reduces charge-transfer resistance and promotes efficient sodium-ion movement across the interface.

Overall, this approach highlights the potential of polymer-based interface engineering to overcome key interfacial challenges in SSSBs, contributing to the development of reliable and sustainable solid-state energy storage systems.

Keywords: Sodium-Ion Batteries, composite polymer electrolyte, interfacial engineering

ACEPS-13, January 11-14, 2026, Bengaluru, India

Cold sintering assisted densification for NASICON-type solid electrolyte for sodium ion battery

Sandipan Bhattacharyya[1,*], Saurabh Sharma[1], Sourav Shyamal[1] , Shobit Omar[1]

[1] *IIT Kanpur, Kanpur, Uttar Pradesh, India*

* sandipan20@iitk.ac.in

Abstract

The cold sintering process (CSP) is a potential method that enables densification at relatively lower temperatures. Sintering of ceramic electrolytes requires high temperature and longer time and is therefore, very energy-intensive. Moreover, high processing temperature causes material volatilisation as well as the formation of secondary phase(s), deteriorating the properties of the electrolyte. $Na_3Zr_2Si_2PO_{12}$ (NZSP), a promising NASICON-type solid electrolyte for sodium-ion batteries, also suffers the same problem of Na and P loss and formation of unwanted secondary phases (e.g. ZrO_2) due to its high temperature sintering at 1250 °C. In the present work, the CSP method is investigated for the sintering temperature of magnesium-doped NZSP, which successfully resulted in the highly-dense pellets at a lowered sintering temperature. X-ray diffraction, scanning electron microscope and impedance spectroscopy were used for the phase analysis, morphological study and ionic conductivity determination. The obtained data was compared further with samples prepared using the conventional route. To evaluate its electrochemical performance, coin cell was fabricated using a dense electrolyte prepared with optimised processing conditions, keeping iron-doped $Na_3V_2PO_{12}$ as cathode and Na-Metal as anode. The cell showed reasonably good cycling performance resulting around ~90% capacity retention over 100 cycles.

Keywords: Cold Sintering Process, Na-ion batteries, NASICON, Solid Electrolyte

Microstructure optimizations of Na_3SbS_4/$Na_3Zr_2Si_2PO_{12}$ composite solid electrolytes for improving cycling performance in Sodium All-solid-state batteries

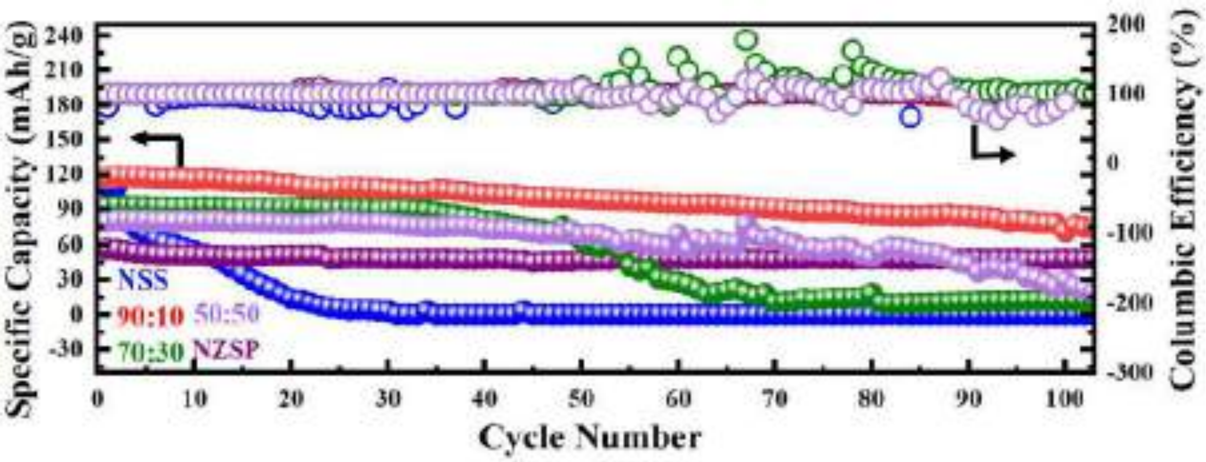
Celastin Bebina Thairiyarayar[1,*], Wei-Ren Liu[1]

[1] *Department of Chemical Engineering, R&D Center for Membrane Technology, Center for Circular Economy, Chung Yuan Christian University, 200 Chung Pei Road, Chung Li District, Taoyuan City, 32023, Taiwan, Republic of China.*

* *WRLiu1203@gmail.com*

Abstract

Solid-state sodium-ion batteries offer improved safety and cost advantages, but sulfide electrolytes such as Na_3SbS_4 (NSS) suffer from interfacial instability, by-product formation, and structural defects that hinder cycling performance [1]. To overcome these issues, we developed a composite electrolyte by incorporating NASICON-type $Na_3Zr_2Si_2PO_{12}$ [NZSP] into NSS. The optimized 90 wt% NSS-10 wt% NZSP composition effectively filled voids, blocked cracks, and enabled dual-phase Na^+ transport, increasing ionic conductivity to 0.37-0.396 mS cm^{-1} and reducing activation energy from 0.25 to 0.22 eV. In a $Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$ | composite | Na half-cell, the battery delivered 118.9 mAh g^{-1} and stable cycling for 100 cycles at 0.05 A g^{-1} as shown in Fig. 1. Cycle life of different compositions of Na_3SbS_4 - $Na_3Zr_2Si_2PO_{12}$ composite solid electrolytes. These results demonstrate that NZSP–NSS composites significantly enhance ionic transport and interfacial stability, advancing the development of high-performance sulfide-based solid-state sodium batteries.



Keywords: Na_3SbS_4; NASICON; Composite electrolyte; all-solid state sodium battery

References

(1) Mwemezi, M.; Park, W. B.; Ikhe, A. B. *Electrochim. Acta* **2024**, *480*, 143919.

ACEPS-13, January 11-14, 2026, Bengaluru, India

To dope fluorine into Halide Solid Electrolyte.

Silvia Begum[1] , Susmita Bera[2], Ripan K. Biswas[3], Lily Mandal[4], Abhik Banerjee*

Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology (TCG CREST), Sector V, Salt Lake, Kolkata 700091, India

* Abhik.banerjee@tcgcrest.org

A solid-state battery is the next-generation energy storage technology that promises high energy density, high power, and ultimate safety.[1] However, Li dendrite formation and high-voltage oxidation stability are two major challenges in developing solid-state batteries. Solid electrolytes are crucial components that provide cathodic and anodic stability. Nonetheless, no single electrolyte can solve all issues at the cathode-anode interface.[2,3] For example, sulphide solid electrolytes can interact chemically and electrochemically with both Li metal and high-voltage cathodes. In contrast, halides are stable up to 4.2V vs. Li on the cathode side but are highly reactive with Li metal. Oxide electrolytes are kinetically stable with Li metal and at high voltages; however, high processing conditions can create additional impedance on the cathode side due to cross-ion diffusion across the SE-oxide cathode interface.[4] Doping with fluorine is an effective strategy to improve both cathodic and anodic stability, with LiF stabilising Li metal and fluorine offering the highest electrochemical potential to enhance oxidation stability with high-voltage cathodes. Yet, fluorine-doping often reduces conductivity. In this abstract, we demonstrate how fluorine doping stabilizes cathodes and anodes through in operando XPS and electrochemical measurements, as well as methods to increase fluorine doping levels without sacrificing ionic conductivity.

Keywords: solid electrolyte1, fluorine substitution2, solid electrolyte interface3, ionic conductivity4

References

(1) Janek, J.; Zeier, W. G. A Solid Future for Battery Development. Nat. Energy 2016, 1, No. 16141..

(2) Schlem, R.; Banik, A.; Ohno, S.; Suard, E.; Zeier, W. G. Insights into the Lithium Sub-Structure of Superionic Conductors Li3YCl6 and Li3YBr6. Chem. Mater. 2021, 33, 327−337.

(3) Kraft, M. A.; Culver, S. P.; Calderon, M.; Böcher, F.; Krauskopf, T.; Senyshyn, A.; Dietrich, C.; Zevalkink, A.; Janek, J.; Zeier, W. G. Influence of Lattice Polarizability on the Ionic Conductivity in the Lithium Superionic Argyrodites Li6PS5X (X = Cl, Br, I). J. Am. Chem. Soc. 2017, 139, 10909−10918.

(4) Kamaya, N.; Homma, K.; Yamakawa, Y.; Hirayama, M.; Kanno,R.; Yonemura, M.; Kamiyama, T.; Kato, Y.; Hama, S.; Kawamoto, K.;et al. A Lithium Superionic Conductor. Nat. Mater. 2011, 10, 682−686.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Graphene and diglyme assisted improved Al^{3+} ion storage in MoO_3 nanorod: steps for high-performance aqueous aluminum-ion battery

Homen Lahan[1, 2,*], Shyamal Kumar Das[1],

[1] *Affication-1, Department of Physics, Tezpur University, Assam, India 784028*

[2] *Affication-2, Centre of Excellence Battery Engineering, Atria University, Bengaluru, India 560024*

* homen,l@atriauniversity.edu.in

Abstract

An approach to improve the Al^{3+} ion storage capacity of MoO_3 in aqueous electrolyte is illustrated here. Graphene as conductive additive and diglyme as electrolyte additive play a pivotal and synergistic role in the improvement. Graphene-MoO_3 composite exhibits stable capacity of 160 mAh g^{-1} over 100 cycles in diglyme mixed aqueous electrolyte with v/v mixing ratio of 50:50, whereas it delivers a capacity of only 75 mAh g^{-1} at the 100th cycle in pristine aqueous electrolyte. Besides, pristine MoO_3 also demonstrates improved stability in diglyme mixed aqueous electrolyte [1, 2].

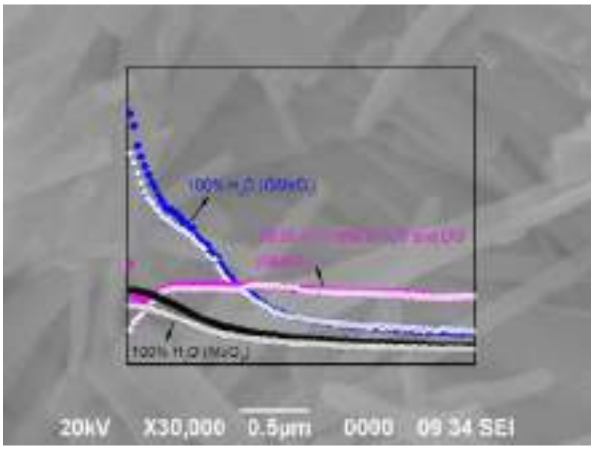


Fig. Graphical Abstract

Keywords (max 5): Aluminum-ion battery, Diglyme, Graphene, Molybdenum trioxide.

References

(1) Lahan, H. and Das, S. K. Graphene and diglyme assisted improved Al^{3+} ion storage in MoO_3 nanorod: steps for high-performance aqueous aluminum-ion battery. *Ionics,* 25:134-138, 2019.

(2) Das, S. K, Mahapatra, S, Lahan, H. Aluminium-ion batteries:developments and challenges. *J Mater Chem A*, 5:6347–6367, 2017.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Zinc-Magnesium Dual ion Battery utilizing spinel $MgMn_2O_4$ as cathode material.

Fahad Abu[1,*], Jitendra Kumar Yadav[2], Bharti Rani[2] , Priyanka Saini[2], Ambesh Dixit[2] , Manoj Kumar Singh[1,*]

[1] *Centre of Material Sciences, University of Allahabad, Prayagraj-211002, India.*

[2] *A-MAD Laboratory, Department of Physics, Indian Institute of Technology Jodhpur, Jodhpur-342030, India.*

* mksingh100@allduniv.ac.in

Abstract

Zinc-Magnesium Dual Ion battery (ZMDIB) was fabricated using $MgMn_2O_4$ as the cathode and metallic zinc sheet as the anode in the presence of an aqueous Zn, Mg dual-ion electrolyte. The cathode material was synthesized using hydrothermal method and the structural purity is confirmed with the physical characterizations, including XRD, RAMAN and EDX analysis. FESEM and BET techniques were used to investigate morphology and surface area of the synthesized material. The electrochemical performances of dual-ion battery were observed by fabricating coin cell and utilizing the techniques such as CV, GCD, and EIS. The performance and stability of dual-ion battery was enhanced by modifying the electrolyte. The highest specific capacity was found to be 177 mA h g^{-1} at 50 mA g^{-1}. It also showed good stability with capacity retention of 85 % after 2000 cycles at a current density of 0.5 A g^{-1}. Ex-situ XRD analysis was performed to check the electrode stability after long term cycling. The results indicated that the developed doped nanomaterial exhibits excellent charge storage characteristics, followed by a watch demonstration.[1,2]

Keywords: Electrochemical Analysis, Galvanostatic Charge/Discharge, Cyclic Voltammetry.

References

(1) Soundharrajan, V.; Sambandam, B.; Kim, S.; Mathew, V.; Jo, J.; Kim, S.; Lee, J.; Islam, S.; Kim, K.; Sun, Y.-K.; Kim, J. Aqueous Magnesium Zinc Hybrid Battery: An Advanced High-Voltage and High-Energy $MgMn_2O_4$ Cathode. *ACS Energy Lett* **2018**, *3* (8), 1998–2004. https://doi.org/10.1021/acsenergylett.8b01105.

(2) Xie, J.; Zhang, Q. Recent Progress in Multivalent Metal (Mg, Zn, Ca, and Al) and Metal-Ion Rechargeable Batteries with Organic Materials as Promising Electrodes. *Small* **2019**, *15* (15). https://doi.org/10.1002/smll.201805061.

Engineering NDI-Derived Organic Anodes for Enhanced Electrochemical Performance in Aqueous Calcium-Ion Batteries

Manisha Sanawa[1], Dipen Biswakarma[1] , Rekha Kumari[1], Aninda Jiban Bhattacharyya[1,2 *]

[1] *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru, Karnataka, 560012*

[2] *2Interdisciplinary Centre for Energy Research, Indian Institute of Science, Bengaluru, Karnataka, 560012*

* anindajb@iisc.ac.in

Abstract

Aqueous multivalent-ion batteries (Zn^{2+}, Mg^{2+}, Ca^{2+}, Al^{3+}) are emerging as safe, cost-effective, and sustainable alternatives to lithium-ion technologies, leveraging earth-abundant materials and the high charge-storage potential of multivalent redox processes. However, commercialization is hindered by the scarcity of electrode materials compatible with these aqueous systems, particularly in calcium-ion sytems. Organic electrode materials offer an attractive route forward, combining structural tunability, low cost, environmental benignity, and potential for multi-electron redox activity. (1)

Our research group has extensively investigated organic materials within aqueous battery systems, probing into mechanistic studies in multivalent systems (Zn^{2+}), both theoretically and experimentally.(2)

In this presentation, we report our development of derivatives of 1,4,5,8-naphthalenetetracarboxylic dianhydride (NDI) as organic anodes tailored for aqueous Ca^{2+} batteries. The optimised electrode exhibit enhanced structural stability and reversible Ca^{2+} redox behavior. Mechanistic insights from ex-situ spectroscopic characterization confirm reversible coordination of Ca^{2+} to carbonyl groups indicating redox conversion rather than traditional intercalation mechanisms.Finally, a full cell has been developed by combining it with prussian blue analogs. These design strategies align with broader efforts to harness aromatic dianhydrides like NTCDA/PTCDA as robust organic hosts in multivalent chemistries and offer a viable pathway toward practical aqueous Ca-ion devices.

Keywords : Organic anode · Naphthalenetetracarboxylic dianhydride (NDI) · Aqueous calcium-ion battery · Redox carbonyl conversion

References

(1) Dai, H.; Guan, L.; Mao, M.; Wang, C. Evaluating the Present and Future of Organic Batteries. *Nat. Rev. Clean Technol.* **2025**, *1*, 493–510.

(2) Venkatesha, A., Gomes, R., Nair, A. S., Mukherjee, S., Bagchi, B., & Bhattacharyya, A. J. (2022). A redox-active 2-D covalent organic framework as a cathode in an aqueous mixed-ion electrolyte Zn-ion battery: Experimental and theoretical investigations. *ACS Sustainable Chemistry & Engineering*, *10*(19), 6205–6216.

Electrolyte Engineering for Dendrite-Free and Long-Life Aqueous Zinc-Ion Batteries

Bhaskar Kakoty[1], Alapan Samanta[1], Premkumar Senguttuvan[1*]

[1] *New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India*

* prem@jncasr.ac.in

Abstract

Aqueous zinc-ion batteries (ZIBs) have garnered significant attention as a sustainable alternative to lithium-ion batteries (LIBs) due to their intrinsic safety, low cost, and abundance of zinc resources. Unlike LIBs, which rely on flammable organic electrolytes and critical raw materials like lithium and cobalt, ZIBs utilize water-based electrolytes and non-toxic materials, making them safer and more environmentally friendly. Additionally, zinc metal anodes offer a higher theoretical capacity and lower redox potential, making ZIBs attractive for large-scale energy storage applications. However, despite these advantages, aqueous ZIBs face several critical challenges that limit their commercial viability. The primary issues in ZIBs stem from the instability of the zinc anode in aqueous environments. Zinc metal is prone to dendrite formation during repeated plating and stripping, leading to short circuits and capacity decay. Moreover, continuous dissolution of cathode in mild acidic electrolyte limit long-term stability of the battery.[1,2]

This work tackles these issues through electrolyte engineering by incorporating organic co-solvents and functional additives into the aqueous electrolyte. These modifications successfully inhibit dendrite growth, suppress cathode dissolution by inducing a well-regulated SEI. The optimized electrolyte exhibits enhanced cycle life, high coulombic efficiency with stable capacity in full- cell configuration. Advanced characterization methods, such as time-of-flight secondary ion mass spectrometry (TOF-SIMS), *in-situ* FTIR, and MALDI spectroscopy are used to probe the SEI composition and its formation mechanism. These findings highlight the importance of electrolyte design in improving the zinc in battery stability and lifespan toward practical safe and sustainable energy storage.

Keywords: Electrolyte, Surface Chemistry, Zinc, Cathode, Aqueous

References

(1) Kakoty, B.; Vengarathody, R.; Mukherji, S.; Ahuja, V.; Joseph, A.; Narayana, C.; Balasubramanian, S.; Senguttuvan, P. *J. Mater. Chem. A Mater*. **2022**, *10* (23), 12597– 12607.

(2) Kakoty, B.; Brahma, D.; Ganguly, S.; Halder, S.; Jain, K, J.; Balasubramanian, S.; Rajaram, S.; Senguttuvan, P. *Chem. Mater.* **2025**, *37*, 8, 2907–2919.

Metal-organic hybrid interface for Zinc batteries

Akash Mukhraj Paswan , C. Retna Raj*.

Functional Materials and Electrochemistry Laboratory, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal-721302, India

* E-mail: crraj@chem.iitkgp.ac.in

Abstract

Energy storage is a stepping stone in the decarbonization of the power sector and the transition to environmentally friendly renewable sources. Aqueous zinc-ion batteries (ZIBs) are among the potential alternatives to replace non-aqueous lithium batteries owing to their high energy density and eco-friendliness. Zinc, with its high theoretical capacity (820 mAh g^{-1} / 5855 mAh cm^{-3}), low cost, and compatibility with aqueous systems, is both safe and environmentally friendly. [1-2] Although zinc batteries are strong contenders, they suffer from short cycle life and capacity fading. Over successive cycles, the anode suffers from dendritic growth, corrosion, and other parasitic reactions, which can cause the battery to short-circuit. The cathode, meanwhile, suffers from low capacity and active material dissolution, leading to capacity decay.[3-4] Herein, we demonstrate an approach for electrolyte engineering using 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPS) to mitigate ZIBs issue. AMPS, along with Zn^{2+}, forms a metal–organic hybrid interface at the electrode surface. This hybrid interface, with uniformly distributed polar functionalities, regulates zinc ion flux during plating, and suppresses corrosion and other parasitic reactions.[3] Electrochemical characterization in half-cell (Zn||Ti) shows a higher nucleation overpotential and improved coulombic efficiency (99.2%) for the modified electrolyte. The galvanostatic charge–discharge cycling of a symmetrical cell (Zn||Zn) made with the additive shows a cycle life >1050 h, compared with the blank electrolyte (200 h). A full cell (Zn||V_2O_5) fabricated with the modified electrolyte showed a high discharge-specific capacity of 304.6 mAh g^{-1} at 0.2 A g^{-1}, with a capacity retention of 59.25% after 200 cycles. Electrolyte engineering effectively suppresses dendritic growth at the anode, increases cycle life, and retards capacity fading at the cathode.

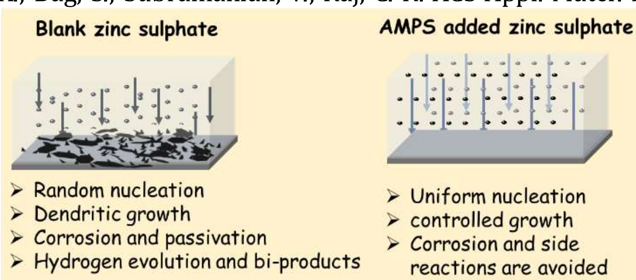
Keywords: zinc battery, electrolyte engineering, AMPS, 2-Acrylamido-2-methyl-1-propanesulphonic acid, metal organic hybrid layer

References

1. Mallick, S.; Raj, C. R. ChemSusChem 2021, 14, 1987– 2022.

2. Paswan, A. M.; Thakur, V. S.; Banerjee, S.; Raj, C. R. Adv. Funct. Mater. 2025, 35 (2), 2412370.

3. Mallick, S.; Choutipalli, V. S. K.; Bag, S.; Subramanian, V.; Raj, C. R. ACS Appl. Mater. Interfaces 2022, 14 (33), 37577– 37586.



ACEPS-13, January 11-14, 2026, Bengaluru, India

Zinc-Based Biopolymer Gel Electrolytes with Dual Crosslinking for High-Performance and High-Power Applications

Arpita Mishra[1], Anshuman Dalvi*

[1] Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Vidya Vihar, Pilani, Rajasthan 333031, India

* p20240474@pilani.bits-pilani.ac.in

Abstract

The growing demand for sustainable, safe, and high-performance energy storage systems has driven intensive research into gel polymer electrolytes, especially those derived from natural biopolymers. This work presents a zinc-based biopolymer gel electrolyte employing a dual crosslinking strategy that combines covalent bonding and zinc ion coordination. The biopolymer matrix—formulated using eco-friendly precursors such as dialdehyde cellulose and gelatin—forms a robust, three-dimensional hydrogel structure that ensures mechanical durability, thermal resilience, and efficient ion transport pathways.

The synergistic effect of dual crosslinking significantly enhances the electrolyte's ionic conductivity and flexibility while effectively mitigating zinc dendrite formation. Electrochemical analyses reveal a wide electrochemical stability window, low interfacial resistance, and prolonged cycling stability under high-rate charge/discharge conditions. In zinc-ion battery (ZIB) applications, the gel electrolyte enables stable and reversible zinc plating/stripping with high Coulombic efficiency. Additionally, its application in supercapacitors demonstrates superior power performance and rapid ion diffusion capabilities. These results highlight the potential of scalable, biopolymer-based dual-crosslinked gel electrolytes as viable candidates for next-generation energy storage technologies requiring both high energy and high-power outputs.

Keywords: Zinc-ion battery, Biopolymer electrolyte, Dual crosslinking, Gel polymer, Energy storage

ACEPS-13, January 11-14, 2026, Bengaluru, India

Photo-assisted self-chargeable aqueous Zn-ion batteries

Ganesh Mahendra[1,2], Rahuldeb Roy [1,3], Ashutosh K. Singh[1,2,3]

[1] *Centre for Nano and Soft Matter Sciences, Bangalore, Karnataka, 562162 India*

[2] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India.*

[3] *Manipal Academy of Higher Education, Manipal, Karnataka, 576104, India*

* Corresponding author's email address: aksingh@cens.res.in, ashuvishen@gmail.com

Abstract

Aqueous zinc ion batteries (ZIBs) have paved the way for manufacturing safe and high-capacity batteries. Photobattery can be a viable solution where solar energy is converted and stored efficiently while being compact [1]. In this study, we present a new self-charging energy storage device by investigating chemical processes for air-based recharging in photo-assisted Zn-ion device, utilizing VO_2/WO_3 as a cathode. Here, hydrated vanadium oxide ($VO_2·xH_2O$) nanoribbons synthesized by hydrothermal method, are used in aqueous ZIB [2]. Aqueous electrolyte is sustainable, due to the Zn-based salts being cost-effective, abundant and ease of preparation. The air-based charging achieves an Open Circuit Potential (OCP) of 1 V, reaching 0.9 V OCP within 140 s. The blend of $VO_2·xH_2O$ and WO_3 resulted in photocathode which can convert solar energy and store it as electrochemical energy in ZIB [3].

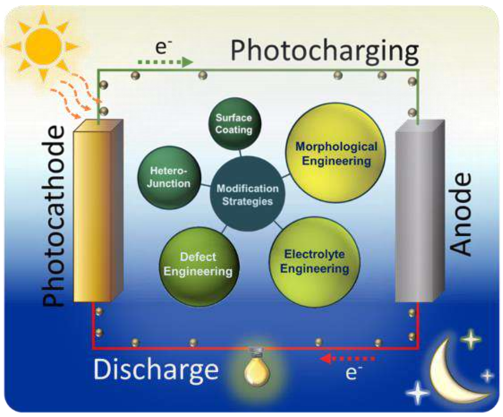


Fig.1. Schematic of the photo-assisted aqueous Zn-ion battery

Keywords (max 5): Zinc ion battery, Self-rechargeable, Photo battery, Energy storage, Metal-air battery

References

(1) Mary, A. S., Mahendra, G., Roy, R., Ganesha, M. K., & Singh, A. K. EES Batteries, (**2025**)

(2) Mahendra, G., Roy, R., and Singh, A. K. J. Power Sources, **624**, 235515 (**2024**).

(3) Roy, R., Mahendra, G., and Singh, A. K. Chem. Eng. J., **500**, 156870 (**2024**).

ACEPS-13, January 11-14, 2026, Bengaluru, India

Electrode/Electrolyte Interphase Engineering for highly stable Zn Anode

Dinesh Patel[1,2], Dr. Xiaolei wang[2], Dr Ashwini Kumar Sharma[1]

[1]Indian Institute of Technology Roorkee, India

[2]University of Alberta, Alberta, Canada

Email: Ashwini@ch.iitr.ac.in, xiaolei.wang@ualberta.ca

Abstract

Aqueous zinc batteries (AZBs) are an emerging energy storage technology that offers enhanced safety, environmental sustainability, and strong potential for grid-scale applications.[1,2] However, the inherent thermodynamic instability of the Zn anode in aqueous electrolytes presents significant challenges, including corrosion, hydrogen evolution reaction (HER), and dendrite formation.[3,4] These issues drastically reduce the cycle life and coulombic efficiency of the zinc anode. To overcome these challenges, the formation of a stable and robust in situ solid electrolyte interphase (SEI) on the anode surface, achieved through the decomposition of electrolyte components, plays a crucial role in suppressing side reactions and improving anode stability and performance. Fluoride-based interphase engineering, incorporating zincophilic and hydrophobic properties through electrolyte modification, offers a simple yet effective approach with promising advantages. Zincophilic materials enhance zinc ion transfer kinetics, while hydrophobic components mitigate water-induced side reactions by reducing water activity near the anode, thereby improving the overall stability of the Zn metal anode. In this study, we utilized an aqueous zinc salt electrolyte with a fluorine-based additive, which promotes the formation of a ZnF_2-rich inorganic inner layer and a fluoride-rich organic outer layer. The synergistic effects of this engineered SEI architecture significantly enhance the cycling stability of the zinc anode, even under high current density.

Keywords: Interphase Engineering, Aqueous battery, Zinc battery, Electrolyte addtives

References:

1. Ponnada, S.; Kiai, M. S.; Krishnapriya, R.; Singhal, R.; Sharma, R. K. Lithium-Free Batteries: Needs and Challenges. *Energy and Fuels*, **2022**, 6013–6026.
2. Wang, J.; Hu, H.; Zhang, H.; Zhao, J.; Li, X.; Song, Z.; Ding, J.; Deng, Y.; Han, X.; Hu, W. Regulating the Catalytically Active Sites in Low-Cost and Earth-Abundant 3d Transition-Metal-Based Electrode Materials for High-Performance Zinc-Air Batteries. *Energy and Fuels* **2021**, *35* (8), 6483–6503.
3. Yue, J.; Suo, L. Progress in Rechargeable Aqueous Alkali-Ion Batteries in China. *Energy and*

Fuels, **2021**, 9228–9239.

4. Xu, C.; Li, B.; Du, H.; Kang, F. Energetic Zinc Ion Chemistry: The Rechargeable Zinc Ion Battery. *Angewandte Chemie* **2012**, *124* (4), 957–959.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Transition Metal–Buffered Tellurium Cathodes for Zinc-Ion Batteries

Meenu C Ignatius[1,], Christie Thomas Cherian[1*]

[1]*School of Electronic Systems and Automation, Digital University Kerala, Thiruvananthapuram, India*
**Email: christie.cherian@duk.ac.in*

Abstract

Zinc-ion batteries (ZIBs) have emerged as a promising solution for sustainable energy storage, owing to their inherent safety, environmental compatibility, and the availability of zinc, positioning them as attractive candidates for both grid-scale and portable energy applications. The overall performance of ZIBs is determined by the choice of cathode material. Conventional cathodes, including manganese oxides, vanadium oxides, and Prussian Blue Analogues(PBA), primarily function via intercalation and surface redox reaction processes, which inherently limit their specific capacity and cycling stability.

Achieving higher energy densities necessitates the development of cathode materials that combine elevated redox potentials with substantial specific capacities, as intercalation-based cathodes are intrinsically constrained in these respects. Chalcogen elements such as sulfur, selenium, and tellurium are particularly promising for advancing ZIB technology, as their high redox potentials and large theoretical capacities combined with the ability of their cathodes to undergo positive valence state conversions, thereby positioning conversion-type cathodes as a compelling avenue for advancing ZIB technology[1]. Among these, tellurium distinguishes itself due to its outstanding electrical conductivity (2×10^2 S m^{-1}) and high volumetric capacity (2621 mAh cm^{-3}), greatly surpassing the corresponding properties of sulfur and selenium[2]. While conversion-type cathodes may be prone to structural degradation during cycling, this challenge can be addressed through the incorporation of buffering systems, such as transition metal. The electrolyte plays a major role in serving as an ion-conducting medium and stabilizing cationic tellurium species[3].

In this study, metal telluride-based electrodes were synthesized, and their structural and morphological features were confirmed through X-ray diffraction (XRD) and scanning electron microscopy (SEM). Electrochemical characterizations were performed in a Zinc||metal telluride battery configuration using a Swagelok cell. The electrochemical behavior was investigated by cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) techniques. The influence of different electrolyte concentrations on battery performance was analyzed in a voltage range of 0–1.8 V.

Keywords: Zinc Ion Battery, Tellurium cathode, Transition metal buffer

References

(1) Chen, Z.; Zhi, C. Chalcogens for High-Energy Batteries. *Nature Reviews Materials*. Nature Research April 1, 2025, pp 268–284. https://doi.org/10.1038/s41578-025-00773-7.

(2) Chen, Z.; Wang, S.; Wei, Z.; Wang, Y.; Wu, Z.; Hou, Y.; Zhu, J.; Wang, Y.; Liang, G.; Huang, Z.; Chen, A.; Wang, D.; Zhi, C. Tellurium with Reversible Six-Electron Transfer Chemistry for High-Performance Zinc Batteries. *J Am Chem Soc* 2023, *145* (37), 20521–20529. https://doi.org/10.1021/jacs.3c06488.

(3) A High-Energy Tellurium Redox-Amphoteric Conversion Cathode Chemistry for Aqueous Zinc Batteries.

Compositional and Defect-Driven Ion Transport in Layered Oxides for Na-Ion and Aqueous Zn-Ion Batteries

Vikas Singh Thakur[a] and Swastika Banerjee*[a]
[a]*Computational Laboratory for Energy Application, Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand, 247667*
***E-mail:** sbanejee@cy.iitr.ac.in

Abstract

The growing demand for large-scale, sustainable energy storage has intensified the search for battery technologies beyond lithium. This shift has driven growing interest in post-lithium systems that employ earth-abundant elements and multivalent-ion chemistries.[1,2] Among emerging alternatives, sodium-ion and aqueous zinc-ion batteries stand out for their low cost, high natural abundance, and potential for scalable energy storage. Realizing the full potential of these systems lies in engineering cathode materials that combine fast ion transport, high redox activity, and structural robustness. Layered transition metal oxides (TMOs) are particularly attractive for their compositional flexibility and rich redox chemistry. However, realizing their full potential requires deeper exploration of the compositional landscape and defect engineering strategies within layered cathodes to enhance ionic conductivity, activate additional redox mechanisms, and maximize reversible capacity.[3,4] In Na-ion chemistry, we explore aliovalent doping, cation vacancies, and their interplay to reveal cooperative and non-cooperative effects that enhance Na^{+} diffusion, promote oxygen redox, and stabilize P2–O3 phase transitions. In aqueous Zn-ion batteries, where Zn^{2+} mobility is intrinsically limited, we provide mechanistic insights into Zn^{2+} transport in layered oxides, highlighting how defect engineering and co-intercalation synergistically improve rate capability. These findings advance our understanding of how structural descriptors regulate ion transport and phase behaviour in layered cathodes, offering valuable design principles for high-performance, next-generation cathode materials.

Keywords: Layered Cathode, Batteries, Redox Chemistry, Energy Storage, Ion Diffusion

References

(1) Thakur, V. S.; Banerjee, S. *The Journal of Physical Chemistry. C,* **2024**, *128* (19), 7865–7875.

(2) Paswan, A. M.; Thakur, V. S.; Banerjee, S.; Raj, C. R. *Advanced Functional Materials* **2025,** *35* (2).

(3) Niu, Y.; Hu, Y.-S. et al. *Energy & Environmental Science* **2024**, *17* (20), 7958–7968.

(4) Janek, J.; Zeier, W. G. et al. *Nature Communications* **2018**, *9*(1), 1656.

Tailoring Charge Carrier Dynamics *via* Atomic-Scale Interface Engineering in S-Scheme $Bi_2WO_6/ZnIn_2S_4$ Photoanodes for Photoelectrochemical Water Splitting

Dipendu Sarkar[1,2], Srabanti Ghosh[1,2,*]

[1]*Energy Materials & Devices Division (EMDD), CSIR - Central Glass and Ceramic Research Institute, Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India*

[2]*Academy of Scientific & Innovative Research (AcSIR), Ghaziabad, 201002, India*

* Corresponding author's email: srabanti@cgcri.res.in, ghosh.srabanti@gmail.com

Abstract

Enhancement of renewable H_2 production *via* water splitting using visible light-driven semiconductor photocatalysts has long received global attention because of its great potential for low cost and sustainability. Bismuth Tungstate (Bi_2WO_6), with its broad band gap, poses challenges to efficient visible light absorption and suffers from rapid electron-hole recombination, limiting its hydrogen production efficiency.[1] We have engineered a heterojunction between Bi_2WO_6 (BWO) and $ZnIn_2S_4$ (ZIS),[2] which enhances visible light absorption and promotes effective charge separation, reducing the recombination of photoexcited charge carriers and increasing the drift velocity of electrons and holes. In this study, assembled rod-like BWO structures are combined with nanoplate-like ZIS, creating a unique hybrid morphology. Interestingly, the metallic Bi formed during the synthesis of the heterojunction significantly enhances charge separation efficiency and creates favourable electronic states that facilitate the accumulation of photogenerated electrons at the semiconductor interface. Furthermore, the reduction of trap states after heterojunction formation reduces electron-hole recombination and extends the lifetime of charge carriers, significantly boosting H_2 generation performance and photoelectrochemical response. The optimized BWIS@0.26 heterojunction exhibits a photocurrent response that is 10 times higher compared to bare BWO owing to the synergistic effects of metallic Bi and trap-state engineering at the interface. Our findings demonstrate that interface engineering of semiconductors is a viable approach to improve the efficiency of photoelectrochemical systems for renewable energy applications.

Keywords: $Bi_2WO_6/ZnIn_2S_4$ heterostructures, S-scheme heterojunction, Photoelectrochemical water splitting, Defect states, Interfacial Bi-S bond

References

(1) Ghosh, S.; Das, P. S.; Bera, S.; Sarkar, D.; Roy, K.; Nath, S.; Ghosh, P.; Ghosh, C. K.; Allu, A. R. Conjugated Polymer-Supported Doped Bi_2WO_6 S-Scheme Heterojunction for Proficient Water Splitting via Dual Regulation of Band Gap Engineering and Improved Charge Separation. *ACS Appl. Energy Mater.* **2024**, *7* , 10906–10920.

(2) Zhao, X.; Xie, S.; Huang, H.; Zhu, X.; Li, J.; Yang, L.; Bai, L.; Wei, D.; Yin, K.; Yang, H.; Chen, H.; Luo, M. $ZnIn_2S_4$ Quantum Dot/Mo-Doped $WO_{2.72}$ Nanowire Heterojunctions Boost the Photocatalytic Desulfurization of Diesel. *ACS Appl. Nano Mater.* **2024**, *7* , 11767–11776.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Zinc-assisted engineering of Co–N_x sites in polymer derived perforated carbon for high performance oxygen reduction reaction

Prakash Subramani [a,b], Sreekuttan M. Unni [a,b]*

a CSIR-Central Electrochemical Research Institute Chennai Unit, CSIR Madras Complex, Taramani, Chennai-600113, Tamil Nadu, India.

b Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

* *sreekuttanunni@cecri.res.in*

Abstract

Electrocatalysts for the oxygen reduction reaction (ORR) are crucial for the development of high-efficiency fuel cells and metal-air batteries. Nonetheless, developing cost-effective catalysts that offer both high activity and durability remains a major challenge. In this context, we present a successful approach to enhance the electrocatalytic performance of Co-N-C by adjusting the density of the active reaction centres through the strategic use of Zn. Zinc acts as an in-situ pore-forming agent to maximise the number of active sites in a Co-N-C catalyst synthesised from a mixture of polyaniline and cobalt chloride hexahydrate using a thermal degradation route (ZC-N/C). The zinc ions in the precursor not only enhance the surface area of the resulting carbon, but also inhibit the formation of cobalt oxide/sulfide, maximising the +2 and +3 oxidation states of cobalt on the carbon surface. The synergistic effect of Zn, Co, and the N-doped carbon matrix alters the electronic structure of the active metal sites and enhances the active reaction density, thus enhancing ORR activity. The ORR onset and half-wave potentials of the synthesised ZC-N/C are on par with those of the state-of-the-art commercial Pt/C under alkaline conditions. Additionally, ZC-N/C shows an exchange current density of 3.23×10-4 A cm-2 and a rate constant of 6.65×10-4 cm s-1 for the ORR, which is comparable to that of Pt/C. ZC-N/C reduces the oxygen molecules through a four-electron transfer pathway with 2% H2O2 production. The distinctive electronic interaction of doped Co/Zn-Nx moieties in ZC-N/C provides excellent stability with a ΔE1/2 of 16 mV even after 10000 cycles between 0.6 - 1 V vs RHE. Moreover, the performance of ZC-N/C as a cathode catalyst in an anion exchange membrane fuel cell (AEMFC) shows a Pmax of 215 mW cm-2, which is similar to that of Pt/C (214 mW cm-2). In addition, a zinc-air cell assembled using ZC-N/C as the cathode demonstrates a power density of 136 mW cm-2, along with outstanding rate capabilities and stability. At a current density of 5 mA cm-2, ZN-N/C achieved a capacity of 777 mAh gZn-1, which represents 95% of the theoretical capacity of the Zn-air cell. These results highlight that Zn/Co–NC is a potentially cost-effective electrocatalyst for the ORR in low-temperature AEMFC and Zn-air batteries.

Keywords: Anion exchange membrane fuel cells (AEMFC), Zinc-air battery (ZAB), Oxygen reduction reaction, Nitrogen-doped carbon, Cobalt sulfite nano particles.

References

(1) Tian, H.; Liu, X.; Dong, L.; Ren, X.; Liu, H.; Price, C. A. H.; Li, Y.; Wang, G.; Yang, Q.; Liu, J. Enhanced Hydrogenation Performance over Hollow Structured Co-CoO *x*@N-C Capsules. *Adv. Sci.* **2019**, *6* (22), 1900807

(2) Jiang, S.; Zhu, C.; Dong, S. Cobalt and Nitrogen-Cofunctionalized Graphene as a Durable Non-Precious Metal Catalyst with Enhanced ORR Activity. J. Mater. Chem. A **2013**, 1 (11), 3593-3599.

(3) Sun, T.; Wu, Q.; Zhuo, O.; Jiang, Y.; Bu, Y.; Yang, L.; Wang, X.; Hu, Z. Manganese Oxide-Induced Strategy to High-Performance Iron/Nitrogen/Carbon Electrocatalysts with Highly Exposed Active Sites. *Nanoscale* **2016**, *8* (16), 8480–8485.

MOF-Driven Electrocatalytic Dioxygen Redox Switching in Rechargeable Air Batteries

Hitesh Kumar[1], Anweshi Dewan[1], Neethu Christudas Dargily[1], Bhojkumar Nayak[1], Biplab Ghosh[2,*], and Musthafa Ottakam Thotiyl[1,*]

[1] *Department of Chemistry, Indian Institute of Science Education and Research (IISER)-Pune, Dr. Homi Bhabha Road, Pashan, Pune 411008, Maharashtra, India*

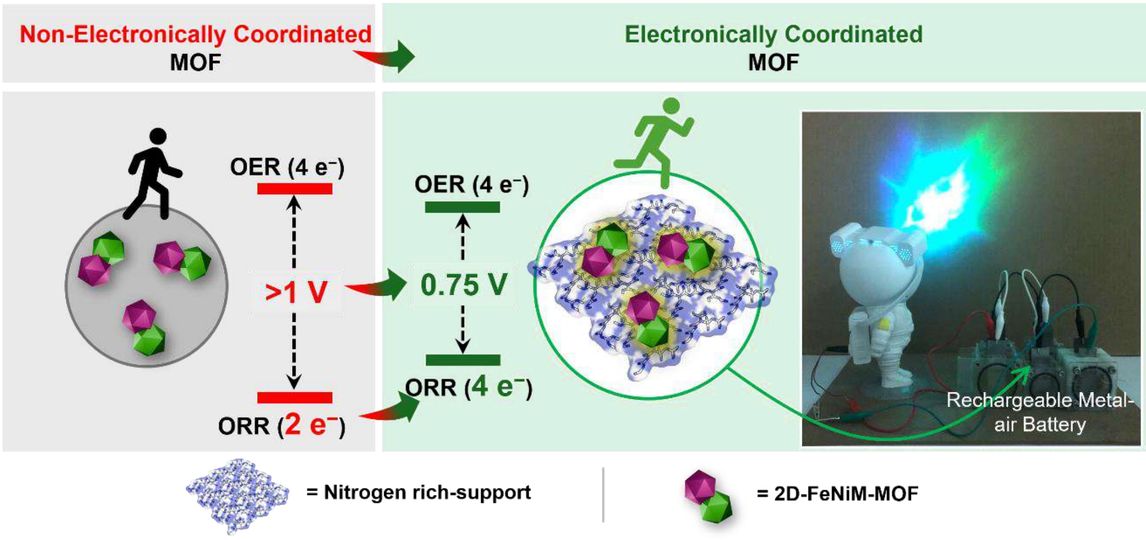
musthafa@iiserpune.ac.in

[2] *Beamline Development and Application Section, Bhabha Atomic Research Centre, Mumbai 400094, India*

biplab@rrcat.gov.in

Abstract

In this work, we engineer a bimetallic Fe-Ni 2D MOF intimately interfaced with nitrogen-rich g-C_3N_5, driving localized charge redistribution at the atomic scale. This dynamic heterostructure shows a unique reorganization of oxidation states, ligand fields and oxygen vacancy distribution, precisely tailoring active site geometry and electronic properties. Such synergy fundamentally alters dioxygen redox processes kinetically as well as mechanistically, reducing voltage gaps by 250 mV alongside unlocking remarkable catalytic efficiencies. Advanced spectroscopic studies confirm electronic restructuring, while high-resolution microscopy reveals the atomic arrangement and defect landscapes responsible for superior activity. Integration of this tuned MOF in a zinc-air battery yields a high peak power density of 163 mW·cm^{-2}, a specific capacity of 778 mAh/g and remarkable stability exceeding 100 hours, with high round-trip efficiency retention of 57.4% compared to Pt/C + RuO_2 system (42.5%). This work elucidates the transformative potential of atomic control and electronic synergy in MOF-based materials, setting new paradigms for designing high-performance, tunable catalysts for sustainable energy solutions.



.

Keywords: (Bimetallic Metal Organic Framework, Oxygen Reduction Reaction, Oxygen Evolution Reaction, Zinc Air Battery)

ACEPS-13, January 11-14, 2026, Bengaluru, India

Design of a High-Performance bifunctional electrocatalyst for Aqueous rechargeable Zn–CO_2 Batteries toward Efficient CO_2 Conversion and Energy Storage

Akriti Gautam, Ravinder Sharma, Aditi Halder*

School of Chemical Sciences, Indian Institute of Technology Mandi, Mandi 175005, Himachal Pradesh, India

*aditi@iitmandi.ac.in

Abstract

The aqueous Zn-CO_2 battery has a high theoretical capacity of Zn (820 mAh g^{-1}) and uphold a unique potential in CO_2 fixation and reduction, as well as energy conversion and storage, which has been developing fast in recent years[1]. Since, CO_2 elimination from the atmosphere is a tedius and expensive process, thus CO_2 conversion and utilization process such as electrochemical CO_2 reduction (E-CO_2R) provide a sustainable approach to convert CO_2 into valuable fuels and feedstocks. The electrochemical reactions that occur at the cathode during charging and discharging, namely the oxygen evolution reaction (OER) and CO_2RR, respectively, are primarily responsible for the performance of aqueous rechargeable Zn–CO_2 batteries (ARZCBs) [2]. Since, these two reactions participates at the cathode and the fundamental mechanisms are also different for both the reaction. Thus, design and development of a bifunctional (CO_2RR-OER) catalyst with optimum activity is primarily needed for the development of ARZCBs. In this work, we utilized Bimetallic transition metal sulfide as a bifunctional catalyst for OER and CO_2RR. To evaluate electrochemical CO_2RR, LSV and chrono-amperometry in three electrode system (H-cell) have been performed and reaction was monitored for various products like ethanol and hydrogen by using NMR and GC technique.

Keywords : Zn–CO_2 battery, Electrochemical CO_2 reduction, Oxygen evolution reaction, Bifunctional catalyst

References

(1) Guo, W.; Wang, Y.; Yi, Q.; Devid, E.; Li, X.; Lei, P.; Shan, W.; Qi, K.; Shi, L.; Gao, L. Research progress of aqueous Zn–CO2 battery: design principle and development strategy of a multifunctional catalyst. *Frontiers in Energy Research* **2023**, *11*, 1194674.

(2) Gupta, D.; Mao, J.; Guo, Z. Bifunctional Catalysts for CO2 Reduction and O2 Evolution: A Pivotal for Aqueous Rechargeable Zn– CO2 Batteries. *Advanced Materials* **2024**, *36* (35), 2407099.

FeCo MOF@ NiCo LDH as an Efficient Catalyst for Electrochemical Oxidation of Biomass Derived 5-Hydroxymethylfurfural in 3D Printed Electrolyser

Prateek Shukla[1], Suddhasatwa Basu[1,*]

Department of Chemical Engineering and Technology, Indian Institute of Technology, Delhi, 110016

**Corresponding author Email:* sbasu@iitd.ac.in

Abstract

Hydroxymethylfurfural (HMF) is one of the important platform chemicals derived from biomass, which is used to synthesise 2,5-furandicarboxylic acid, a precursor for green polymer polyethene furanoate [1]. Electrochemical oxidation of HMF takes place at near-ambient conditions and has significant advantages over conventional processes, but the high cost of flow electrolysers and the dearth of robust electrodes restricts the research to batch processes. Nickel and Cobalt-based layered double hydroxide (NiCo-LDH) catalysts have shown enhanced catalytic activity due to their adaptable layered structure and chemical compatibility for the HMF oxidation reaction [1]. However, they suffer from low conductivity, which limits their performance. Nevertheless, the heterostructure interface can improve their catalytic properties, thereby enhancing the charge transfer and leading to better contact between the electrolyte and the catalyst. Herein, we report the two-step process for the synthesis of CoFe metal-organic framework over NiCo LDH, which could be used as a cathode in a 3D printed flow electrolyser. The synergy between MOFs and LDH catalysts allows for a greater surface area, improved controlled coordination environments, and increased molecular adsorption. The as-prepared CoFe MOF over NiCo LDH at Nickel foam demonstrated around 94% conversion of 10 mM HMF in 1 M KOH with 95% FDCA selectivity at a potential of 1.4 V vs RHE in batch process studies. Accordingly, a 3D-printed flow electrolyser is fabricated for the continuous HMFOR [2]. This strategy facilitates the development of lightweight, cost-effective, highly efficient electrolysers and enables rapid scalability for HMFOR.

Keywords: 3D printed electrolyser, HMF oxidation, metal organic framework, layered double hydroxides

References

[1] Yang, Y.; Mu, T. Electrochemical Oxidation of Biomass Derived 5-Hydroxymethylfurfural (HMF): Pathway/Mechanism, Catalysts and Coupling Reactions. *Green Chemistry* **2021**. https://doi.org/10.1039/d1gc00914a

[2] Singh, A.; Singh, K.; Dixit, R. J.; De, B. S.; Basu, S. Co-Generation of Hydrogen and FDCA from Biomass-Based HMF in a 3D-Printed Flow Electrolyzer. *Industrial & Engineering Chemistry Research* **2024**. https://doi.org/10.1021/acs.iecr.4c01213

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhanced Hydrogen Evolution Reaction via Wet-chemical Synthesis of Mixed-Phase 1T/2H MoS_2

Sukanti Behera[1,*] Ramesh Avala[1]

[1] *Chemistry department, Maulana Azad National Institute of Technology Bhopal-462003, India.*

* sukantib.manit@gmail.com

Abstract

This work investigates at the electrocatalytic characteristics of two-dimensional (2D) molybdenum disulfide (MoS_2) phases for the hydrogen evolution reaction (HER), which is an important pathway for production of sustainable hydrogen fuel. 2D transition metal dichalcogenides (TMDs) are known for their distinct electrical and optical properties, making them suitable for a variety of applications, including catalysis. Specifically, MoS_2 is a viable alternative to high-cost platinum catalysts in HER process, with the mixed 1T/2H phase renowned for its higher activity than more frequent 2H phase. We present the bulk synthesis of 2H-MoS_2-C and mixed 1T/2H-MoS_2 by a wet-chemical approach, and investigate the effect of reaction time on their characteristics. Our findings demonstrate the enhanced HER efficiency of the combined 1T/2H-MoS_2 phase. Quantitative electrochemical experiments demonstrate that mixed 1T/2H-MoS_2 has a low overpotential of 260 mV at 10 mA/cm^2 and a Tafel slope of 65 mV/dec. These values outperform those of MoS_2-C (470 mV at 10 mA/ cm^2, 99 mV/dec) and pristine 2H-MoS_2 (530 mV at 7.7 mA/ cm^2, 204 mV/dec). The mixed-phase MoS_2 increased electrocatalytic activity is ascribed to the conductive 1T phase, which has a greater active surface area that includes both basal planes and edges, giving it a considerable advantage over the 2H phase of edge-limited activity.

Keywords: 1T/2H-MoS_2, 2D-TMDs, HER, Wet-chemical, MoS_2-C

NiFe Boride-Derived Catalysts for Efficient and Stable Oxygen Evolution in AEM Electrolyzers

Palash Jyoti Gogoi[1,2], Neena S. John[1,2]

[1]*Centre for Nano and Soft Matter Sciences (CeNS), Shivanapura, Bengaluru 562162, India*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*

* jsneena@cens.res.in

Abstract

Metal alloyed borides are gaining attention as next-generation catalysts for the oxygen evolution reaction (OER), a crucial step in water splitting. Their high conductivity, tunable composition, and abundance make them appealing alternatives to noble metals[1]. However, their long-term stability under industrially relevant conditions, including high current densities and elevated temperatures, remains underexplored. In this study, we employ a phase composition modulation strategy to design efficient and durable OER catalysts based on metal alloyed borides. This approach facilitates in situ phase evolution during electrocatalysis, forming catalytically active borate/oxide species[2]. In situ X-ray absorption spectroscopy (XAS) confirms that the transformation of metal borides into metal borates is essential to achieving high activity and durability. A nickel–iron alloyed boride-derived catalyst demonstrates an overpotential of 250 mV at 10 mA cm^{-2} in 1 M KOH, along with remarkable stability at 100 mA cm^{-2} for over 50 hours. These results highlight its strong performance under practical current densities. To further validate its applicability, the catalyst is incorporated into an anion exchange membrane (AEM) water electrolyzer paired with a Pt/C cathode. The device operates stably at 1.8 V and 50 °C for over 70 hours, showcasing excellent durability under industrial conditions.

Our findings provide valuable insights into the structure–activity relationships of boride-based catalysts and emphasize the significance of phase engineering in designing scalable, cost-effective materials for green hydrogen production.

Keywords (max 5): OER, AEM electrolyser, *in situ* XAS, metal alloyed boride

References

(1) Cai, W.; Yang, H.; Zhang, J.; Chen, H.-C.; Tao, H. B.; Gao, J.; Liu, S.; Liu, W.; Li, X.; Liu, B. Amorphous Multimetal Alloy Oxygen Evolving Catalysts. *ACS Mater Lett* **2020**, *2* (6), 624–632. https://doi.org/10.1021/acsmaterialslett.0c00146.

(2) Zou, X.; Zhang, W.; Zhou, X.; Song, K.; Ge, X.; Zheng, W. The Surface of Metal Boride Tinted by Oxygen Evolution Reaction for Enhanced Water Electrolysis. *Journal of Energy Chemistry* **2022**, *72*, 509–515. https://doi.org/10.1016/j.jechem.2022.05.039.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Escalating OH- desorption in bimetallic HER electrocatalyst for anion exchange membrane water electrolysis

Vipin Yadav[1], Vanshree parey[2], Ayush Kumar Shaw[1], Sudip Chakraborty[2*] and M. M. Shaijumon[1*]

[1] *School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Maruthamala PO, Kerala, 695551, India.*

[2] *Harish-Chandra Research Institute (HRI), Jhunsi, Prayagraj – 211019, U.P., India.*

* Email: shaiju@iisertvm.ac.in

Abstract

Ruthenium-based nanoclusters are emerging as promising electrocatalysts for alkaline hydrogen evolution reaction (HER), owing to their strong water dissociation capability.[1] However, their catalytic performance is often limited by the strong adsorption of hydroxide ions (OH^-), which is crucial for anion exchange membrane water electrolyser (AEMWE) for achieving the amperes level current density.[2] To address this limitation, we have designed a ruthenium–cobalt bimetallic nanocluster anchored on a nitrogen-doped carbon matrix, which improves the OH^- desorption from Ru sites, lowers water dissociation energy, resulting in enhanced HER kinetics. The improved OH^- desorption has been validated by cyclic voltammetry and in situ Raman spectroscopy in 1.0 M KOH. In particular, an anion exchange membrane electrolyser has been assembled for the practical implementation of Ru-Co-NC as a cathode, which shows the industrial level current density of 2 A cm-2 at 2.35 volts and high stability over 140 hours. The high cell efficiency of 61.7% and low cost H2 production of $1.08 per GGE H_2 at 0.5 A cm^2 demonstrate the potential of Ru-Co-NC for green hydrogen production on an industrial scale. The density functional theory (DFT) calculations provide mechanistic insights, revealing reduced water dissociation energy, favourable hydrogen binding energy, and mitigated OH^- adsorption on the Ru-Co-NC surface. These results highlight the importance of concurrently engineering water activation and OH^- desorption to optimize HER activity for industrial-level current density.

Keywords: Water splitting, Hydrogen evolution reaction, AEM Water Electrolyser, OH- desorption, Density functional theory.

References

(1) Yadav, V.; Megha; Sen, P.; Shaijumon, M. M. Electrosynthesis of Ruthenium Nanocluster Incorporated Nickel Diselenide for Efficient Overall Water Splitting. J Mater Chem A Mater 2024, 12 (9), 5319–5330. https://doi.org/10.1039/D3TA06988E.

(2) McCrum, I. T.; Koper, M. T. M. The Role of Adsorbed Hydroxide in Hydrogen Evolution Reaction Kinetics on Modified Platinum. Nat Energy 2020, 5 (11), 891–899. https://doi.org/10.1038/s41560-020-00710-8.

Poster-72

Hierarchical nanoflakes anchored mesoporous Ni-MOF microspheres for efficient overall electrocatalytic water splitting

Ajay Patil [a] , Manopriya Samtham [a] , Ekta Choudhary [a,b] , Ankit Yadav [a] , Aayushi Miglani [b] , Santosh Bimli [a] , Harshada Jadhav [a] , Rupesh S. Devan [a,c]*

a Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

b Department of Physics, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

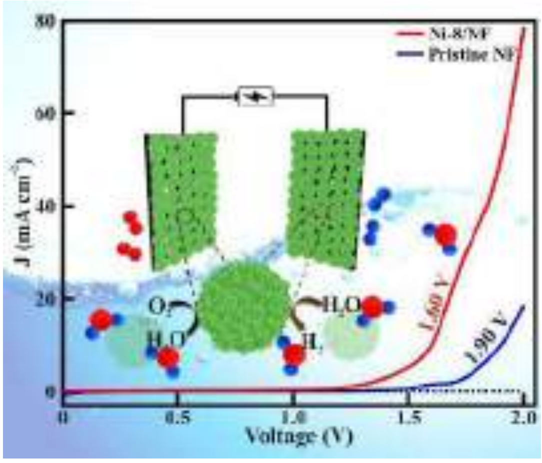
c Centre for Electric Vehicle & Intelligent Transport System, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

*Email: rupesh@iiti.ac.in

Abstract

Metal-organic frameworks (MOFs) have garnered considerable attention for water electrolysis due to their larger surface area, tailorable topology, and abundant electroactive sites. This study investigates 3D nanoflake-anchored hierarchical mesoporous pure Ni-MOF microspheres with tailored crystallinity and surface morphology for efficient overall electrocatalytic water splitting. The optimized Ni-MOF (Ni8) offering a specific surface area of 146.96 m^2/g, providing abundant electroactive sites and featuring Ni^{2+}/Ni^{3+} redox states that facilitate efficient mass transport and gas release during electrolysis demonstrated superior electrocatalytic performance. Notably, Ni8 demonstrated excellent electrocatalytic performance, achieving overpotentials of 337 mV for the oxygen evolution reaction (OER) and 559 mV for the hydrogen evolution reaction (HER) at 10 mA/cm^2 in 1M KOH electrolyte. Ni8 resulted in a cell voltage of 1.60 V for overall water splitting, with an electrochemical surface area (ESCA) of 7.80 cm^2 and turnover frequency (TOF) of 1.02 1/s. These findings emphasize the significance of 3D hierarchical mesoporous structures in enhancing catalytic activity and positioning Ni-MOF as a cost-effective alternative to noble metal based catalysts for sustainable hydrogen. If you include Figure(s) and Table(s), those materials must be incorporated into the text together with their captions.

Keywords (max 5): Metal-organic frameworks (MOFs), Hierarchical mesoporous structure, Water electrolysis, Hydrogen production, Bifunctional electrocatalyst.



References

(1). Vincent, I., Lee, E., & Kim, H. Highly Active Ni–Fe Based Oxide Oxygen Evolution Reaction Electrocatalysts For Alkaline Anion Exchange Membrane Electrolyser. Catalysts, 12(5), 476 (2022). https://doi.org/10.3390/catal12050476

2. Zhou, D., Li, P., Xu, W., Jawaid, S., Mohammed-Ibrahim, J., Liu, W., Kuang, Y., & Sun, X. Recent Advances In Non-Precious Metal-Based Electrodes For Alkaline Water Electrolysis. ChemNanoMat, 6, 336–355 (2020). https://doi.org/10.1002/cnma.202000002

3. Cao, X., Yang, Z., Wu, X., Wang, X., Teng, X., Yun, J., Zhang, J., & Liang, X. Multilayered NiMo/CoMn/Ni Cathodic Electrodes With Enhanced Activity And Stability Toward Alkaline Water Electrolysis. ACS Appl. Mater. Interfaces, 15(28), 34181–34194 (2023). https://doi.org/10.1021/acsami.3c03727

4. Ahn, S. H., Park, H. Y., Choi, I., Yoo, S. J., Hwang, S. J., Kim, H. J., Cho, E., Yoon, C. W., Park, H., & Son, H. Electrochemically Fabricated NiCu Alloy Catalysts For Hydrogen Production In Alkaline Water Electrolysis. Int. J. Hydrogen Energy, 38, 13493–13501 (2013). https://doi.org/10.1016/j.ijhydene.2013.07.086

5. Chen, H., Huang, H. B., Li, H. H., Zhao, S. Z., Wang, L. D., Zhang, J., Zhong, S. L., Lao, C. F., Cao, L. M., & He, C. T. Self-Supporting Co/CeO_2 Heterostructures For Ampere-Level Current Density Alkaline Water Electrolysis. Inorg. Chem., 62, 3297–3304 (2023). https://doi.org/10.1021/acs.inorgchem.2c03687

Green synthesized MgO nanomaterials for the application of Hydrogen Evolution Reaction- Synthesis and Characterizations

Vinay Prasad V, Bhargavi Somapur and Nagaiah Kambhala*

Materials Research Lab, Department of Physics and Electronics, School of Sciences, Jain (Deemed-to-be) University, J.C. Road, Bangalore, 560027, India.

Abstract

The increasing the demand for clean hydrogen has creats the significant interest in developing efficient and sustainable methods and materials for green hydrogen production. Hence here we have synthesized the Magnetium oxide (MgO) nano materials as electrocatalysts for hydrogen evolution using the green synthesis method. Aloe vera gel has been used as a reducing and used various concentrations (5g, 10,15 and 20g) of Aloe vera gel. The main objective of the report is to study the effect of the Alovera concentration on MgO nano materials for alkaline water electrolysis activity for hydrogen evolution. XRD data confirms the crystalline cubic phase of MgO. Optical absorption data has been shown the decrease in band gap energy from 4.84 to 3.27 eV as Aloevera concentration increased. Scanning Electron Microscope (SEM) images of the samples show the diverse nanostructures with different morphological changes with respect to the change in Aloe vera concentration. Functional groups presence and Mg-O (800- 890 cm^{-1}) in FTIR spectroscopic and Raman sprectroscopic data confirms the functional groups like C-O and C=O due to the residues derived from the Aloe vera during the synthesis.

The greeen synthesized materials (G-MgO-A, G-MgO-B, G-MgO-C, and G-MgO-D, samples) are behaved as a good electrocatalysts for hydrogen evolution using the alkaline water. Among these samples, G-MgO-B has been shown the superior properties of electrocatalysts with lower overpotential of 175 mV at 10mA/cm2 current density with lower Tafel slope of 108 mV/Dec. Hence, We believe that the low cost and earth abundant materials of green synthesized MgO nano materials (G-MgO-B) are best electrocatalyst for the alkaline water electrolysis for hydrogen production due to rich defects like functional groups on the surface, carbon coating and oxygen vacancies of the green synthesis of MgO nano materials.

Keywords : Green synthesis method; MgO; Hydrogen evolution reaction; alkaline water electrolysis

- **Corresponding Author: Dr. Nagaiah Kambhala (k.nagaiah@jainuniversity.ac.in)**
  Presenting author: Mr. Vinay Prasad V (vinaygowda15121994@gmail.com)

Experimental and theoretical study of mixed phase 1T/2H-MoS_2 via dual metal Cu and Fe doped for Hydrogen Evolution Reaction

Ramesh Avala[1,*], Sukanti Behera[1]

[1] *Chemistry department, Maulana Azad National Institute of Technology Bhopal-462003, India.*

* rameshavala92@gmail.com

Abstract

MoS_2 has been researched as a cost-effective and environmentally friendly alternative to Pt in the production of hydrogen fuel. MoS_2 appear in various phases, such as mixed 1T/2H, 1T, and 2H phases. The combined 1T/2H phase has better qualities than the metallic 1T phase and semiconduter 2H phase. The metastable 1T phase is stabilized by the interaction between the 1T and 2H phases in the mixed 1T/2H-MoS_2, which increases its catalytic activity. Here, we examined the performance of dual-metal-doped (copper and iron) mixed 1T/2H-MoS_2 with varying compositional ratios in the hydrogen evolution process (HER) both experimentally and through density functional theory (DFT). In experimrntal results shows that a minimum Tafel slope of 40 mV/dec and an overpotential of -20 mV at a current density of -10 mA/cm^2. Additionally, after 1000 voltammetry cycles, the material showed remarkable potential stability with negligible change in potential. The stability of the system for HER was validated by theoretical tests using DFT. We studied on four possible combinations of dual metals doped into 1T/2H-MoS_2. Such as include 1) Cu and Fe doped in 1T phase, 2) Cu in 1T and Fe in 2H phase, 3) Cu in 2H and Fe in 1T phase, and 4) Cu and Fe in 2H phase. Copper and iron doping in the 2H phase resulted in a low ΔG value of 0.7 eV for the combined 1T/2H-MoS2. In comparison to others, CuFe-1T, Cu-1T/Fe-2H, and Cu-2H/Fe-1T are -10.7, -5.6, and -2.6 eV, respectively. Our work dual metal-doped engineering method for improving the hydrogen evolution reaction (HER) of 1T/2H-MoS_2 is a very efficient and simple method.

Keywords: 1T/2H-MoS_2, Dual metal doped, HER, Hydrothermal, DFT

From Waste to Power: Transforming Used Zn/MnO_2 Batteries into Advanced Cathode Materials for Zinc-Ion Batteries

***M. Jenitha*[1] · *R. Ajay Rakkesh*[1*]**

Functional Nano-Materials (FuN) Laboratory, Department of Physics and Nanotechnology,

Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur – 603203, India

**Corresponding author: Email: ajayr1@srmist.edu.in; ajayrakkesh@gmail.com*

Abstract

The growing demand for sustainable and cost-effective energy storage solutions has intensified interest in recycling strategies that align with circular economy principles. This study presents a novel approach to synthesizing cathode materials for aqueous zinc-ion batteries by reclaiming active components from fully discharged Zn/MnO_2 batteries. The recovered materials were composited with vanadium oxide to enhance conductivity and structural stability. Further surface modifications, such as metal oxide integration and carbon coating, were implemented to address inherent limitations like poor electronic conductivity and structural degradation. Comprehensive physicochemical and electrochemical characterizations confirmed that the regenerated cathode materials exhibited improved performance, including stable cycling behavior, high reversibility, and efficient charge storage. This research not only demonstrates the feasibility of using battery waste to develop functional electrodes but also highlights a promising pathway toward environmentally responsible and economically viable zinc-ion battery technologies.

Keywords: Zinc-ion batteries, Cathode recycling, Vanadium oxide composite, Sustainable energy storage, circular economy.

References

(1) Lu, Y.; Wei, M.; Wang, Z.; Evans, D. G.; Duan, X. Structure and properties of layered manganese–vanadium oxide as a cathode material for lithium secondary batteries. *Electrochemistry Communications* **2004**, *6* (7), 672–677. https://doi.org/10.1016/j.elecom.2004.04.023.

(2) Chen, J.; Zhou, Y.; Islam, M. S.; Cheng, X.; Brown, S. A.; Han, Z.; Rider, A. N.; Wang, C. H. Carbon fiber reinforced Zn–MnO2 structural composite batteries. Composites Science and Technology 2021, 209, 108787. https://doi.org/10.1016/j.compscitech.2021.108787.

(3) Shangguan, E.; Wang, L.; Wang, Y.; Li, L.; Chen, M.; Qi, J.; Wu, C.; Wang, M.; Li, Q.; Gao, S.; Li, J. Recycling of Zinc–Carbon Batteries into MnO/ZnO/C to Fabricate Sustainable Cathodes for Rechargeable Zinc‐Ion Batteries. ChemSusChem 2022, 15 (15). https://doi.org/10.1002/cssc.202200720.

Electrooxidation of Biomass-Derived Furfural Using Low-crystalline Catalysts: A Sustainable Route to Value-Added Chemicals Beyond the OER

Vigneshraaj A S[1,2], Abhijeet Singh[1], Kavita Pandey*[1,2,3]

[1]Centre for Nano and Soft Matter Sciences (CeNS), Shivanapura, Bengaluru 562162, India

[2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India

[3]Manipal Academy of Higher Education, Manipal, Karnataka 576104, India

*kavitapandey@cens.res.in

Abstract

Hydrogen production through water electrolysis has garnered significant attention as a clean and sustainable energy solution. Innovative hybrid electrolysis strategies have emerged, aiming to overcome this bottleneck by replacing the OER with more efficient organic oxidation reactions. Biomass has emerged as a promising feedstock in renewable hybrid electrolysis strategies, offering efficient conversion into high-value-added chemicals. Electrochemical oxidation of biomass-derived furfural (FF) into value-added furoic acid (FA) offers a sustainable and efficient strategy to replace the kinetically sluggish oxygen evolution reaction (OER) at the anode[1,2]. Herein, we report the in situ fabrication of a layered double hydroxide catalyst on carbon cloth for the electrocatalytic furfural oxidation reaction (FOR). To optimize its performance, we systematically varied the synthesis conditions for obtaining low-crystalline LDH. The low-crystalline catalyst exhibits exceptional electrocatalytic activity towards FOR, delivering a notably low onset potential of 1.39 V vs. RHE. In contrast, the competing oxygen evolution reaction (OER) displays a higher onset potential of 1.52 V vs. RHE, highlighting the advantage of FF oxidation as a more energy-efficient anodic pathway. Dynamic structural transformations and mechanistic insights into the catalyst were investigated using in-situ Raman spectroscopy and electrochemical impedance spectroscopy–Distribution of Relaxation Time (EIS-DRT) analysis. This study presents a strategy for biomass valorization while concurrently enhancing anodic reaction kinetics through an efficient, earth-abundant electrocatalyst.

Keywords: Furfural Oxidation Reaction (FOR), Dynamic structural transformation, EIS-DRT, In-situ Raman

References:

1. Fan, H.; Jiao, D.; Fan, J.; Wang, D.; Zaman, B.; Zhang, W.; Zhang, L.; Zheng, W.; Cui, X. Enhancing Water-Dissociation Kinetics and Optimizing Intermediates Adsorption Free Energy of Cobalt Phosphide via High-Valence Zr Incorporating for Alkaline Water Electrolysis. *J. Energy Chem.* 2023, *83*, 119–127. DOI: 10.1016/j.jechem.2023.04.014.
2. Xiang, K.; Wu, D.; Deng, X.; Li, M.; Chen, S.; Hao, P.; Guo, X.; Luo, J.-L.; Fu, X.-Z. Boosting H_2 Generation Coupled with Selective Oxidation of Methanol into Value-Added Chemical over Cobalt Hydroxide@Hydroxysulfide Nanosheets Electrocatalysts. *Adv. Funct. Mater.* 2020, **30** (01), 1909610. DOI: 10.1002/adfm.201909610.

Triggering Exothermic Water Dissociation on Copper via foreign atom Implantation for Enhanced Alkaline Hydrogen Generation

Bhargav Rajbongshi[1], Pragyan Tripathi[2], Abhishek Kumar Singh[2]* and Manikoth M. Shaijumon[1]*

[1]School of Physics and Centre for Advanced Materials Research with International Engagement (CAMRIE), Indian Institute of Science Education and Research Thiruvananthapuram, Maruthamala PO, Thiruvananthapuram, Kerala, 695551, India

[2]Materials Research Centre, Indian Institute of Science, Bangalore, Karnataka-560012, India

* shaiju@iisertvm.ac.in, abhishek@iisc.ac.in

Abstract

Implantation of foreign elements into a host lattice can enhance catalytic activity by modulating electronic properties. Copper, a low-cost and abundant material, shows great potential in energy conversion applications. However, its high water dissociation energy barrier limits its catalytic performance in alkaline hydrogen evolution reactions (HER). Herein, we present a highly scalable co-electrodeposition method to enhance the electrocatalytic performance of copper for alkaline HER by incorporating rhenium(Re) into the copper lattice. The incorporated Re improves electrocatalytic activity by promoting exothermic water dissociation and enhancing water adsorption. The optimised catalyst, CuRe-10/CP, achieves an overpotential of 46 mV to drive a current density of 10 mA cm^{-2}, demonstrating excellent electrochemical stability for 450 h at 50 mA cm^{-2} in an alkaline medium (1.0 M KOH). Additionally, we evaluated the electrochemical activity of the CuRe-10/CP in simulated seawater and alkaline seawater, where it exhibited exceptional activity and stability. Electrochemical impedance spectroscopy (EIS), electrochemical surface area measurement (ECSA), and turnover frequency (TOF) analyses confirm the significant enhancement in catalytic performance following Re incorporation. Furthermore, in-situ Raman spectroscopy, EIS and density functional theory (DFT) studies reveal that the Re incorporation into the copper lattice significantly improves the water dissociation and intermediate adsorption. This study gives a scalable strategy for designing platinum group element free electrocatalysts for alkaline hydrogen evolution.

Keywords:Hydrogen generation, Hydrogen evolution reaction, Water dissociation, Electrocatalysis, Water splitting

References

(1)B. Rajbongshi, P. Tripathi, A. K. Singh, M. M. Shaijumon, *Small* **2025**, 2504300

Defect-Tuned Spinel Oxides via Sol–Gel Synthesis for Selective and Efficient Electrochemical Ammonia Production from Nitrate

Mannil Thodi Muhthasin [ab] Ashida P Hamsa [ab] and Sreekuttan M Unni [*ab]

[a] *CSIR-Central Electrochemical Research Institute Madras Unit, CSIR Madras Complex, Taramani, Chennai 600113, Tamil Nadu, India.*

[b] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.*

E-mail: sreekuttanunni@cecri.res.in

Electrocatalytic nitrate reduction (eNO_3RR) is gaining attention as a dual-benefit strategy for sustainable ammonia production and environmental remediation. By providing a low-energy and decentralized alternative to the traditional Haber–Bosch process, eNO_3RR not only reduces carbon footprint but also helps mitigate nitrate pollution in water systems. However, the multi-electron transfer steps involved in this reaction, along with competing hydrogen evolution reaction (HER), make it a challenging process. Achieving high selectivity and activity demands precise tuning of catalyst surface and electronic properties.

In this work, we report the design of a highly efficient spinel oxide electrocatalyst synthesized via a simple and scalable sol–gel method. This synthesis approach allows precise control over composition and morphology, producing phase-pure nanostructured spinels with abundant active sites. To further boost catalytic performance, we implement a synergistic strategy that combines compositional doping, engineered structural defects, and oxygen vacancy modulation.[1] These modifications create an optimized surface electronic environment that enhances the adsorption and activation of key intermediates ($*NO_3$, $*NO_2$, $*NOH$), accelerates the rate-determining steps, and effectively suppresses undesired HER pathways.[2]

Even without advanced structural modifications, the catalyst exhibits outstanding activity under ambient and neutral pH conditions, delivering an ammonia yield rate of 8.33 mg h^{-1} mg^{-1}cat at –0.4 V vs. RHE, along with a Faradaic efficiency of 95.84% at –0.3 V vs. RHE. These results underscore the intrinsic catalytic potential of the spinel oxide framework and highlight the effectiveness of the sol–gel synthesis in exposing reactive facets and preserving surface integrity.

This work reveals that even unmodified spinel oxides can achieve high-performance eNO_3RR, serving as a strong baseline for future studies involving defect engineering or doping. Moreover, it emphasizes how scalable, low-cost synthesis routes can yield practical catalysts for green ammonia production and environmental cleanup.

Keywords: Electrocatalytic nitrate reduction, Ammonia production, Spinel oxide, Defect engineering, Oxygen vacancies.

References

(1) Qi, S.; Lei, Z.; Huo, Q.; Zhao, J.; Huang, T.; Meng, N.; Liao, J.; Yi, J.; Shang, C.; Zhang, X.; Yang, H.; Hu, Q.; He, C. Ultrathin High-Entropy Fe-Based Spinel Oxide Nanosheets with Metalloid Band Structures for Efficient Nitrate Reduction toward Ammonia. *Advanced Materials* **2024**, *36* (27). https://doi.org/10.1002/adma.202403958.

(2) Hu, Q.; Qi, S.; Huo, Q.; Zhao, Y.; Sun, J.; Chen, X.; Lv, M.; Zhou, W.; Feng, C.; Chai, X.; Yang, H.; He, C. Designing Efficient Nitrate Reduction Electrocatalysts by Identifying and Optimizing Active Sites of Co-Based Spinels. *J Am Chem Soc* **2024**, *146* (5), 2967–2976. https://doi.org/10.1021/jacs.3c06904.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Atomic-Level Modulation of Boron–Nitrogen–Carbon Frameworks for Enhanced Ambient Electrochemical Ammonia Synthesis

Ashida P Hamsa [ab], Mannil Thodi Muhthasin [ab] and Sreekuttan M Unni *[ab]

[a.] *CSIR-Central Electrochemical Research Institute Madras Unit, CSIR Madras Complex, Taramani, Chennai 600113, Tamil Nadu, India.*

E-mail: sreekuttanunni@cecri.res.in

[b.] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India.*

Abstract:

Electrochemical nitrogen reduction (eNRR) under ambient conditions offers a sustainable pathway for decentralised ammonia production, yet remains fundamentally challenged by the high activation barrier of dinitrogen and the competitive hydrogen evolution reaction (HER). Boron–nitrogen codoped carbon (BNC) materials have emerged as a promising class of metal-free catalysts due to their tailored charge distribution, defect-rich architecture, and favourable interaction with nitrogen molecules. Here, we report a systematic approach to enhance eNRR performance by engineering the nitrogen chemistry within the BNC matrix through precise control over synthesis parameters—optimising the nature and density of nitrogen configurations and their interaction with boron-centred active sites. To further amplify activity, atomically dispersed metal species are introduced into the optimised BNC framework, modulating the local electronic structure and spin density near boron, thus strengthening N_2 adsorption and facilitating the activation of key intermediates. This integrated design achieves an ammonia yield rate of 67 μg h^{-1} mg_{cat}^{-1} at −0.2 V vs RHE, with a Faradaic efficiency of 65%, outperforming many state-of-the-art systems. The work demonstrates the power of coupled heteroatom and atomic metal engineering within carbon frameworks, offering new insights into the rational design of advanced eNRR catalysts.

Keywords: nitrogen configurations, boron and nitrogen codoping, nitrogen reduction reaction, boron nitride, ammonia electrosynthesis

References:

(1) Hamsa, A. P.; Muhthasin, M. T.; Unni, S. M. Tailoring Nitrogen Chemistry in Boron- and Nitrogen-Codoped Carbon for Enhanced Electrochemical Ammonia Synthesis. *ACS Appl. Eng. Mater.* **2025,** *3* (6), 1686–1695. https://doi.org/10.1021/acsaenm.5c00204.

(2) Bhardwaj, S.; Alli, S. J.; Barman, N.; Thapa, R.; Dey, R. S. Ternary Heteroatom-Doped Carbon As a High-Performance Metal-Free Catalyst for Electrochemical Ammonia Synthesis. *ACS Appl. Mater. Interfaces* **2025,** *17* (18), 26661–26670. https://doi.org/10.1021/acsami.5c02039.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Ultrasmall Ru nanoparticles decorated nitrogen-doped CNTs encapsulated CoNi alloy for efficient glycerol oxidation coupled with nitrate reduction

Loknath Thapa[1] and C. Retna Raj[1]*

[1] *Functional Materials and Electrochemistry Lab,*

Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur 721302 West Bengal, India,

Email: crraj@chem.iitkgp.ac.in

Abstract

Paired electrocatalysis combines two complementary half-cell reactions in a single electrolytic system, allowing for the simultaneous generation of valuable products while reducing overall cell voltage and enhancing energy efficiency through strategic coupling of oxidation and reduction processes.[1] Upcycling pollutants and byproducts like glycerol and nitrate (NO_3^-) contributes to sustainable waste management and chemical production. We synthesized ultrasmall Ru NPs (2-3 nm) (Figure 1a) decorated over nitrogen-doped CNTs encapsulated CoNi alloy (Ru-CoNi@NCNTs) as a bifunctional catalyst for electrochemical oxidation of glycerol coupled with nitrate reduction. Ru-atoms play a crucial role in regulating the local proton concentration around the active sites essential for the proton-coupled electron transfer (PCET) process during NO_3^- reduction to NH_3. Ru-CoNi@NCNTs delivered a high current density of >450 mA cm^{-2} at -0.2 V *vs.*RHE in the presence of 0.1 M NO_3^-, and a maximum yield of 22.9 mg h^{-1} cm^{-2} with 90% FE for NH_3 at -0.3 V *vs.*RHE. At anode, the catalyst delivered a high yield of 20.4 mg$_{formate}$ h^{-1} cm^{-2} with over 90% FE at 1.4 V *vs.*RHE. Ru-CoNi@NCNTs is highly stable even after prolonged electrolysis with no change in crystallinity and morphology. The glycerol-nitrate paired electrocatalytic system (NO_3RR||GlyOR) (Figure 2) enables upcycling of waste while simultaneously producing valuable chemicals, offering higher energy efficiency compared to conventional single reaction systems.

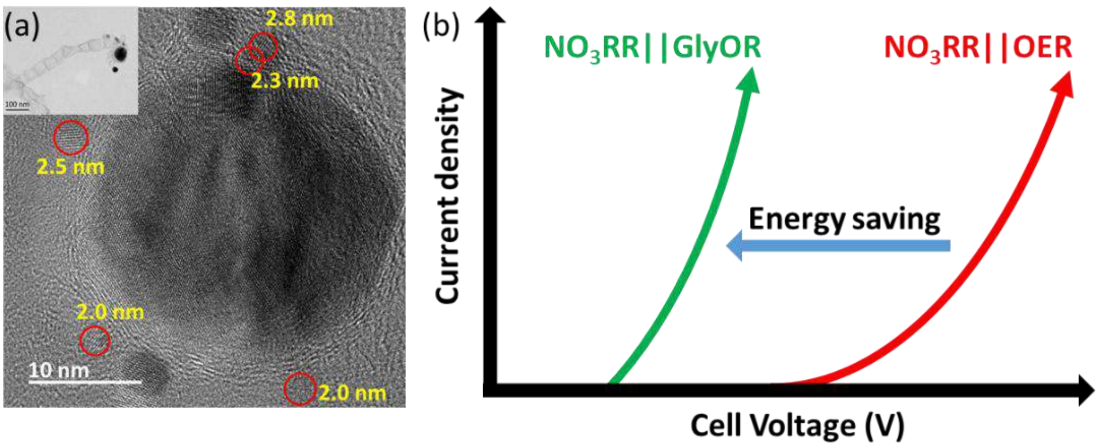


Figure 1: (a) HRTEM image of Ru-CoNi@NCNTs (inset TEM image), (b) Schematic representation of reduction in Cell voltage in NO_3RR||GlyOR system compared to conventional NO_3RR||OER.

Keywords: Paired electrocatalysis, Nitrate reduction, Glycerol oxidation, Ammonia, CNTs

Reference

(1) Thapa, L.; Bhaumik, A.; Mondal, S.; Raj, C. R. A Heterostructured Electrocatalyst for the Electrochemical Valorization of 5-Hydroxymethylfurfural Coupled with the Hydrogen Evolution Reaction. J. Mater. Chem. A 2023, 11 (47), 26242-26251.

Unlocking Energy Potential: Zinc Peroxide in Energy Storage

Shivangi Mehta, Sarbjit Kaur, Chirag and Tharamani C. Nagaiah*

Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab-14001, India

Corresponding author: tharamani@iitrpr.ac.in

Abstract

As global community shifts from non-renewable to renewable sources of energy such as solar and wind power, the challenge of balancing energy generation with fluctuating demand becomes increasingly critical.[1] The advancement in the energy storage devices and carrying out electrocatalytic reactions in an efficient way is the need of the hours. One such approach is fusing energy conversion and storing system enabling the two-electron oxygen reduction reaction ($2e^-$ ORR), to value added hydrogen peroxide (H_2O_2) product and its utilization in the energy storage devices using suitable bifunctional catalyst, without any external H_2O_2 source.[2] H_2O_2 is a dynamic energy carrier and oxidizing agent that has been widely contributed to diverse industries.[3] The real time H_2O_2 production analyze by rotating ring disk electrode (RRDE) and various spectroscopic techniques. Furthermore, this study explores the development of an aqueous rechargeable Zn-H_2O_2 battery that utilizes a bifunctional electrocatalyst for sustainable H_2O_2 production while simultaneously generating electricity.[4] The zinc–peroxide battery exhibits remarkable cycle life and energy efficiency. Moreover, the battery deliver a continuous electro generated H_2O_2 output during discharge and achieve a notable power density which indicate its viability as an energy solution. These findings position the Zn-H_2O_2 battery system as a promising next-generation technology, offering both environmental and economic advantages for future energy systems.

Keywords: Two-electron oxygen reduction reaction (ORR), in-situ H_2O_2 generation, bifunctional electrocatalyst, Zinc- peroxide battery.

References

1. San Roman, D.; Krishnamurthy, D.; Garg, R.; Hafiz, H.; Lamparski, M.; Nuhfer, N. T.; Meunier, V.; Viswanathan, V.; Cohen-Karni, T., Engineering Three-Dimensional (3D) Out-of-Plane Graphene Edge Sites for Highly Selective Two-Electron Oxygen Reduction Electrocatalysis. *ACS Catalysis* **2020,** *10* (3), 1993-2008.
2. Mehta, S.; Kaur, S.; Garg, K.; Singh, M.; Nagaiah, T. C. J. A. C., Unveiling an In Situ H2O2 Production: Rechargeable Zinc-H_2O_2 Battery Powering 26 LEDs. **2025**, e202505593.
3. Zhang, H.; Wang, Z.; Wang, Z.; Wang, L.; Wang, Y. J. A. A. E. M., Valence state modulation of chromium in selective hydrogen peroxide production electrocatalysts. **2021,** *4* (9), 10114-10123.
4. Ko, Y.-J.; Choi, K.; Yang, B.; Lee, W. H.; Kim, J.-Y.; Choi, J.-W.; Chae, K. H.; Lee, J. H.; Hwang, Y. J.; Min, B. K. J. J. o. M. C. A., A catalyst design for selective electrochemical reactions: direct production of hydrogen peroxide in advanced electrochemical oxidation. **2020,** *8* (19), 9859-9870.

Enhanced Methanol Production through Electrochemical CO2 Reduction Reaction via a Bimetallic Electrocatalyst.

Muzamil Majeed, Prof Tharamani C.N*.

Department of chemistry Indian institute of technology Ropar, Rupnagar, 140001, India (tharamani@iitrpr.ac.in)

Abstract

The limited adsorption and activation of CO_2 on catalyst and the high energy barrier for intermediate formation hinder the development of electrochemical CO_2 reduction reactions (CO_2RR).[1] The development of efficient and selective electrocatalysts for electrochemical CO_2 reduction reaction (eCO_2RR) is critical for advancing carbon-neutral energy technologies. In this work, we have designed a bimetallic Bi@Co catalyst as cathode material for the CO_2RR . Methanol (CH_3OH) is a highly energy efficient product of the electrochemical CO_2 reduction reaction (CO_2RR). [2] Bismuth-based catalysts have shown promise in the conversion of CO_2 to methanol , but there is still a great need for further improvement in selectivity and activity. Herein, we report the preparation of Bi nanosheets decorated by cobalt oxide cube morphology with high $Co^{2+}/Co^{3+}/Co^{4+}$ ratio and rich oxygen vacancies.[3] The Cobalt oxide affect the electronic structures of bismuth, enhance CO_2 adsorption, and thus promote the CO_2RR properties of Bi nanosheets. [4] Compared with elemental Bi nanosheets, the hetero-structured Cobalt oxide/Bi oxide nanosheets exhibit much higher activity over a wide potential window, showing a current density of 10 mA cm^{-2} with a Faradaic efficiency of 53% at −0.9 V after half hour *vs*. RHE.

Keywords : Electrochemical CO_2 reduction, mechanism of CO_2RR, Electrocatalysts, CO_2 adsorption.

References

1. Ko, E.; Kim, Y. S.; Kim, B.; Mule, A. R.; Chung, C. H., Efficient CO_2 utilization and sustainable energy conversion via Zn–CO2 batteries using gaseous CO_2. *Journal of CO_2 Utilization* **2024,** *80*, 102681.

2. Weng, C.; Wang, C.; Song, Y.; Zhang, Y.-X.; Zou, K.; Chen, H.; Yang, X.; Lin, W., In-situ reconstruction of active bismuth for enhanced CO_2 electroreduction to formate. *Chemical Engineering Journal* **2025,** *505*, 159732.

3. Nankya, R.; Xu, Y.; Elgazzar, A.; Zhu, P.; Wi, T.-U.; Qiu, C.; Feng, Y.; Che, F.; Wang, H., Cobalt-Doped Bismuth Nanosheet Catalyst for Enhanced Electrochemical CO_2 Reduction to Electrolyte-Free Formic Acid. **2024,** *63*, (36), e202403671.

4. Ruan, S.; Zhang, B.; Zou, J.; Zhong, W.; He, X.; Lu, J.; Zhang, Q.; Wang, Y.; Xie, S., Bismuth nanosheets with rich grain boundaries for efficient electroreduction of CO_2 to formate under high pressures. *Chinese Journal of Catalysis* **2022,** *43*, (12), 3161-3169.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Unveiling the Electrocatalytic Mechanism of Carbonophosphates Towards Water Oxidation Catalysis

Nikhil Doddi[1,*], Abhisek Padhy[1], Prabeer Barpanda[1]

[1] *Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India.*

* nikhildoddi@iisc.ac.in

Abstract

Transition metal phosphates hold promise as efficient oxygen evolution reaction (OER) catalysts, but a clear picture of the OER mechanism and its link to structural changes remains elusive, particularly the role of surface reconstruction on activity.[1,2] Herein, we unveil the origin of the electrocatalytic activity of the carbonophosphate class of polyanionic insertion frameworks towards the electrochemical water oxidation reaction. These isostructural compounds, denoted by $Na_3MPO_4CO_3$ (M=Ni, Co, Mn), possess a *sidorenkite*-type structure with the monoclinic symmetry ($P2_1/m$).[3] Notably, $Na_3NiPO_4CO_3$ exhibits remarkable catalytic performance with an activation overpotential of 320 mV at 20 mA/cm^2 with good long-term durability in alkaline KOH solution. By integrating electrochemical OER measurements with a combined suite of *operando* Raman and *in-situ* X-ray absorption (XANES/EXAFS) analysis, we elucidate the *in-situ* self-reconstruction of $Na_3NiPO_4CO_3$ catalyst into disordered $Ni(OH)_2$/γ-NiOOH electroactive phases with simultaneous leaching of phosphorus into the electrolyte. Depth-resolved XPS studies further confirmed the dynamic evolution of these reconstructed electrocatalytic phases into the bulk structure (upto 500 nm). The enhanced catalytic performance can be attributed to the abundance of surface-exposed OER-active Ni^{+3} sites, generated through the electrochemical activation of the *sidorenkite* precatalyst. This study underscores the role of *in-situ* techniques in unravelling the real-time structural transformations of phosphate-based electrocatalysts and their extensive impact on catalytic activity.

Keywords: *Sidorenkite*, Electrocatalysts, Reconstruction, Activation, Leaching,

References

(1) Gond, R.; Zhu, J.; Barpanda, P. Phosphate-based Polyanionic Insertion Materials for Oxygen Electrocatalysis. *Mater. Chem. Front.* **2024**, 8, 1170.
(2) Kim, H.; Park, J.; Park, I.; Jin, K.; Jerng, E. S.; Kang, K. Coordination Tuning of Cobalt Phosphates Towards Efficient Water Oxidation Catalyst. *Nat. Commun.* **2015**, 6, 8523.
(3) Chen, H.; Hautier.; Ceder, G. Synthesis, Computed Stability, and Crystal Structure of a New Family of Inorganic Compounds: Carbonophosphates. *J. Am. Chem. Soc.* **2012**, 48, 19619.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Green ammonia production through electrochemical nitrate reduction utilizing MOF-based composite

Himanshu Chauhan[1,*], Ashish Yadav[1]

[1] *Indian Institute of Technology Roorkee, India*

* ashish@ch.iitr.ac.in

Abstract

The electrochemical reduction of nitrate (NO_3^-) to ammonia (NH_3) offers a promising strategy for addressing two critical global challenges: nitrate pollution and sustainable ammonia production. Traditional methods for NH_3 synthesis, such as the Haber–Bosch process, are highly energy-intensive and contribute significantly to greenhouse gas emissions. Simultaneously, excessive nitrate discharge from agricultural and industrial activities poses serious environmental and health risks. In this context, electrochemical nitrate reduction (e-NRA) under ambient conditions has emerged as an attractive alternative for decentralized and energy-efficient ammonia generation. However, achieving high selectivity, activity, and stability in e-NRA remains a significant challenge due to the complex multi-electron transfer process and competing side reactions.

In this work, we report the design and synthesis of a metal–organic framework (MOF)-based composite catalyst tailored for efficient e-NRA. The composite integrates a high-surface-area MOF scaffold with catalytically active metal nanoparticles, supported on a conductive substrate. The MOF structure provides abundant coordination sites for nitrate adsorption and confinement of reaction intermediates, while the embedded metal centers facilitate electron transfer and activation of NO_3^- molecules. Electrochemical tests demonstrated a high ammonia yield rate and Faradaic efficiency, along with excellent stability over extended operation. Mechanistic studies suggest that the synergistic interaction between the MOF and metal sites enables favorable adsorption geometries and promotes proton-coupled electron transfer, suppressing undesired by-products such as N_2 or NO_2^-. Our study highlights the potential of MOF-based composite catalysts for selective nitrate electroreduction and paves the way for integrated technologies that combine environmental remediation with value-added chemical production. The tunable nature of MOFs, coupled with the modularity of composite design, opens new avenues for tailoring active sites and reaction environments for enhanced performance in electrocatalytic nitrogen transformation processes.

Keywords: MOF, multi-electron transfer, green ammonia,

ACEPS-13, January 11-14, 2026, Bengaluru, India

CO_2 Electroreduction on CeO_2: Influence of Rare Earth Doping on Oxygen Vacancy Formation

Soham Raychowdhury, Vipin Kamboj, Chinmoy Ranjan*

[1,2,3] *Department of Inorganic and Physical Chemistry, Indian Institute of Science (IISc), Bengaluru, India*

* Email : ranjan@iisc.ac.in

Abstract

Keywords: CO_2 utilisation, CO_2 electrolysis, Solid oxide electrolysers, Mixed ionic electronic conductor, Oxygen defect chemistry

The shift away from fossil fuels is essential for reducing greenhouse gas emissions. A promising approach involves CO_2 electroreduction powered by renewable energy. Although converting CO_2 into hydrocarbons (CH_x) is energetically demanding due to complex multielectron transfer steps, the selective reduction of CO_2 to CO presents a more energy-efficient alternative. CeO_x-based electrodes are widely employed in this process because of their mixed ionic-electronic conductivity (MIEC).

In this study, DFT+U calculations were used to explore the impact of Pr and Gd doping on CeO_2 electrodes. Oxygen abstraction energies were computed to assess defect formation in both pristine and doped systems. The presence of hydrogen was found to lower these energies, promoting the formation of Ce^{3+}. Bader charge analysis indicated that hydrogen occupies oxygen vacancy sites in CeO_x as hydridic species. In Pr-doped CeO_2, oxygen abstraction was even more favorable; however, the strong formation of O–H bonds in molecular hydrogen limited oxygen release, maintaining the material in a more oxidized state. In the Ce{Pr}O_2 lattice, hydrogen exhibited protic behavior.

Adsorption analyses revealed that CO binds more strongly to Ce-metal sites in doped Ce{M}O_x than in undoped CeO_x, supporting an oxygen-vacancy-driven mechanism involving the formation of a "metal–carbonyl" intermediate.

ACEPS-13, January 11-14, 2026, Bengaluru, India

CoSn Intermetallic Bifunctional Oxygen Electrocatalyst for Zn-Air Batteries

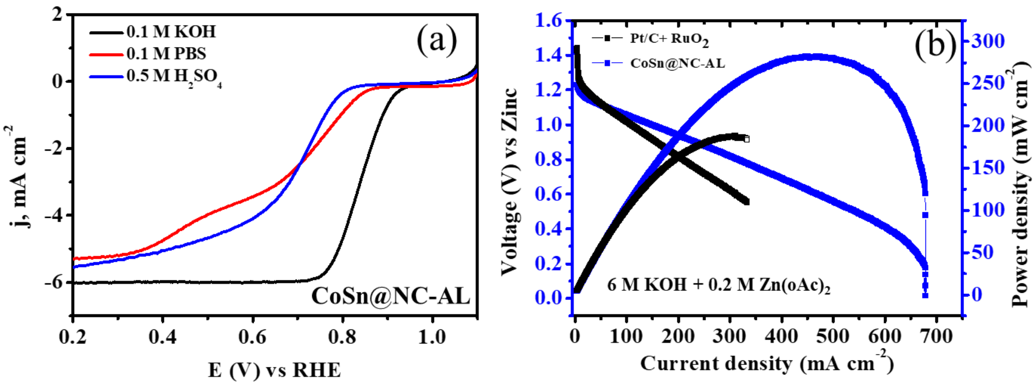
Santanu Ghora, and C. Retna Raj*.

Functional Materials and Electrochemistry Laboratory, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal-721302, India

* E-mail: crraj@chem.iitkgp.ac.in

Abstract

The rising demand for efficient, durable, and affordable energy storage has accelerated research beyond Li-ion batteries. Zinc-air batteries with high theoretical energy density (1084 Wh kg^{-1}), eco- friendliness, and low cost, are the promising alternatives for next-generation clean energy technologies. However, their practical implementation is hindered by the sluggish kinetics of the oxygen reduction reaction (ORR) and oxygen evolution reaction , which govern the discharge and charge processes, respectively. Conventional catalysts such as Pt, Ir, and Ru are either expensive or lack bifunctional activity.[1]



Intermetallic nanostructures, owing to their ordered crystal structure, uniform active sites, and unique electronic properties, are a promising choice for a low-cost bifunctional catalyst.[3] Herein, We synthesized an electrocatalytically active CoSn intermetallic catalyst embedded within a nitrogen-doped carbon shell (CoSn@NC-AL) via a novel shape-controlled approach using a Co–Sn bimetallic charge-transfer complex ($[Co(bpy)_3][Sn(OH)_6]$) and ZIF-8 precursor. The CoSn@NC-AL catalyst exhibits remarkable pH-universal ORR activity, with onset potentials of 0.94, 0.89, and 0.85 V, and half-wave potentials of 0.84, 0.76, and 0.69 V *vs.* RHE in alkaline, neutral, and acidic media, respectively. Impressively, it retains its catalytic performance with negligible change after 25,000 cycles in 0.1 M KOH. The rechargeable ZAB delivers a high peak power density of 282 mW cm^{-2} at 463 mA cm^{-2} in alkaline electrolyte, and 44 mW cm^{-2} at 80 mA cm^{-2} in neutral electrolyte. Furthermore, the device shows excellent charge–discharge cycling stability for >99 h in alkaline and 270 h in neutral media, with negligible voltage decay, highlighting the robust bifunctional activity of the catalyst in both environments.

Keywords: bimetallic complex, intermetallic, CoSn@NC, oxygen electrocatalyst, zinc-air battery

References

(1) Ghora, S.; Chakraborty, R.; Bag, S.; Kumar, M. M.; Raj, C. R. *Chem. Commun.,* **2025**, *61*, 2636-2657.

(2) Kundu, A.; Mallick, S.; Ghora, S.; Raj, C. R. *ACS Appl. Mater. Interfaces* **2021**, *13*, 40172–40199.

(3) Ghora, S.; Satpati, B.; Jena, B. K.; Raj, C. R. *ACS Appl. Mater. Interfaces* **2025**, *17*, 2, 3426–343.

ACEPS-13, January 11-14, 2026, Bengaluru, India

F-based Ni-Fe systems for improved OER application

Rinya Rubu[1], Divya Bhutani[2], Premkumar Senguttuvan[1, *]

[1]*New Chemistry Unit, International Centre for Materials Science, and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064 Karnataka, India*

[2]*Chemistry and Physics of Materials Unit, and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064 Karnataka, India*

*prem@jncasr.ac.in

Abstract

Hydrogen (H_2), with its high energy density, is emerging as a sustainable alternative and a vital clean energy source over fossil fuels. The commercial H_2 generation via the steam reforming process results in the emission of carbon dioxide and carbon monoxide, adversely affecting the fuel-cell electrodes and the environment.[1] Alternatively, electrochemical water-splitting generates H_2 at the cathode, i.e., Hydrogen Evolution Reaction (HER). The sluggish kinetics of the Oxygen Evolution Reaction (OER) at the counter electrode require additional overpotential (E^o = 1.23 V). Hence, improving the kinetics of OER can positively affect the overall efficacy of water electrolysis. The state-of-the-art catalysts for OER and HER include noble metals like Pt, RuO_2, and IrO_2, which are scarce and costly. Engineering the catalytic surfaces of the earth-abundant transition metal alternatives with defects and dopants is known to improve the efficiency of fuel production. Nickel-based catalysts act as pre-catalysts with active conversion to NiOOH species in alkaline conditions. [2] The catalytic activity of Ni improves through regulating the electronic structure with other metal ions or anions. Fe has been widely reported to enhance the catalytic activity of Ni, attaining ampere-level currents and high stability towards OER. As an anion, fluorine assists electron transfer from one metal site to another, facilitating surface reconstruction, thus enhancing overall activity. [3]

In this direction, we explored the Fe-based $NH_4M^{2+}M^{3+}F_6$ defect-pyrochlore system, synthesized by a soft-chemical method. The NiFe-pyrochlore showed a very high current density of 1.6 A cm^{-2} at a low overpotential of 310 mV in alkaline conditions with a stable performance for 550 hours (1 A cm^{-2}) in potentiostatic conditions. Post-reaction characterizations and control electrochemical studies conclude the in-situ modifications in electronic structure with the existence of active metal sites in higher oxidation states and oxyfluoride species. The easy synthesis, high stability, and reproducibility of the catalyst make it suitable for future utilization in sustainable energy generation and conversion.

Keywords: *OER, Pyrochlore, Fluorine, Ni-Fe, alkaline*

References

(1) Cho H.H.; Vladimir Strezov V.; Evans T.J. Environmental impact assessment of hydrogen production via steam methane reforming based on emissions data. *Energy Rep.*, **2022**, *8*, 13585–13595.

(2) Wygant B. R.; Kawashima K.; Mullins C. B. Catalyst or Precatalyst? The Effect of Oxidation on Transition Metal Carbide, Pnictide, and Chalcogenide Oxygen Evolution Catalysts. *ACS Energy Lett.* ,**2018**, 3, 2956–2966.

(3) Zhang J.; Ye Y.; Wang Z.; Xu Y.; Gui L.; He B.; Zhao L. Probing Dynamic Self-Reconstruction on Perovskite Fluorides toward Ultrafast Oxygen Evolution. *Adv. Sci.*, **2022**, *9*, 2201916.

Visible-Light-Responsive Carbon-Nanotube-Integrated $In_2S_3/FeVO_4$ Photoanode: A Synergistic Band-Alignment Strategy for Enhanced Oxygen Evolution

Nitika Garg[1], Ashok K. Ganguli[1,2,*]

[1] *Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016*

[2] *Department of Chemical Sciences, Indian Institute of Science Education and Research Berhampur, Ganjam, Odisha-760003, India*

* Corresponding author's email address: ashok@chemistry.iitd.ac.in

Abstract

The development of high-performance and durable photoelectrodes is crucial for advancing photoelectrochemical (PEC) water-splitting technologies, which are vital for achieving efficient oxygen evolution reactions (OER) and sustainable hydrogen production.[1] This study introduces a novel ternary composite, $In_2S_3/FeVO_4$/CNT, designed for enhanced PEC oxygen evolution.[2] The $In_2S_3/FeVO_4$ heterostructure significantly improves PEC performance through its type-II band alignment,[3] which effectively reduces electron-hole recombination and enhances charge separation. Incorporating carbon nanotubes (CNTs) further optimizes performance by providing efficient conductive pathways that facilitate electron transport and lower charge transfer resistance.[4] As a result, the $In_2S_3/FeVO_4$/CNT ternary composite achieves an impressive current density of 14.70 mA cm^{-2} at 1.8 V vs. RHE, marking a significant performance enhancement compared to pristine In_2S_3 and $FeVO_4$. Electrochemical impedance spectroscopy (EIS) reveals that the ternary composite exhibits the lowest charge transfer resistance, while Bode phase analysis highlights a prolonged carrier lifetime, indicative of improved charge separation. The applied bias photon-to-current efficiency (ABPE) shows a dramatic 32-fold increase compared to pristine In_2S_3, underscoring the synergistic effects of heterostructure engineering and CNT integration. Additionally, the ternary composite demonstrates excellent stability and reliability during transient photocurrent cycling, maintaining consistent performance under repeated chronoamperometric ON/OFF cycling.

Keywords: Type-II heterostructure, Photoelectrochemical Oxygen Evolution, Photoanode

References

(1) K. Sathiyan, T. Mondal, P. Mukherjee, S. G. Patra, I. Pitussi, H. Kornweitz, R. Bar-Ziv, T. Zidki, Nanoscale 2022, 14, 16148.

(2) N. Garg and A. K. Ganguli, Chemistry–An Asian Journal, e202401192.

(3) M. D. Sharma, M. Basu, Langmuir 2022, 38, 12981.

(4) V. Georgakilas, V. Tzitzios, D. Gournis, D. Petridis, Chemistry of Materials 2005, 17, 1613.

ACEPS-13,January 11-14,2026,Bengaluru,India

P,S co-doped nanomaterials for alkaline sea water electrolysis

Divya Bhutani[1], Yadhu Krishnan P[1], Eswaramoorthy Muthuswamy[1*]

[1] Chemistry and Physics of Material Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore,560064, Karnataka, India

* eswar@jncasr.ac.in

Abstract

Hydrogen fuel from green alternatives have been gaining lot of attention lately due to socio economic barriers and global energy crisis. Water electrolysis has been able to replace commercial steam reforming for high purity hydrogen production. In water electrolysis, Hydrogen Evolution Reaction (HER) occurs at cathode, while Oxygen Evolution Reaction (OER) happens at anode. Due to the corrosivity issue associated with acidic pH and high cost of state of art catalysts (Pt/RuO_2/IrO_2), alternatives like non-noble metal catalysts can be considered. Heteroatom doping and surface heterogeneity is known to modify electronic structure of active sites.

This issue associated with high amount of fresh water can be tackled by utilizing abundant sea water sources. Chloride ion interruption and oxidation is a competitive reaction while using sea water electrolysis.[1] This can be overcome by very simple strategy of electrostatic repulsion from groups like phosphates or sulphates.[2] Herein we utilized P,S- co-deposited on Fe based catalyst showing high activity (1.6Acm^{-2} at 390mV, -1.4Acm^{-2} at 520mV) towards OER and HER respectively. The catalyst also showed good performance of 1.8Acm^{-2} at 2.4V. Moreover, the catalyst showed high catalytic stability towards OER, HER and full cell in galvanostatic mode to achieve a high current density of 1Acm^{-2}.

Keywords: Sea water electrolysis, Co-doping, Electrostatic repulsion.

References

(1) Gao, F.-Y.; Yu, P.-C.; Gao, M.-R. Seawater Electrolysis Technologies for Green Hydrogen Production: Challenges and Opportunities. *Curr Opin Chem Eng* **2022**, *36*, 100827. https://doi.org/https://doi.org/10.1016/j.coche.2022.100827.

(2) Wu, Y.; Du, X.; Zhang, X. P Doping Transition Metal Sulfides as Bifunctional Electrocatalyst for Overall Seawater Splitting. *Int J Hydrogen Energy* **2025**, *103*, 174–182. https://doi.org/10.1016/J.IJHYDENE.2025.01.181.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Harnessing Magnetism: Self-Supported $NiCo_2O_4$ on Magnetic Substrate for High-Performance Alkaline Water Electrolysis

Minakshi Sharma[1,*], Vijay K. Singh[2], Ambesh Dixit[1]

[1]Advanced Materials and Devices (A-MAD) Laboratory, Department of Physics, Indian Institute of Technology Jodhpur, Jodhpur, Rajasthan-342030, India

[2]Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab-140001, India

*Corresponding authors: ambesh@iitj.ac.in, vksingh@iitrpr.ac.in

Abstract

Alkaline water electrolysis under an external magnetic field has attracted considerable interest owing to its potential to accelerate electrochemical reaction kinetics and minimize energy losses[1]. Recent studies demonstrate that applying a magnetic field to a ferromagnetic working electrode can enhance catalytic activity; however, the underlying mechanism and the interplay between ferrimagnetic (FiM) and ferromagnetic (FM) interfaces in driving such improvements remain unclear[2]. In this work, we report a simple one-step hydrothermal synthesis of a self-supported FiM Nickel Cobaltite ($NiCo_2O_4$) electrocatalyst grown directly on FM Nickel Foam. X-ray diffraction analysis confirms the phase-pure synthesis, while field emission scanning electron microscopy reveals a nanostructured flower-type morphology. The efficacy of electrocatalyst is tested via electrochemical characterizations in 1 M KOH . The electrocatalyst under no magnetic field (0 mT) shows an overpotential for 10 mA cm^{-2} current density (η_{10}) of ~ 207 and 296 mV for HER and OER respectively. However, the overpotential η_{10} shows a significant reduction to 168 and 272 mV for HER and OER respectively upon subjected to a static external magnetic field of 35 mT. Thus, applying magnetic field significantly boosts its HER and OER performance with the enhancement of ~ 178 % and ~ 540 % in current densities, respectively. This enhancement is attributed to magnetic gradients established between the FiM/FM interface and the diamagnetic electrolyte, which results in FiM-FM superexchange, ultimately reducing the magnetoresistance of the electrode. The chronoamperometry test reveals that the electrocatalyst sustains its activity under magnetic field for ~ 40 h. Our work demonstrates the importance of fabricating magnetic electrocatalysts over magnetic substrates for energy-efficient overall alkaline water electrolysis.

Keywords: Water electrolysis, Green hydrogen, Magnetoelectrocatalysis, Ferrimagnetic, Ferromagnetic.

References

(1) Luo, L.; Xu, L.; Wang, Q.; Shi, Q.; Zhou, H.; Li, Z.; Shao, M.; Duan, X. Recent Advances in External Fields-Enhanced Electrocatalysis. *Adv. Energy Mater.* **2023**, *13* (36). https://doi.org/10.1002/aenm.202301276.

(2) Zhang, Y.; Chen, M.; Chen, J.; Zhang, M.; Xu, P. A Perspective on Magnetic Field-Enhanced Electrocatalytic Water Splitting. *Appl. Phys. Lett.* **2024**, *125* (11). https://doi.org/10.1063/5.0229187.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Synergistic Catalysis of CuNPs and rGO for Electrochemical Nitrate Reduction

Pooja Kumari[1,*], Mahesh Kumar [2], Kirti Sankhala[2]

[1] *Internet of Things- IDRP, Indian Institute of Technology Jodhpur, India*

[2] *Electrical Department, Indian Institute of Technology Jodhpur, India*

[2] *Centre for Emerging Technologies for Sustainable Development*, *Indian Institute of Technology Jodhpur, India*

* P23IoT003@iitj.ac.in

Abstract

Plants must obtain adequate nitrogen (N) from the soil for their growth and development. Nitrate (NO_3^-) serves as the primary nitrogen source for plants in aerobic soils. In addition, the increasing contamination of water resources with nitrate ions poses a significant risk to human health and the environment, highlighting the need for rapid, sensitive, and cost-effective detection strategies. To address the global need for developing long-term sustainable solutions we present a copper nanoparticles-decorated reduced graphene oxide (CuNPs/rGO) nanocomposite as a highly efficient electrochemical sensing platform for nitrate detection. CuNPs were deposited onto a glassy carbon electrode (GCE) via drop-casting, followed by functionalization with rGO to enhance the sensing performance. Calibration plots for paraquat detection in the concentration range of 10–100 μM were obtained at the CuNPs/rGO-modified GCE, exhibiting a linear response with increasing paraquat concentration. The modified electrode demonstrated a markedly enhanced current response approximately threefold higher compared to CuNPs-only modified electrodes. Furthermore, the sensor achieved a theoretical limit of detection (LOD) of 0.104 nM, as estimated from the linear fitting curve, highlighting its high sensitivity toward paraquat detection. The interaction of the NO_3^- molecule with the sensor film was examined by density functional theory (DFT) simulations, which indicated that oxygen-vacant spots on the CuNPs/rGO surface are optimal for NO_3^- adsorption. This durable sensor serves as an efficient instrument for real-time environmental evaluation of NO_3^-, contributing to public health safeguarding.

Keywords: Copper nanoparticles, Reduced graphene oxide, Electrochemical sensor, Nitrate detection, Density Functional Theory

Efficient Recovery of Cobalt and Graphite from Spent Lithium-Ion Batteries Using a Guanidine Hydrochloride –Citric Acid monohydrate Based Deep Eutectic Solvent

Vibhor Bhatnagar[1], Sarita Yadav[1] and Yogesh Sharma[1,2] *

[1]Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India
[2]Centre for Sustainable Energy, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India

*Corresponding author email: yogesh.sharma@ph.iitr.ac.in

Abstract

The global challenge caused by substantial increase in discarded lithium-ion batteries (LIBs) has resulted in serious environmental contamination which requires urgent intervention of environmentalists. Deep Eutectic Solvents (DESs) as green solvents are on a merge to replace toxic mineral acids used in hydrometallurgical process to recover spent LIBs. Here, we propose a less viscous, highly acidic, and strongly reducible DES to selectively extract Cobalt and Graphite from industrially processed LIB black mass. A hydrated DES composed of guanidine hydrochloride (GHC) and citric acid monohydrate (CAM) can extract cobalt and graphite from LIB Black Mass under optimal reaction conditions of 120°C and 4 hours. Due to the strong acidity and abundant chloride coordinating ions of CAM/GHC, the $LiCoO_2$ black mass exhibits significant solubility in this DES system, with partial dissolution observed even at room temperature without stirring. Cobalt is precipitated as Cobalt oxalate dihydrate by adding oxalic acid dihydrate whereas Lithium remains into the solution as Lithium oxalate ions, which require further anti-solvent precipitation technique to convert $Li_2C_2O_4$ to Li_2CO_3. The process of leaching mechanism by our novel DES is compared with traditional choline chloride- citric acid (ChCl:CA) based DES and results offer perfect evidence for utilization of DES in the extraction of critical metals from spent LIB electrode materials. To enhance the recovery efficiency of cobalt and graphite, key leaching parameters—including temperature, hydrated DES composition, and metal–ligand coordination behavior were systematically optimized. Furthermore, CAM/GHC could be recycled with a similar dissolving performance. This work addresses critical challenges in metal recovery and contributes to the advancement of sustainable battery recycling by demonstrating a green and efficient alternative to conventional hydrometallurgical routes.

Keywords: Spent Lithium-ion Batteries, Deep Eutectic Solvents, Hydrometallurgy, Green solvents

References

(1) Tian, Y.; Chen, W.; Zhang, B.; Chen, Y.; Shi, R.; Liu, S.; Zhang, Z.; Mu, T. A Weak Acidic and Strong Coordinated Deep Eutectic Solvent for Recycling of Cathode from Spent Lithium-Ion Batteries. *ChemSusChem* 2022, *15* (16), e202200524.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Modeling and simulation of Mg-AgCl Seawater activated batteries

M.Senthilkumar[1,*], TVSL.Satyavani[1], Venkatasailanathan Ramadesigan [2]

[1] *Naval Science and Technological Laboratory , Visakhapatnam, India*

[2] *Indian Institute of Technology, Bombay, India*

* senthilmathi.nstl@gov.in

Abstract

For underwater vehicle applications, Mg-AgCl sea water activated (SWA) batteries are being used for propulsion power. These batteries are capable of providing high power during discharge, which is the requirement for underwater vehicle. Mathematical models have been used extensively to simulate physical and electrochemical processes occurring inside the battery. Comparison of modeling results with experimental data have revealed greater scientific information of the processes inside the battery. In order to gain a better understanding of Mg-AgCl SWA battery, it is necessary to conduct detailed modelling and simulation work into the different operation conditions of Mg-AgCl SWA battery. In this current work, a one dimensional model is established to simulate the voltage profile of Mg-AgCl SWA battery. A scheme of principal equations for Mg-AgCl SWA battery is derived based on single domain method. A set of mathematical equations is solved for discharging process of Mg-AgCl SWA batteries. The entire Mg-AgCl cell is considered as single domain and the equations are solved for 1 dimensional. The model predicts the voltage profiles at different flow rates of electrolyte, current density, temperature and inter electrode spacing. Kinetics of electrochemical process and transport of species with in the cell are solved and integrated. The voltage profiles were predicted by means of COMSOL Multiphysics 6.0.The results are compared with experimental results obtained from testing of a basic Mg-AgCl battery setup employing AP65 magnesium alloy as anode and AgCl as cathode.

Keywords (max 5): Seawater, Reserve battery, Flow rate, Magnesium, Silver

References

(1) Paruvayakode, S.; Athulya, O. V.; Thomas, K. A.; Fasmin, F. *Modeling and Simulation of Discharge Behavior of Mg-H2O Seawater Battery*. *J. Power Sources,* 2023, 578**,** 233175.

(2) Madhavan, A. S., Thomas, K. A., & Rajith, L.,Electrochemical characterization and discharge performance of AZ31, AZ61 and AZ91 alloys as anodes for seawater battery. *Journal of Power Sources*, 2025, 628, 235863.

Machine learning assisted Ni-Fe Hydroxide (NFH)/Carbon Black electrode for electrochemical sensing and isomeric discrimination of di Hydroxybenzene isomers

Suman Mondal, Shirsendu Mitra*, Kalisadhan Mukherjee *

Pandit Deendayal Energy University, Raysan, Gandhinagar, Gujarat, India 382007

*Corresponding Author: Dr. Kalisadhan Mukherjee, kalisadhan.mukherjee@sot.pdpu.ac.in

Detecting, discriminating, and quantifying dihydroxybenzene (DHB) isomers like catechol (CT) and hydroquinone (HQ) presents significant analytical challenges due to their nearly identical redox potentials and similar electrochemical behaviors. Quantification becomes more complex in binary mixtures, where signal interference occurs and selective, concentration-dependent calibration is required. Currently, there is a lack of simple, low-cost, handheld strip-based sensors for reliable discrimination and quantification of DHB isomers. In this work, we report the development of a Nickel-Ferric Hydroxide (NFH)/carbon black nanocomposite-based, non-enzymatic electrochemical working electrode and a corresponding strip sensor for the detection, discrimination, and quantification of CT and HQ. The working electrode, used in a standard three-electrode setup, achieves detection limits as low as 10 nM for both isomers, while the strip sensor shows a limit of detection of 50 nM. Both platforms effectively discriminate CT and HQ signals even in 1:1 mixture. Statistical parameters such as skewness and kurtosis of the sensing signals have been modeled to support robust real-time discrimination. The sensors demonstrate excellent repeatability (over 5000 measurements) and reproducibility over time. Detailed synthesis and structural characterization of the sensing materials provide valuable insights into the underlying mechanisms

Keywords: Metal oxide, MWCNT, Electrochemical sensor, Phenolic compound, Machine Learning.

References.

1. Mondal, S. et al. ACS Appl. Nano Mater. 2025, 8, 42, 20463–20476
2. Ranjbar, S. et al. ACS Sens. 2023, 8, 11, 4281–4292

ACEPS-13, January 11-14, 2026, Bengaluru, India

Membraneless Natural Seawater Electrolyzer

Hemanga Pradhan and Musthafa Ottakam Thotiyl*

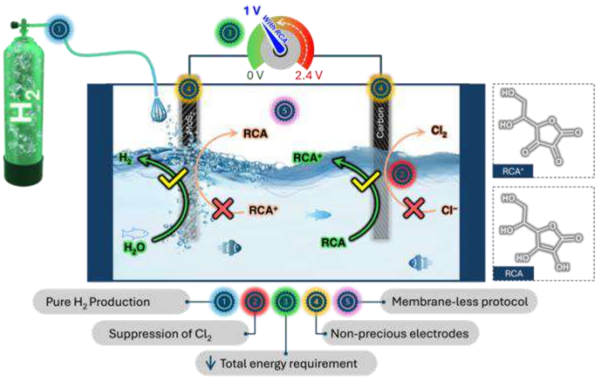
Department of Chemistry, Indian Institute of Science Education and Research, Pune, Dr. Homi Bhabha Road, Pune, 411008, India.

* Email: musthafa@iiserpune.ac.in

Abstract

Seawater electrolysis poses electrochemical challenges due to the concurrent chlorine evolution reaction (CER), which leads to fuel contamination and typically requires segmented cell designs with costly membranes and precious metal anodes. In this work, we introduce a membrane-free, scalable strategy for green hydrogen production from natural seawater by employing a unidirectional competitive redox reaction. The oxidized redox species remains stable on a carbon electrode, effectively suppressing CER while promoting hydrogen evolution through additional proton release. This approach enables a lab-scale, unsegmented, precious-metal-free electrolyzer operating at voltages as low as 1 V, sustaining pure hydrogen generation for over 100 hours with energy consumption nearly one-third that of conventional systems.[1] This offers a highly energy-efficient and cost-effective route for centralized green hydrogen production, aligning with global climate goals.

Keywords: Seawater Electrolyzer, Hydrogen Production, Competitive Redox, Membraneless



Schematic diagram of the sea-water splitting device in an undivided cell architecture containing a unidirectional redox competition agent (RCA).

References

(1) Pradhan, H.; Mondal, R.; Nayak, B.; Thimmappa, R.; Mendhe, R. M.; Ottakam Thotiyl, M. Unidirectional Competitive Redox Enabled Unsegmented Natural Sea-Water Splitting for Green Hydrogen Production. *Green Chem.* **2025**, *27* (3), 770–781.

A non-isothermal water formation cell for electrochemical heat recovery

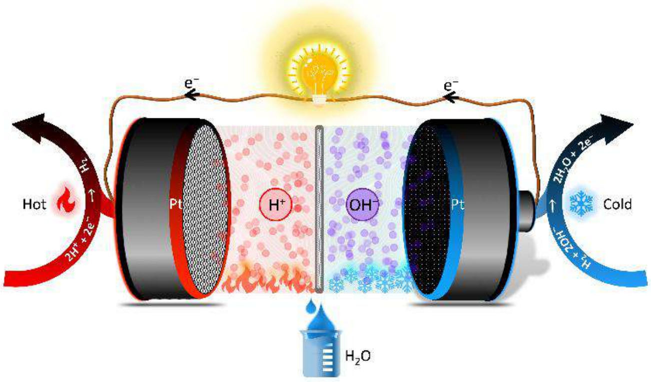
Shyaam Srirangadhamu Yuvaraj and Musthafa Ottakam Thotiyl*

Department of Chemistry, Indian Institute of Science Education and Research, Pune, Dr Homi Bhabha Road, Pune, 411008, India.

musthafa@iiserpune.ac.in

Abstract

Low-grade heat harvesting represents a promising route for converting ambient waste heat into electrical energy. However, conventional thermogalvanic systems predominantly rely on metal ion or halide-based redox couples, which are constrained by low heat-to-electricity conversion efficiencies. Here, we demonstrate a non-redox thermogalvanic approach based on water formation via a net-zero hydrogen redox process. This reaction exhibits a favorable positive entropy change with an inherent asymmetry in their temperature-dependent response, enabling the conversion of nearly 30% of absorbed thermal energy into electrical output, with a resulting thermodynamic efficiency exceeding unity. The developed device achieves a temperature-insensitive maximum power density of approximately 33.55 $mW \cdot m^{-2} \cdot K^{-2}$, which is ~70 times greater than that of state-of-the-art ferrocyanide–ferricyanide systems. This work significantly broadens the scope of electrochemical heat harvesting by moving beyond traditional redox-based mechanisms.



Schematic diagram of electrochemical water formation assisted galvanic–thermogalvanic device for waste heat recovery.

Key words: Thermogalvanic device, Hydrogen redox, Heat harvesting, Seebeck coefficient.

References

(1) Mondal, R.; Yuvaraj, S. S.; Nayak, B.; Pradhan, H.; Thotiyl, M. O. A Non-Isothermal Water Formation Cell for Electrochemical Heat Recovery. *Chem. Sci.* **2025**, 7751–7758.

Thermodynamics of Sodium-Tin Alloys for Negative Electrodes from First-Principles

Javeed Ahmad Dar[1,*], Sai Gautam Gopalakrishnan[1]

1 Materials Engineering, Indian Institute of Science, Bengaluru, India Indian Institute of Science, CV Raman Road, Bengaluru, Karnataka-560012 India.
* javeeddar@iisc.ac.in

Sodium-ion batteries (NIBs) are an alternative option to state-of-the-art lithium-ion batteries (LIBs) due to their low cost and natural abundance of sodium. Significant progress has been made in NIB cathode materials such as layered metal oxides and polyanionic compounds with promising results. On the anode side, graphite, which is the anode for LIBs, shows insignificant capacity for sodium due to the unfavorable thermodynamics, resulting in the use of low energy density hard carbon. Thus, it is crucial to identify anode materials that are more energy dense and exhibit good cycle life compared to hard carbon for improving the cell-level performance of NIBs. In this context, metals that can form alloys with sodium, such as tin, antimony, germanium, and lead are promising anode materials for NIBs due to their high capacities. Particularly, tin exhibits a high theoretical capacity of 847 $mAhg^{-1}$, calculated till formation of the $Na_{15}Sn_4$ intermetallic. However, it is important to understand the alloying reaction of Na and Sn for the optimization of tin-based anodes for NIBs. Herein, we investigate the thermodynamic properties and estimate the Na-alloying voltage for the sodium-tin system using first principles calculations. Additionally, we construct a cluster expansion Hamiltonian based on density functional theory calculations and perform semi-grand canonical Monte Carlo simulations to estimate the solubility of Na within the Sn body-centered cubic and body-centered tetragonal structures, at different temperatures. Construction of the temperature-composition phase diagram enables us to estimate the extent of (metastable) sodium-solubility in tin and the corresponding alloying voltages. Our work should improve the fundamental understanding of the thermodynamics of the sodium-tin alloy system and aid in the optimization of alloying anodes for usage in NIBs.

Multifunctional Na–CO_2 Electrochemical System: Experimental Validation and Modeling for Sustainable Hydrogen and $NaHCO_3$ Co-Production

Raman Kumar Singh[1], Dipannita Saha[2], Sreyanka Karmakar[2], Prakash C Ghosh[1], Amartya Mukhopadhyay[2], Venkatasailanathan Ramadesigan[1*]

[1] *Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India, 400076*

[2] *Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India, 400076*

* venkatr@iitb.ac.in

Abstract

The atmospheric CO_2 concentration has reached an unprecedented level of approximately 427 ppm, contributing significantly to environmental degradation. Existing mitigation techniques are often limited by high costs and low efficiency[1]. Electrochemical conversion of CO_2 in aqueous electrolytes, offers a promising route for transforming CO_2 into value-added products while mitigating anthropogenic emissions. In the aqueous solution, CO_2 dissolves and produces HCO_3^-, H^+, and CO_3^{2-}. Continuous purging of CO_2 further decreases the pH, enhancing H^+ production[2]. In this study, we present a $Na - CO_2$ system to utilize the produced H^+ from CO_2 using Na-metal as an anode, an organic electrolyte, NASICON separator, aqueous electrolyte (CO_2 saturated NaOH solution) and Pt/C coated cathode. A Pt/C-coated cathode facilitates the hydrogen evolution reaction (HER), while sodium oxidation occurs at the anode. The Na^+ ions produced at the anode migrate through the NASICON separator and react with bicarbonate ions (HCO_3^-) in the catholyte to form sodium bicarbonate ($NaHCO_3$). This process enables the simultaneous production of hydrogen gas, sodium bicarbonate, and electrical energy.

A multiphase transient mathematical model using dilute solution theory, binary electrolyte theory, and laminar bubble flow in aqueous electrolyte is developed and validated against experimental results. The model provides insights into the system's behavior by resolving concentration fields, reaction zones, local currents, and potentials. Additionally, a parametric study is performed to assess the impact of key design parameters, including cathode–separator distance, anode size, electrode porosity, and chemical reaction rate constant. This combined experimental and modeling approach offers comprehensive insights into the operation and optimization of $Na - CO_2$ electrochemical systems for sustainable energy and CO_2 utilization.

Keywords: Na-CO_2 battery, CO_2 utilization, Energy Conversion, Bubbly flow, Hydrogen Production

References

(1) Kaur, S.; Zhang, Y.; Song, J.; Zhang, C.; Liu, J.; Cheng, F. Efficient CO_2 Utilization and Sustainable Energy Conversion via Aqueous Zn–CO_2 Batteries. *Nano Energy* **2023**, *109*, 108242. https://doi.org/10.1016/j.nanoen.2023.108242.

(2) Jain, D.; Sharma, M.; Ghoshal, A. K. Numerical Modeling of Carbon Dioxide Chemisorption in Sodium Hydroxide Solution in a Micro-Structured Bubble Column. Chem. Eng. Sci. 2015, 137, 685–696. https://doi.org/10.1016/j.ces.2015.06.043.

Analysis of the sensing performance of Ti3C2 MXene coated Screen Printed Electrodes for Electrochemical Detection of Cortisol

Harini Loganathan[1], Durgalakshmi Dhinasekaran[1,*], Ajay Rakkesh Rajendran[2]

[1] 1Department of Medical Physics, CEG Campus, Anna University, Chennai, India -600025

2Functional Nanomaterial Laboratory, Department of Physics and nanotechnology, Faculty of Engineering and technology, SRM Institute of Science and technology, Chennai, India -603203

* durgalakshmi@annauniv.edu

Abstract

MXenes are a class of 2D materials that exhibit a large surface-to-volume ratio, with exceptional electrocatalytic properties and tunable surface chemistry. It is formed by chemically etching the "A" layer from the 3D MAX phase and offers a novel platform for electrochemical biosensing applications. Titanium Carbide (Ti_3C_2) MXenes can be employed as a working electrode due to their 2D sheet-like morphology and high porosity, which is achieved through the intercalation of the etching agent. The partially filled d-orbitals in the Titanium transition metal in Ti_3C_2 MXenes leads to the formation of a large number of active sites promoting efficient electron transfer during redox reactions for enhanced sensitivity and selectivity of electrochemical sensors. Cortisol detection plays a vital role in today's world, as its irregular levels serves as an indicator for psychological stress which leads to obesity, anxiety and depression. Hence, timely detection is crucial for regulating overall health. When cortisol interacts with Ti_3C_2 MXenes, the electrons from cortisol binds with oxygen containing surface terminations (O, OH) through combination of covalent, vanderwaals and hydrogen bonds at the electrode electrolyte interface. In this work, a novel Ti_3C_2 MXene screen-printed electrode is fabricated to analyse the reaction mechanism at the electrode-electrolyte interface during the addition of cortisol in the electrolyte. The real time performance and the analytical figures of merit of the sensor, such as sensitivity, selectivity, and detection limit, is evaluated through voltametric and amperometric techniques. The screen-printed electrodes can be optimized and developed as point-of-care devices for real-time and continuous monitoring of cortisol using whole blood in the future.

Keywords: Electrochemical, Ti_3C_2 MXenes, screen printed electrodes, cortisol, sensors.

References

(1) Usman, K. A. S.; Judicpa, M.; Bacal, C. J. O.; Marquez, K. P.; Zhang, J.; Dharmasiri, B.; Randall, J. D.; Henderson, L. C.; Razal, J. M. A One-Pot Strategy for Modifying the Surface of Ti3C2Tx MXene. Surf Coat Technol 2024, 494. https://doi.org/10.1016/j.surfcoat.2024.131522.

(2) Vignesh, V.; Castro-Dominguez, B.; James, T. D.; Gamble-Turner, J. M.; Lightman, S.; Reis, N. M. Advancements in Cortisol Detection: From Conventional Methods to Next-Generation Technologies for Enhanced Hormone Monitoring. ACS Sensors. American Chemical Society April 26, 2024, pp 1666–1681. https://doi.org/10.1021/acssensors.3c01912.

Impedance Spectroscopy Unveils Interfacial Dynamics in NiO-Modified Electrodes for Glucose Detection

Arya K[a,b] , Kavita Pandey [a,b*]

[a] *Centre for Nano and Soft Matter Sciences (CeNS), Shivanapura, Bengaluru 562162, India,*

[b] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*

*kavitapandey@cens.res.in

Electrochemical impedance spectroscopy (EIS) is a powerful tool for probing the interfacial properties and reaction mechanisms of electrochemical sensors. In this study, we extensively utilized EIS to analyze the interaction between nickel oxide (NiO) polyhedra and glucose at the electrode interface, providing deep insights into the performance of nonenzymatic glucose sensors. NiO polyhedra were synthesized via the direct thermal decomposition of nickel nitrate hexahydrate ($Ni(NO_3)_2 \cdot 6H_2O$), a scalable and straightforward method that remains underutilized in electrochemical sensing applications. The synthesized NiO was used to modify glassy carbon electrode (GCE) and screen-printed electrodes (SPE). The electrochemical glucose-sensing properties of these NiO-modified electrodes were assessed using cyclic voltammetry (CV) and chronoamperometry (CA), with EIS playing a crucial role in elucidating the electrode interface interactions. The NiO/GCE demonstrated high sensitivity for glucose detection, achieving 1109 μA mM^{-1} cm^{-2} in the glucose concentration range of 5 μM to 1 mM and 737.7 μA mM^{-1} cm^{-1} from 1 mM to 6 mM, with a detection limit of 1.1 μM. Notably, the sensitivity decreased at higher glucose concentrations, indicating two distinct linear ranges. EIS measurements were conducted at varying potentials for two constant glucose concentrations to investigate this phenomenon. The EIS analysis revealed a flip in the impedance spectra or negative resistance at higher glucose concentrations, providing detailed information about charge transfer resistance and interfacial kinetics, which explained the observed changes in sensitivities in CV and CA experiments. The electrode exhibited excellent selectivity over common interferents, along with reproducible and stable performance. The extensive use of EIS not only provided a deeper understanding of the electrode processes but also highlighted the effectiveness of the thermally decomposed NiO polyhedra in enhancing sensor performance. This work underscores the potential of NiO-modified electrodes for nonenzymatic glucose sensing and demonstrates the critical role of EIS in advancing electrochemical sensing technologies.

Keywords :Impedance spectroscopy, Glucose oxidation, Nickel oxide, semsitivity

References

(1) **A. Kannathvalappil**, V. A. S., N. Bhat, N. K. Gupta, K. **Pandey**, *The Journal of Physical Chemistry C* 2025, *129*, 7387.

ACEPS-13, January 11-14, 2026, Bengaluru, India

High-throughput screening of intercalation electrodes for electrochemical ion capture and desalination

Sougat Purohit[1*], Andreas Kuhlmann[2], Marten Huck[2], Hans-Georg Steinrück[2], Sai Gautam Gopalakrishnan[1]

[1] *Department of Materials Engineering, Indian Institute of Science, Bengaluru, India*

[2] *Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy (INW), Germany*

**Email: sougatp@iisc.ac.in*

Abstract

The increasing salinity of freshwater sources, driven by rising sea levels and human activities, demands efficient management of industrial brine [1]. Desalination offers a solution by transforming waste brine into a resource, extracting valuable minerals like Li, Na, K, Mg, and Ca while producing clean water. Desalination also provides a sustainable method for extracting important ions like Li from unconventional sources such as geothermal brines, seawater, and industrial wastewater. We focus on electrochemical desalination using intercalation electrodes, an energy-efficient method that selectively extracts specific ions (or multiple ions) from varied brine compositions. While much of the research in this field has focused on overcoming the shortcomings of the most common intercalation electrodes - olivine-$FePO_4$ and spinel-MnO_2 [2], our approach explores alternative electrode frameworks with superior properties. Lithium-ion battery (LIB) and beyond LIB cathodes are promising candidates for potential desalination electrodes. However, the stability of these battery cathodes in water is not well understood. Utilizing high-throughput computational data generated using density functional theory-based calculations, we construct multi-element Pourbaix diagrams to assess their thermodynamic stability in water (at different salt concentrations) and calculate the intercalation voltage of water-stable frameworks. We filter frameworks based on the optimum operating voltage for aqueous electrolytes and identify electrodes that can intercalate either multiple or selective ions. Our high-throughput computational study proposes promising candidate electrodes for experimental trials, advancing electrochemical desalination for sustainable mineral extraction and water purification.

Keywords: Desalination, beyond LIB cathodes, Pourbaix diagrams, aqueous electrolytes

References

(1) Kaushal, Sujay S., et al. "The anthropogenic salt cycle." *Nature Reviews Earth & Environment* 4.11 (2023): 770-784.

(2) Xiong, Yuecheng, et al. "Electrochemical lithium extraction from aqueous sources." *Matter* 5.6 (2022): 1760-1791.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhanced Diffusion Kinetics in FeS_2 Electrodes via Lattice Relaxation Mechanisms

Manjeet Jakhar[1,*], Kanhaiya Lal Yadav[1]

[1] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee, India*

* manjeet1@ph.iitr.ac.in

Abstract

Electrochemical energy storage systems are emerging as pivotal components of the global energy landscape. Among various strategies to enhance material performance, structural modification has proven to be a powerful tool for tailoring electrochemical properties. In this work, iron sulfide (FeS_2) was synthesized via a hydrothermal method and systematically studied to understand the impact of lattice relaxation on its charge storage behavior. Structural analysis using XRD and TEM confirmed lattice relaxation, which is correlated with improved ion diffusion kinetics. XPS analysis revealed a shift in binding energies toward lower values, indicative of altered electronic structure due to defect formation. Electrochemical performance, evaluated using a three-electrode configuration, demonstrated a significant enhancement in specific capacitance from 433 F/g to 946 F/g at a current density of 1 A/g. The Nyquist plot further confirmed the contribution of both diffusive and capacitive processes, marked by a transition from blocking to absorbing behavior in EIS. These findings highlight the role of lattice-level modifications in optimizing FeS_2-based electrodes and underscore their potential for next-generation energy storage technologies.

Keywords: Gamma Irradiation, Electrochemical kinetics, Ionic Conductivity, Energy Storage

References

(1) Ghorbani-Asl, M.; Kretschmer, S.; Krasheninnikov, A. V. Two-Dimensional Materials under Ion Irradiation: From Defect Production to Structure and Property Engineering. Defects Two-Dimensional Mater. 2022, 259–301. https://doi.org/10.1016/B978-0-12-820292-0.00015-X.

(2) Zhao, Z.; Padhiar, M. A.; Zhang, S.; Ma, T.; Khan, N. Z.; Ji, Y.; Maroof, Z.; Pan, S. Gamma Radiation-Induced Changes in the Structural and Optical Properties of CsPbBr3 Thin Films for Space Applications. Ceram. Int. 2024, 50 (23), 48995–49002. https://doi.org/10.1016/j.ceramint.2024.09.239.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Detection of Soft Short Circuits in Lithium Metal Batteries in the Early Stages by Using FFT and Welch's Algorithm

Rehbar Hasan[1,*], She Huang Wu[2,3], Wei Nien Su[2,3], and Bing Joe Hwang[1,3]

1. Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan.

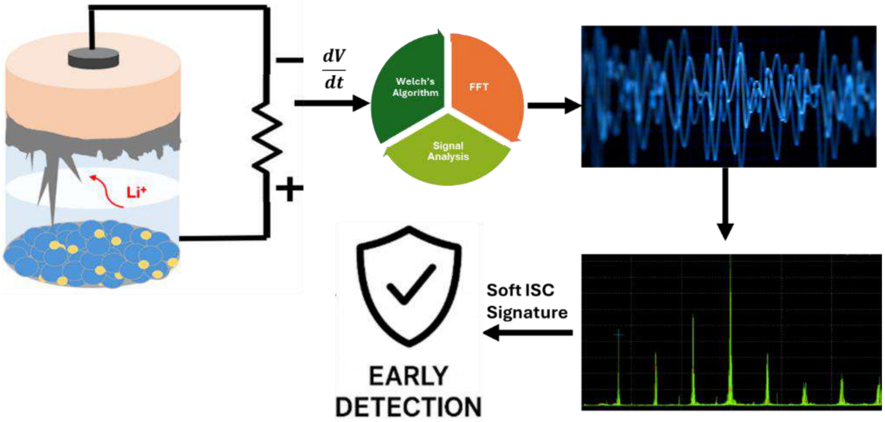
2. Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei 10607, Taiwan.

3. Sustainable Electrochemical Energy Development Center (SEED), National Taiwan University of Science and Technology, Taipei 10607, Taiwan.

E-mail: wush@mail.ntust.edu.tw, wsu@mail.ntust.edu.tw, bjh@mail.ntust.edu.tw

Abstract

Lithium batteries are vital for contemporary energy storage and are integral to the global shift towards sustainable energy. Nonetheless, their safety and reliability present considerable hurdles, particularly in high-power applications. Internal short circuits (ISCs), frequently caused by the proliferation of lithium dendrites, are a primary contributor to battery thermal runaway, occasionally leading to catastrophic incidents such as fires and explosions. Although numerous investigations have suggested diverse methodologies for the early detection of ISCs, they frequently necessitate complex methods or intricate configurations. This study presents an innovative methodology for the early detection of soft short circuits in lithium metal batteries (LMBs) through the application of signal processing techniques to cycle data from diverse battery designs, eliminating the need for abusive conditions. Model the battery as an RC circuit with periodic resistance variations, correlating these fluctuations to the occurrence of ISCs. This methodology, which combines the Fast Fourier Transform (FFT) and Welch's technique for frequency domain analysis, enables the identification of distinctive peaks and power spectral distributions linked to ISC development. Our system presents an innovative method for the early detection of proactive ISC and significantly enhances battery safety while mitigating the risk of serious disasters.



Keywords: Soft ISC, early detection, periodic resistance, safety, non-abusive technique

Manganese-based energy materials derived from low grade manganese ore

MeghaDash [1,2], Sushree Pattanaik [1,2], Satyaswini Sahu [1,2], T. Pavan Kumar [1,2] and Mamata Mohapatra*[1,2]

[1]*CSIR-Institute of Minerals and Materials Technology, Department of Hydro, Bio & Electrometallurgy, Bhubaneswar, 751013, Odisha, India*

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh, India*

* Corresponding author's email address: mamata@immt.res.in

Abstract

Recovery of value-added minerals (like manganese) from low-grade manganese ore is gaining significant interest because manganese is highly earth abundant, cheaper and exhibits variable oxidation states. Therefore, these manganese-based products are increasingly used in energy applications. From energy perspective, the development of cost-effective catalysts for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in water splitting has garnered significant attention, owing to its potential to address pressing environmental and energy challenges, including CO_2 emissions and the depletion of fossil fuel reserves [1]. In our present study, an environmentally friendly, microwave-assisted leaching approach was employed to extract manganese from primary sources. Additionally green, cost-effective and safe lixiviant composed of organic acids were utilized. Following optimisation of the leaching parameters, manganese was effectively leached from low-grade manganese ore achieving a leaching efficiency of >90%, whereas iron remained in the residue. Subsequently, transition metal oxalate dihydrate (t-MOX) was recovered from the optimized leach liquor solution. The recovered material was further evaluated for its application in water splitting reaction showing bifunctional electrochemical performance. In terms of OER, the recovered t-MOX showed favourable onset overpotential of 340 mV along with a lower Tafel slope of 65 $mV.dec^{-1}$ demonstrating excellent electrocatalytic and charge transfer kinetics. In terms of HER, the recovered t-MOX shows an onset overpotential of 302 mV recorded at a current density of 10 $mA.cm^{-2}$. Thus, the recovered material demonstrates favourable onset potential and can act as electrocatalyst for both OER and HER in water-splitting processes.

Keywords : Low-grade manganese ores, microwave assisted leaching, organic acid, energy conversion

References

(1) H. Belhadj, Y. Messaoudi, M.R. Khelladi, A. Azizi, A facile synthesis of metal ferrites (MFe_2O_4, M = Co, Ni, Zn, Cu) as effective electrocatalysts toward electrochemical hydrogen evolution reaction, Int. J. Hydrogen Energy. 47 (2022) 20129–20137. https://doi.org/10.1016/j.ijhydene.2022.04.151.

Designing Dual-Metal Catalysts for Sulfur Reduction Reaction through First Principles Calculations

Sahil Kumar[1], Adithya Maurya K R[1] and Mudit Dixit[1,2*]

muditdixit@clri.res.in; dixitmuditk@gmail.com

[1]CSIR-Central Leather Research Institute (CSIR-CLRI), Chennai - 600020, India

[2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India

Abstract

The practical utilisation of lithium-sulfur (Li-S) batteries is hindered by challenges such as the shuttle effect, polysulfide dissolution, and sluggish reaction kinetics. To overcome these challenges, we design a series of dual-atom catalysts (DACs) anchored on N-doped graphene using a computational approach that combines Machine Learning interatomic potentials (MLIPs) as well as we develop a method named PACE (Precise and Accurate Configuration Evaluation) to accurately identify the adsorption configurations on the graphene layer with help of MACE-MP0 to pre-screen adsorbate configurations before performing first-principles density functional theory (DFT) calculations. Our findings reveal that Fe and Co-based DACs (with other 3d and 4d transition metals) exhibit superior polysulfide anchoring capacity compared to single-atom catalysts (SACs), due to the favourable metal-S interactions arising from inter-site synergistic effects. Additionally, we identify key descriptors, such as d-band center, electronegativity, and number of sulfur atoms, that largely influence the Gibbs free energy of the sulfur reduction reaction (SRR). A detailed understanding of the SRR mechanism and atomic-level insights will help improve the electrocatalytic activity of existing graphene-based materials as well as design new materials experimentally.

Keywords: Lithium-sulfur batteries, Density Functional Theory, binding energy, machine learning.

References

1. Wang, Y.; Xu, C.; Li, B.; Tian, M.; Liu, M.; Zhu, D.; Dou, S.; Zhang, Q.; Sun, J., Tailoring a Transition Metal Dual-Atom Catalyst via a Screening Descriptor in Li-S Batteries. *ACS Nano* **2024,** *18* (51), 34858-34869.

2. Tao, X.; Chen, F.; Xia, Y.; Huang, H.; Gan, Y.; Chen, X.; Zhang, W., Decoration of sulfur with porous metal nanostructures: an alternative strategy for improving the cyclability of sulfur cathode materials for advanced lithium–sulfur batteries. *Chemical Communications* **2013,** *49* (40), 4513-4515.

3. Zhang, X.; Yang, T.; Zhang, Y.; Wang, X.; Wang, J.; Li, Y.; Yu, A.; Wang, X.; Chen, Z., Single Zinc Atom Aggregates: Synergetic Interaction to Boost Fast Polysulfide Conversion in Lithium-Sulfur Batteries. *Advanced Materials* **2023,** *35* (6), 2208470.

ACEPS-13, January 11-14, 2026, Bengaluru, India

In Situ Monitoring of Redox Electrochemistry of Perylene Diimide Electrodes by UV–Vis–NIR Spectroscopy

Narendra Kurra[1,*], Kotagiri Venkata Rao[2*], Priyaranjan Sahoo[1], Soujanya H Goudar[2]

[1] *Department of Chemistry, Inidan Institute of Technology Hyderabad, Kandi, Sangareddy*

[2] *Department of Chemistry, Inidan Institute of Technology Hyderabad, Kandi, Sangareddy*

* kvrao@chy.iith.ac.in, narendra@chy.iith.ac.in,

Abstract

By virtue of sustainability and redox functionality, organic materials are an emerging class of electrodes for multivalent metal-ion batteries. However, the inevitable dissolution of radical anions in electrolyte media during electrochemical reduction poses a challenge to electrochemical reversibility and stability.[1] The stable and electrochemical reversible formation of dianions of cationic perylene diimide (*c*PDI) in aqueous calcium-ion electrolyte is reported. Electrostatically assembled *c*PDI onto functional titanium carbide $Ti_3C_2T_x$ MXene is processed in the form of semi-transparent thin films to probe characteristic spectral changes during reduction–oxidation cycles. In situ UV–Vis-NIR spectroscopy studies confirm the potential dependent reversible formation of radical anions and dianions of *c*PDI at −0.3 and −0.6 V versus Ag wire, respectively. Moreover, the bridging of Ca^{2+} ions between two molecules of perylene diimide also causes the change of electron density at the titanium atoms, as observed from the shift in the transverse surface plasmonic peak of MXene. This clearly signifies the role of non-covalent interactions between $Ti_3C_2T_x$ and perylene diimide in stabilizing dianions in aqueous media, thus suppressing the dissolution effects. This study opens avenues for the exploitation of non-covalent interactions in the design of stable functional organic charge storage hosts for multivalent metal ions.[2]

Keywords: MXene, Perylene diimide, In situ UV-visible, Radical anion, Dianion

References

(1) Nimkar, A.; Bergman, G.; Ballas, E.; Tubul, N.; Levi, N.; Malchik, F.; Kukurayeve, I.; Chae, M. S.; Sharon, D.; Levi, M. Polyimide Compounds For Post-Lithium Energy Storage Applications. *Angew. Chemie* **2023**, *135* (50), e202306904.

(2) Sahoo, P.; Goudar, S. H.; Rao, K. V.; Kurra, N. In Situ Monitoring of Redox Electrochemistry of Perylene Diimide Electrodes by UV–Vis–NIR Spectroscopy. *Small* **2025**, 21, 2412429.

Strontium and Aluminum doped Lanthanum Cerate Electrolyte for Dry Reforming of Methane in Protonic Ceramic Electrochemical Cell

Suddhasatwa Basu[1,*], Manas Mishra[1] , Vaibhav Dev[1]

[1]Department of Chemical Engineering , Indian Institute of Technology, Delhi

*Corresponding Author: sbasu@chemical.iitd.ac.in

Dry reforming of methane (DRM) is considered an effective approach to simultaneously fix CH_4 and CO_2 which are malefic greenhouse gases (GHGs) responsible for global warming while producing syngas ($CO+H_2$) which is a feedstock for valuable chemical synthesis (1). Protonic ceramic fuel cells (H-SOFCs) have emerged as a plausible alternative to oxygen ion conducting solid oxide fuel cells (O-SOFCs) attributed to the relatively low activation energy associated with the migration of H^+ ions as compared to O^{2-} ions, effectively allowing them to operate at temperatures below 600^0C (2). In this regard significant research has been carried out on barium based cerate and zirconates for H-SOFC electrolyte application(3).However severe coke deposition in the presence of hydrocarbon fuels and carbon dioxide containing environments is one of the major drawbacks which retards the overall cell performance and ultimately leads to cell degradation. One more important aspect of hydrogen generation from CH_4 and CO_2 mixture is the electrode material since the widely used nickel-cermet suffer from degradation and nickel evaporation in humidified atmospheres. To evade this issue, we have used $Sr_{1.95}Fe_{1.4}Ni_{0.1}Mo_{0.5}O_{6-\delta}$ (SFNM) double perovskite because of its moderate electrical conductivity, higher stability in reducing and CO_2 containing atmosphere as well as its bifunctionality attributed to its stability in oxidizing atmosphere which makes it suitable for its usage as oxygen electrode (4). In this work we have explored barium free ceramic electrolyte , strontium and aluminum doped lanthanum cerate (LSCA) for potential application as proton conducting electrolyte in H-SOFCs. In this regard, we have designed lanthanum cerate ($LaCeO_3$) ; LCO and Lanthanum Strontium Cerium Aluminate ($La_{0.9}Sr_{0.1}Ce_{0.8}Al_{0.2}O_3$); LSCA and 1 wt.% nickel oxide (NiO) added as sintering aid to LSCA (LSCA-NiO) electrolytes and SFNM electrodes in symmetrical configuration, considering the bifunctionality of the double perovskites. The electrical conductivity of the as designed electrolytes has been evaluated in dry air using AC 2 probe technique from 500^0 C to 750^0 C. At 750^0C, the conductivity value for LCO was 2.96 mS cm^{-1} while for LSCA, a 2.6-fold increase in conductivity was observed which is 7.89 mS cm^{-1}. ascribed to the increased basicity at the B-site cation with trivalent metal ion doping and increased acidity at A-site with bivalent metal ion doping respectively enhancing the oxygen vacancy which is pivotal for proton conduction (5).The addition of NiO as sintering aid improves the conductivity and LSCA-NiO exhibits conductivity value of 1.67×10^{-2} S cm^{-1} at 750^0C. The protonic conductivity of LSCA-NiO measured by ion blocking electrode cell between 450^0C to 750^0C method depicts the electrolyte offers a conductivity value of 3.89×10^{-3} S cm^{-1} at 750^0C and 8.85×10^{-4} S cm^{-1} at 500^0C. The electrochemical testing of the symmetrical cells based on LSCA and SFNM has been performed in fuel cell mode CH_4 + CO_2 mixture as fuel and air. A maximum power density of 31 m W cm^{-2} was obtained at 800^0 C .Impedance spectroscopy results indicate a decrease in polarization resistance(R_p) value with an increase in temperature. The lowest R_p was observed to be 2.5 Ω cm^{-2} at 800^0C .

Key Words : Protonic Ceramic Fuel Cells (H-SOFCs), dry reforming of methane (DRM), lanthanum cerate ($LaCeO_3$);LCO, strontium and aluminium doped lanthanum cerate ($La_{0.9}Sr_{0.1}Ce_{0.8}Al_{0.2}O_3$);LSCA .

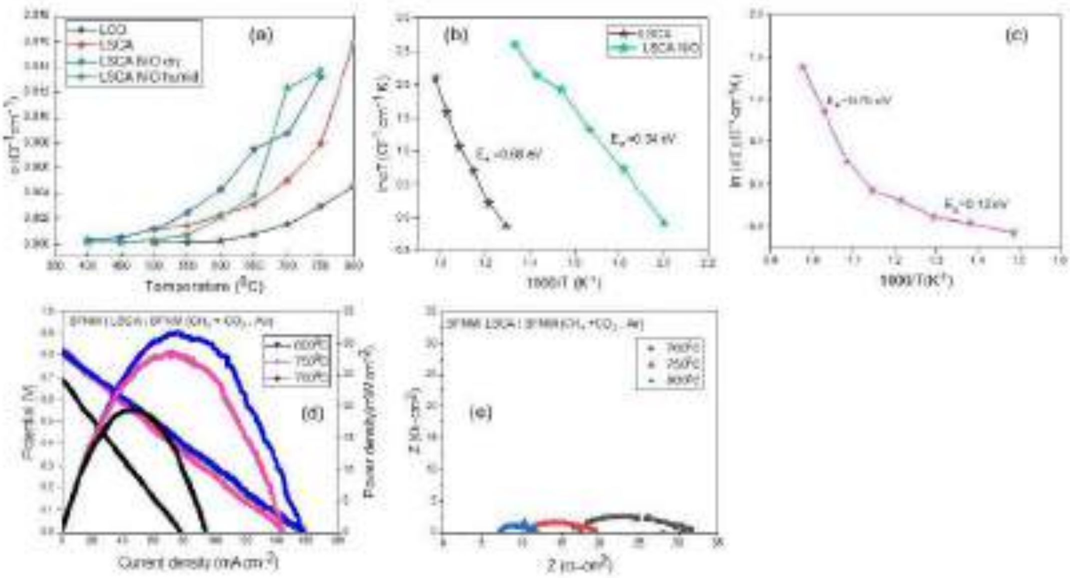


Figure 1. (a) Comparison of conductivities of LCO, LSCA and LSCA-NiO electrolyte materials with temperature, (b) Arrhenius plots of conductivities of LSCA and LSCA-NiO , (c) Arrhenius plots of proton conductivities of LSCA and LSCA-NiO, (d) Current density- voltage -power density characteristics curves of SFNM| LSCA| SFNM symmetrical cells in CH_4 + CO_2 mixture as fuel and air and (e) Nyquist plots of SFNM| LSCA| SFNM symmetrical cells in CH_4 + CO_2 mixture as fuel and air

References

1. Liu F, Deng H, Ding H, Kazempoor P, Liu B, Duan C. Process-intensified protonic ceramic fuel cells for power generation, chemical production, and greenhouse gas mitigation. Joule. 2023 Jun;7(6):1308–32.

2. Duan C, Huang J, Sullivan N, O'Hayre R. Proton-conducting oxides for energy conversion and storage. Applied Physics Reviews. 2020 Mar 1;7(1):011314.

3. Dai H, Kou H, Wang H, Bi L. Electrochemical performance of protonic ceramic fuel cells with stable BaZrO3-based electrolyte: A mini-review. Electrochemistry Communications. 2018 Nov;96:11–5.

4. Osinkin D, Tropin E. Hydrogen production from methane and carbon dioxide mixture using all-solid-state electrochemical cell based on a proton-conducting membrane and redox-robust composite electrodes. Journal of Energy Chemistry. 2022 Jun;69:576–84.

5. Cao J, Ji Y, Shao Z. Perovskites for protonic ceramic fuel cells: a review. Energy Environ Sci. 2022;15(6):2200–32.

ACEPS-13, January 11-14, 2026, Bengaluru, India

NiOS@ANF Electrodes for stable Long-Term Alkaline Water Splitting Using Untreated River Water

Sonu Kumari [1], Aditi Halder[1,*]

[1] *School of chemical sciences, Indian institute of technology, Mandi, India*

* aditi@iitmandi.ac.in

Abstract

Green hydrogen production through water electrolysis powered by renewable energy is a key enabler for global decarbonization and aligns closely with the United Nations Sustainable Development Goals, particularly SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action). In this study, we present a rapid and energy-efficient fabrication strategy for NiOS-decorated activated nickel foam (NiOS@ANF) electrodes using a scalable electrodeposition method completed within 2 hours. The developed electrodes exhibit strong electrocatalytic activity and long-term operational stability in untreated river water, even under fluctuating power inputs—conditions representative of real-world renewable energy sources. This work not only addresses key challenges in electrode design for alkaline water electrolysis (AWE) but also demonstrates the feasibility of integrating low-cost, durable materials into decentralized green hydrogen production systems. Our findings contribute to the broader effort of building sustainable hydrogen infrastructure for a carbon-neutral future.

Keywords: Hydrogen evolution reaction; Oxygen evolution reaction; total water splitting; untreated River water splitting; industrial scale electrocatalyst

References

(1) Kumari, S.; et al. An Efficient and Robust Noble-Metal-Free Self-Standing Bifunctional Water Electrolysis Catalyst: Co_3S_4@Ex. NiFe-LDH for Alkaline Water Electrolysis. Int. J. Hydrogen Energy 2024, 80, 1164–1173.

Modelling Reversible Phase-Change in Cathodes of Sodium-Ion Batteries

Annanya Rout [1,#], Sindhuja Renganathan [2,*]

[1]Center for Education (CFE) , [2]Electro Chemical Power Source Division,
CSIR-Central Electrochemical Research Institute, Karaikudi,Tamil Nadu, India – 630 003
E-mail: * rsindhuja.cecri@csir.res.in, #annanya.rout@gmail.com

Abstract

Reversible phase transformations in cathode materials are critical for the long-term performance of sodium-ion batteries (SIBs). These transformations typically occur either as solid solutions or via two-phase coexistence, with the latter often resulting in characteristic voltage plateaus, as seen in NASICON-type or olivine-type cathodes. A comprehensive understanding of such cathodes necessitates accurate characterization of interfacial dynamics, diffusional pathways within distinct phases, and the structural differences between these phases. While physics-based modeling, particularly the shrinking-core approximation, has been widely applied to phase-change materials like $LiFePO_4$ in lithium-ion batteries, its adaptation to sodium-ion systems remains less explored.

In this work, we extend the shrinking-core model, previously established for lithium systems, to a sodium-ion framework, using $Na_3V_2(PO_4)_2F_3$ (NVPF) as a representative phase-change cathode. This theoretical model effectively captures the intricate interface dynamics during de-sodiation/sodiation processes, encompassing solid-state diffusion limitations and the movement of the phase boundary. Our framework leverages experimental parameters reported for sodium-ion systems, specifically NVPF cathodes [2-3], building upon early modelling efforts in this domain. By utilizing literature-based parameters, the model provides a robust tool for exploring the interplay between diffusion dynamics and phase transformation within the system. This approach offers crucial insights into concentration gradients and the movement of the shell-core interface, directly correlating these phenomena to the cathode's voltage performance. Ultimately, this work presents a foundational approach for the rational design and optimization of sodium-ion cathodes, and when integrated into a complete full-cell model, can predict the overall performance of the entire SIB system.

Keywords: Sodium-ion batteries (SIB), cathode, Shrinking-Core model, Reversible phase transformation, Physics-based modelling

References

1. Jagannathan, K. J. Electrochem. Soc., 2009, 156, A1028–A1033.
2. Chayambuka, K. et al. Electrochim. Acta, 2022, 404, 139726.
3.Chayambuka, K. et al. Electrochim. Acta, 2022, 405, 139727.

Economical 550 V energy harvesting from plastic and electronic waste using human motions

Man Singh,[a] Sameer Kumar,[a] Faisal Hussain Malik,[a] Alankar Kafle,[a] Kalpana Garg,[a] Parimal Sharma,[b] C. C. Reddy[b] and Tharamani C. Nagaiah[a]

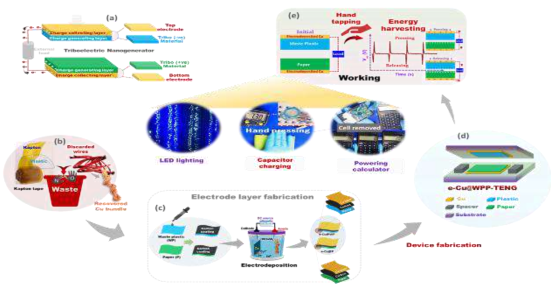
Department of Chemistry, Indian Institute of Technology, Ropar, Punjab-140001, India,

Corresponding author: tharamani@iitrpr.ac.in

Abstract

The disposal of plastic and electronic artifacts is an expensive and time-consuming process. Versatile measures are needed to address the significant environmental hazard posed by excessive plastic consumption and improper disposal of technological trash[1]. Here, we have demonstrated a very simple and affordable method for creating a triboelectric nanogenerator (TENG) out of plastic and electronic debris. Triboelectric layers were made using recovered polyethylene terephthalate (PET) from old Kapton tape and printing paper[2]. More crucially, a straightforward copper sacrificial electrodeposition method was used to create the electrode layers instead of complex and extensive procedures. It is an excellent approach to recycle discarded plastics and create gadgets that collect and generate energy from them[3]. The copper was taken from discarded electrical wires from malfunctioning UPS batteries. The fabricated TENG produced a high-quality electric output maximum open circuit voltage of ~552 V, a short circuit current of 18.8 μA and a high-power density of 7.68 W m^{-2} under contact-separation triggered by human hand tapping. This work stresses the importance of implementing economically viable strategies for utilizing plastic and electronic waste to harvest valuable energy.

Keywords : Triboelectric nanogenerator, Waste plastic, Electrodeposition, Energy generation and storage.



References

1. Bukhari, M. U.; Khan, A.; Maqbool, K. Q.; Arshad, A.; Riaz, K.; Bermak, A., Waste to energy: Facile, low-cost and environment-friendly triboelectric nanogenerators using recycled plastic and electronic wastes for self-powered portable electronics. *Energy Reports* **2022,** *8*, 1687-1695.

2. Nawaz, S. M.; Saha, M.; Sepay, N.; Mallik, A., Energy-from-waste: A triboelectric nanogenerator fabricated from waste polystyrene for energy harvesting and self-powered sensor. *Nano Energy* **2022,** *104*, 107902.

3. Kwon, S.; Kang, J.; Lee, B.; Hong, S.; Jeon, Y.; Bak, M.; Im, S.-k., Nonviable carbon neutrality with plastic waste-to-energy. *Energy & Environmental Science* **2023,** *16* (7), 3074-3087.

Atmospheric Pressure CVD Growth of WS_2/WO_3 Hybrid Architectures for Energy Storage Applications

Nishtha Sagta[1], Ajay Kumar Mishra[2]

[1]*National Institute of Technology Puducherry, Karaikal, India, 609609*

**Email: ph21d1001@nitpy.ac.in*

Abstract

With the growing demand for flexible and high-performance energy storage devices, the development of scalable electrode architectures has become increasingly important. Transition metal dichalcogenides and oxides offer great promise due to their tunable redox behavior and structural versatility[1]. Herein, we report the synthesis of a hybrid tungsten disulfide/tungsten trioxide (WS_2/WO_3) heterostructure via atmospheric pressure chemical vapor deposition (APCVD), offering a facile and scalable route to functional electrode materials. The resulting WS_2/WO_3 hybrid features a unique mixed morphology comprising flower-like and rod-like nanostructures, fostering a synergistic combination of electric double-layer capacitance (EDLC) and faradaic pseudocapacitance. This hybrid architecture was directly integrated onto carbon cloth substrates to fabricate a symmetric two-electrode supercapacitor device. The assembled device exhibits excellent capacitive performance, delivering a specific capacitance of 381 F/g at a scan rate of 100 mV/s.

Our findings highlight the potential of TMD/oxide hybrids as next-generation electrode materials for high-performance supercapacitors, combining scalable fabrication with superior electrochemical characteristics.

[1] A. Subhramaniyan Rasappan *et al.*, "Battery-type WS2 decorated WO3 nanorods for high-performance supercapacitors," *Mater. Lett.*, vol. 357, no. December 2023, p. 135640, 2024, doi: 10.1016/j.matlet.2023.135640.

Studies on ionic conduction in polymer electrolyte membranes

Amita Pandey, Chinmoy Ranjan*

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bengaluru 560012, India, ranjan@iisc.ac.in

Abstract

Polymer electrolyte membranes are gaining significant attention due to their crucial role in various applications and their potential in advancing clean energy technologies, particularly fuel cells and electrolysers. Among these polymers, perfluorinated sulfonic-acid (PFSA) ionomers stand out due to their exceptional ionic conductivity and robust chemical and mechanical stability.

Understanding the ionic conduction mechanisms within Nafion, along with the factors that affect its conductivity and strategies for addressing these challenges, is essential for the development of more effective electrolyte membranes. Such advancements are directly linked to improving the efficiency and performance of energy conversion devices.

Conductivity of Nafion is essentially a function of relative humidity and temperature. Relative humidity itself is a function of temperature. It is hence crucial and challenging to maintain these parameters to study the conductivity of Nafion whilst simultaneously using the spectroscopic methods to develop molecular level understanding during conduction of ions. Electrochemical Impedance Spectroscopy and in-situ Raman scattering measurements upon equilibration at a particular temperature and relative humidity provide important insights to correlate structural changes with the conduction of cations in the membrane. The shifts in the Raman peaks on exchanging Nafion with different cations, particularly -SO3- stretching vibrations on varying temperature and relative humidity provide information about the conductivity mechanism of the Nafion. Distribution of Relaxation Times analysis of the impedance data elucidates the timescales of processes involved in the transport of cations along the complex morphology of the polymer electrolyte membrane.

Keywords : Polymer Electrolytes, Ionic Conductivity, Impedance, In-situ Raman Scattering

References

(1) Kusoglu, A.; Weber, A. Z. New Insights into Perfluorinated Sulfonic-Acid Ionomers. Chem. Rev. 2017, 117 (3), 987–1104. DOI: 10.1021/acs.chemrev.6b0015

(2) Gruger, A.; Régis, A.; Schmatko, T.; Colomban, P. Nanostructure of Nafion Membrane at Different States of Hydration: An IR and Raman Study. Vib. Spectrosc. 2001, 26 (2), 215–225.

(3) Tabuchi, Y.; Ito, R.; Tsushima, S.; Hirai, S. Analysis of In Situ Water Transport in Nafion® by Confocal Micro-Raman Spectroscopy. J. Power Sources 2011, 196 (2), 652–658

ACEPS-13, January 11-14, 2026, Bengaluru, India

Analysis of Li-ion transport in varied solvent systems for Li–S batteries using multi-scale mathematical models

Ritwik Roy[1] , Venkatasailanathan Ramadesigan[1,*]

[1] *Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India, 400076*

* venkatr@iitb.ac.in

Abstract

Lithium-sulphur (Li-S) batteries are irrefutably one the most promising technologies for future applications in electric vehicles for their high theoretical energy density (2567 Wh kg^{-1}) and electrochemical capacity (1675 mAh g^{-1}), but practical performance is relatively poor. This high energy density arises from multi-electron redox reactions involving polysulphides. These reactions alter the electrolyte composition dynamically; consequently, the transport characteristics evolve during cell operation. Furthermore, the crossover of solvated polysulphides to the anode lead to capacity degradation. These highlight the need to understand the effects of electrolyte-transport dynamics. Most continuum scale simulation studies employ dilute solution theory, which neglects inter- and intra-species interactions. The concentrated solution theory, based on the Onsager–Stefan–Maxwell framework, captures these interactions at the continuum level, but it is not easy to apply since it requires several transport parameters, namely the cross diffusivities, which are challenging to obtain from experiments. Hence, we adopt a multiscale approach, combining molecular dynamics with physics-based 1-D model for solvent systems of variable solvation properties. The 1-D model flux equations are modified using the formulations given in Mistry et al.[1] Here, we examine dimethyl ether (DME), 1,3-dioxolane–dimethyl ether (DOL-DME, 1:1 vol) and dimethyl ether-1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether (DME-TTE, 1:1 vol) as the solvents and 1M Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as salt. To simplify the model, we truncate the sulphur reduction reaction to consider three representative polysulphides: S_8^{2-}, S_4^{2-},and S^{2-}. The self and cross diffusivities, and the transference numbers, included in the 1-D model is calculated from the MD analysis. The simulated concentration gradients of various soluble polysulphides across the cell depicts how solvation shell structure change at the microscopic scale affect extent of shuttle and ionic conductivity and thus affect the capacity fading in lean electrolyte cells at the continuum scale. The insights obtained thus serves a tool for understanding electrolyte structure, its effect on the ion transport and efficient prediction of the battery performance, which will help in design and optimization of better electrolyte for Li-S battery.

Keywords: Mathematical modelling, Lithium-Sulphur, Electrolyte

References

(1) Mistry, A. N.; Mukherjee, P. P. "Shuttle" in Polysulfide Shuttle: Friend or Foe?. The Journal of Physical Chemistry C 2018, 122 (42), 23845–23851. https://doi.org/10.1021/acs.jpcc.8b06077

ACEPS-13, January 11-14, 2026, Bengaluru, India

Decoupling Oxygen Redox Irreversibility and TM Migration in Li-Rich Nickel Manganese Oxide by Creating a Disordered Rocksalt Phase

Susim Sabuj Sarkar[1], Subham Ghosh[1], Arup Chakraborty[2] , Maria Diaz-Lopez[3] and Urmimala Maitra[1]*

[1] *School of Materials Sciences, Indian Association for the Cultivation of Sciences, Kolkata, India*

[2] *Department of Materials, University of Oxford, Oxford, United Kingdom*

[3] *Institut Neel CNRS, Grenoble, France*

* urmimala.maitra@iacs.res.in

Abstract

Over the past few decades, there has been considerable debate regarding the oxygen redox in lithium-rich cathodes and, more specifically, the nature and fate of the oxidized oxygen species.[1–4] O-loss has been loosely associated with TM-migrations at elevated states of charge, which eventually leads to Li and O loss from the surface regions (a process called "densification") of the cathode. Another school of thought has proposed the utilization of a cation-disordered rock-salt crystal structure (DRS) to achieve large compositional flexibility and prevent the ill effects of TM-migrations.[5,6] We study the O-redox behaviour of typical Li-rich cathode $L_{1.2}Ni_{0.2}Mn_{0.6}O_2$; with the material crystallizing in two distinct crystal structures: the commonly occurring cation-ordered layered structure and the cation-disordered DRS structure. Distinct disparities in the O-redox behavior of the cathodes within two distinct crystal structures are manifestly evident. The DRS cathode exhibits an accelerated onset and and greater propensity of O-redox as compared to the cathode in the layered structure. More significantly we observe that the oxidized O-species in the DRS structure exhibits a notable degree of freedom, which renders it susceptible to loss from the lattice. In contrast, in layered cathodes the spectroscopic signature of oxydized O species can be found to persist for atleast upto a week suggesting its “trapped” nature. By comparing the differences in environments around the oxydized O-species in the DRS and layered structure the study conclusively relates the O-loss behaviour to TM-migrations and rock-salt phase formation. This finding therefore clearly relates O-loss to rock-salt phase formation and resolves a long-standing ambiguity in the field.

Keywords: Li-ion battery, Cathode Material, Disorder Rocksalt, Anionic Redox

References

(1) Luo, K *et al. Nat. Chem.* **2016**, *8* (7), 684–691.

(2) House, R. A. *et al. Nat Energy* **2021**, *6* (8), 781–789.

(3) Li, B. *et al. Nat. Mater.* **2023**, *22* (11), 1370–1379.

(4) Gao, X. *et al. Nat Mater.* **2025**, *24* (5), 743–752.

(5) Guin, S. *et al. Chem. Mater.* **2024**, *36* (21), 10421–10450.

(6) Clément, R. J. *et al. Energy Environ. Sci.* **2020**, *13*, 345–373.

Accelerating Sodium-Ion Battery Innovation: Integrating DFT, Machine Learning, and AI for Materials Discovery

Kanchan Gangwar[1], Prof. Ashish Yadav [1]*, Prof. Shishir Sinha [2]*

Department of Chemical Engineering, Indian Institute of Technology, Roorkee, India

Corresponding authors email: ashish@ch.iitr.ac.in , shishir@ch.iitr.ac.in

Abstract

Sodium-ion batteries (SIBs) are gaining attention as a safer, more affordable alternative to lithium-ion batteries for large-scale energy storage. However, they still face major problems like low energy density, slow sodium-ion diffusion, unstable cathode materials during cycling, and poor lifespan due to side reactions at the electrode–electrolyte interface. These challenges limit their commercial success. Traditional experimental methods for solving these problems are expensive and time-consuming. To speed up progress, researchers are now combining **Density Functional Theory (DFT)** with **Machine Learning (ML)** and **Artificial Intelligence (AI)** to predict and screen battery materials before making them in the lab. For example, ML models trained on DFT data have successfully predicted the voltage and stability of new cathode materials like NASICON-type compounds. Similarly, ML-driven simulations of hard carbon have revealed how sodium ions move and get stored inside the anode, helping improve energy capacity. AI tools are also being used to design new liquid and solid electrolytes by predicting SEI formation and chemical compatibility. Together, DFT and ML make it possible to test thousands of materials virtually, reducing the need for costly experiments and accelerating the discovery of high-performance battery components. This computational approach is helping SIBs overcome their limitations and move closer to real-world use in grid storage, electric vehicles, and backup power systems.

Keywords: Sodium-ion batteries, DFT, Machine Learning, Artificial Intelligence, Materials Discovery

References

1. Hossain, M. A.; Azhari, A.; Yildiz, B. Deep Neural Network Framework to Predict Electrode Voltages for Sodium-Ion Batteries Using Density Functional Theory Database. *arXiv* **2024**, *arXiv:2503.13067*.

2. Xu, Y.; Long, Y.; Lin, Z.; Xu, T.; Li, Y. Machine Learning-Based Prediction of Formation Energy for Sodium-Ion Battery Cathode Materials. *Batteries* **2024**, *10* (12), 431.

3. Shim, H.; Ahn, J.; Kang, Y.; Park, J. Machine-Learning-Assisted Discovery of High-Voltage NASICON-Type Cathodes for Sodium-Ion Batteries. *Batteries Supercaps* **2024**, *7* (6), 2400186.

4. Cheng, Q.; Zhang, J.; Kitchaev, D. A.; Liu, Y.; Urban, A. Interpretable Machine Learning Uncovers Sodium Storage Mechanisms in Disordered Carbon Anodes. *arXiv* **2024**, *arXiv:2412.00340*.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Molecular Engineering of HOMO–LUMO Levels of Organic Chromophores for Visible-Light-Driven Lignin Valorization

Hyeong Cheol Kang[1], Chan Ki Jeon[1], Lorenzo Zani[2] and Jae-Joon Lee[1*]

[1] *Department Energy & Materials, Research Center for Photoenergy Harvesting & Conversion Technology (phct), Dongguk University, Seoul, 100-715, Republic of Korea*

[2] *Istituto Di Chimica Dei Composti Organometallici, Sesto Fiorentino, Florence, Italy*

* *jjlee@dongguk.edu*

Abstract

A new series of benzothiadiazole (BTD) based organic chromophores was developed by tuning the donor group in the D–DTP–benzothiadiazole–phenyl–acceptor framework with alkoxy-phenyl moieties (BTD-DTP4, 5 and 6). The design aimed to lower the HOMO level by ~300 mV compared to conventional photocatalysts, thereby enabling efficient electron transfer from low-potential HAT mediators such as 4-acetamido-(2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (ACT). Simultaneously, the LUMO level was reduced, extending light absorption beyond that of the reference dye (E)-3-(5-(4-(bis(2',4'-dibutoxy-[1,1'-biphenyl]-4-yl) amino)phenyl)thiophen-2-yl)-2-cyanoacrylic acid (D35) and affording a significant photocurrent gain. Among the series, BTD-DTP5 delivered the best performance, yielding photocurrents of 4.0 mA/cm^2 with ACT, respectively. It also achieved >90% conversion of secondary alcohols to C_α-ketones. These results highlight the critical role of donor engineering in controlling redox levels and absorption profiles, offering a promising strategy for visible-light-driven biomass conversion.

Keywords: Dye-sensitized photoelectrochemical cell; visible-light photocatalysts; alcohol oxidation; biomass conversion

ACEPS-13, January 11-14, 2026, Bengaluru, India

Effect of dispersion of conducting phase on impedance of porous electrode

Lalith Kishore AK, Yadul Sethi[1*] and Bharatkumar Suthar[1]

[1] *Indian Institute of Technology, Bombay, India*

* *sethiyadul@gmail.com*

Abstract

Efficient design of the conductive phase in porous electrodes can significantly reduce overall impedance and improve the performance of electro-chemical systems. Recent work by Ramaswamy et al. demonstrated that surface treatment of platinum-supported carbon catalysts to optimize the distribution of the ionomer phase can enhance fuel cell performance.[1] In solid-state batteries, achieving effective contact between the solid-electrolyte and the electrode active material (AM) remains a major bottleneck limiting performance.[2] Similarly, in Li-ion batteries, the morphology of the carbon-binder domain (CBD) critically influences both ionic and electronic conduction pathways.[3]

Our preliminary computational analysis using an in-house developed impedance code suggests that uniform ion-conductive coatings (white color coatings in Figure 1) can significantly reduce impedance (see Figure 1 impedance). We studied two designs on artificially generated electrodes as shown in Figure 1 where red circles refer to AM. Design 1: a uniform coating of conductive material (white) around the AM, Design 2: the conducting phase is uncoated. In both designs 1 and 2 the conducting material (white) does not entirely occupy the non-AM space and has some empty void space (blue) which does not participate in ion/e- conduction. For the chosen parameter ($\varepsilon_{\mathrm{AM}} = 0.53$, $\varepsilon_{\mathrm{ion-conductive}} + \varepsilon_{\mathrm{void}} = 0.47$) the resistance of the coated electrode was reduced by 22% with just 2.5% increase in conductive phase volume fraction. As expected, the coated electrode also has highest capacitance (i.e active surface area). This indicates that coated electrode may lead to a better design, leading to overall lower impedance. Impedance behaviour is finger-print of various losses within the electrode. Tailored design of the conductive phase can reduce such losses. Therefore, in this work, we systematically investigate various designs of conductive phase in porous electrode and their impedance characterstics.

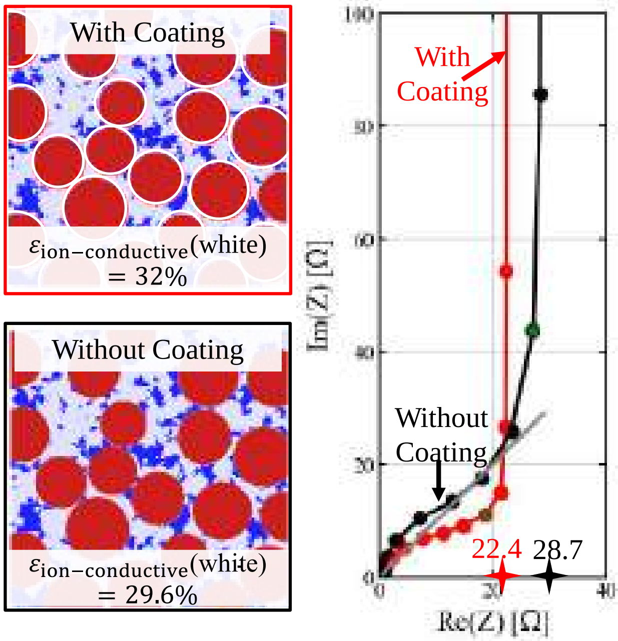


Figure 1: Effect of ion conducting coating on the impedance of a porous simulated electrodes .

Keywords: Impedance, Batteries, Fuel-cell, Ionic, Electronic

References

1. N. Ramaswamy and J. Wortman, *ACS Energy Lett.*, 6170–6177 (2024).

2. T. Famprikis et al., *Nat. Mater.*, 18, 1278–1291 (2019).

3. B. L. Trembacki et al., *J. Electrochem. Soc.*, 165, E725–E736 (2018).

Development of High-Performance Proton Conducting Solid Oxide Cell (H-SOC) Electrodes: Pr-substituted $La_{0.7-x}Pr_xSr_{0.3}Co_{0.8}Fe_{0.2}O_{3-\delta}$ and Nd/Cu Co-doped Bio-Template Enhanced $Pr_2NiO_{4+\delta}$

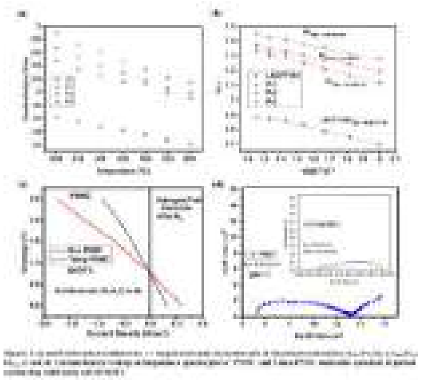
Subhrajyoti Ghosh and Suddhasatwa Basu *

Department of Chemical Engineering, Indian Institute of Technology Delhi, Delhi, India

*Email: sbasu@chemical.iitd.ac.in

Abstract

Proton conducting solid oxide cell (H-SOC), an energy efficient electrochemical device, that converts the chemical energy of fuels (H_2, CH_4 etc.) to electrical energy in fuel cell mode and vice-versa in electrolyzer mode, operating at intermediate temperature (500-700 ^oC).The oxygen reduction reaction (ORR) and water oxidation reaction (WOR) are the rate limiting steps, requiring robust air / steam electrode with enhanced triple ($H^+/O^{2-}/e^-$) conductivity. [1] This study investigated A-site Pr^{3+} substitution in $La_{0.7-x}Pr_xSr_{0.3}Co_{0.8}Fe_{0.2}O_{3-\delta}$ [X=0, (LS), X=0.2 (Pr1),0.35 (Pr2)]. All composition showed metallic conductivity behavior as in figure 1 (a), with Pr3 showing lowest activation energy (E_a=0.01964 eV), followed by Pr1 (E_a=0.0199 eV), LS (E_a= 0.02177eV) and Pr2 (E_a=0.0258 eV) as shown in Arrhenius plot of total conductivity, figure 1 (b). Additionally, A-site 'Nd' and B -site 'Cu' doping in ($Pr_2NiO_{4+\delta}$): PNNC, have been explored as a cobalt free ruddlesden popper air / steam electrode material for H-SOC. PNNC showed semiconducting behavior with highest conductivity of 27.54 S/cm at 750 ^oC, increasing to 31.659 S/cm in humid conditions due to the formation of protonic defects. Single cell: NiO-BZCYY/BZCYY (300μm) / PNNC, achieved current density of 186 mA /cm^2 (fuel cell, at 0.3 V) and -650 mA/cm^2 (electrolysis, at 2 V) at 650 ^oC. Bio-template modified PNNC (Temp PNNC), significantly improved performance achieving 370 mA/cm^2 (fuel cell, at 650 ^oC,0.3V) and -1259 mA/cm^2 (electrolysis, at 650^oC,2V) are achieved, with reduced polarization resistance from 5.18 to 0.322 Ω cm^2. The corresponding current density-voltage curve and impedance spectra for both PNNC and temp-PNNC electrodes are presented in Figure 1 (c) and (d).



Keywords: Proton conducting solid oxide cell, Triple conductors

References

Li, B.; Boulfrad, S.; Traversa, E. Steam Electrolysis by Solid Oxide Electrolysis Cell (SOEC) with Proton-Conducting Oxides. *Chem. Soc. Rev.* **2014**, *43*, 8255.

Highly nanostructured MnFe-LDH@nickel foam synthesized via electrochemical method enhancing the rapid movement of ions in Zinc-ion hybrid capacitors

Shivani,[1] Navpreet Kamboj,[1,*] and Sanjeev Kumar,[1,*]

[1]*Physics Department, Punjab Engineering College (Deemed to be University), Sector-12, Chandigarh, India-160012*
Corresponding author's email- Sanjeev@pec.edu.in

Abstract

By leveraging the synergistic effects of LDHs and conductive networks like nickel foam (NF), the study aims to develop cost-effective, high-performance materials for next-generation metal-ion capacitors. Comprehensive physical characterization of the MnFe-LDH@NF was performed with electrochemical testing. MnFe-LDH stand out due to their tunable composition, high surface area, and excellent ion-exchange properties. The synergistic integration of LDH nanosheets with a conductive substrate like NF significantly enhanced charge transport and electrochemical performance. The deposited MnFe-LDH@NF electrode exhibited a high specific capacitance of 1456 mF cm^{-2}, with an energy density of 102 µWhcm^{-2} and a power density of 357 µWhcm^{-2}. For practical application, MnFe-LDH@NF was assembled with a zinc plate in 1 M KOH electrolyte to construct a hybrid zinc-ion capacitor. This configuration demonstrated a specific capacitance of 220 mF cm^{-2}, along with an energy density of 36 µWh cm^{-2} and a power density of 1090 µW$cm^{-2,}$ while retaining 99.99% of its capacitance and achieving 100% coulombic efficiency over prolonged cycling also reaching to cell voltage upto 0.8 V to 2 V. Furthermore, a planar solid-state device was fabricated, which showed excellent performance with a specific capacitance of 878.8 mF cm^{-2}, energy density of 101 µWh cm^{-2}, and power density of 970 µW cm^{-2}. The device retained 81% of its capacitance after cycling and exhibited a coulombic efficiency of 99% after 2000 charge/discharge cycles. Impressively, it could power an LED for 3 minutes, demonstrating its practical applicability for real-world energy storage solutions.

Keywords: Zinc-ion capacitors, Energy density, Specific capacitance, Power density, Layered double hydroxides.

Hierarchical MXene@Nickel phosphide on 3D Ni Foam for Superior Electrochemical Performance in Zinc-Ion Capacitors

Radhika,[1] Navpreet Kamboj,[1,*] and Sanjeev Kumar,[1,*]

[1] *Physics Department, Punjab Engineering College (Deemed to be University), Sector-12, Chandigarh, India-160012*
Corresponding author's email- Sanjeev@pec.edu.in

Abstract

Various cathode materials, such as transition metal phosphides (TMPs) and carbon-based materials like MXenes, have been explored to enhance the electrochemical performance of zinc-ion capacitors (ZICs). MXenes, particularly $Ti_3C_2T_X$, exhibit excellent electrical conductivity, large surface area, and abundant active sites, making them promising candidates for energy storage applications. However, their performance is often limited by restacking of nanosheets and oxidation in alkaline medium. To overcome these limitations, a hybrid electrode was developed by integrating $Ti_3C_2T_X$ MXenes with nickel phosphide (NP) on a 3D nickel foam (NF) substrate. This hybrid structure leverages the synergistic effects between the high conductivity of MXene and the pseudocapacitive nature of nickel phosphide, resulting in improved specific capacitance, energy density, and cycling stability. The $Ti_3C_2T_X$/NP@NF hybrid electrode was synthesized via a two-step process: electrochemical deposition of nickel phosphide onto nickel foam, followed by hydrothermal growth of MXene. The resulting electrode demonstrated an excellent specific capacitance of 763.64 mF cm^{-2} at a current density of 0.95 mA cm^{-2} in 1 M KOH electrolyte, with a corresponding energy density of 23 μWh cm^{-2} and power density of 223 μW cm^{-2}. Furthermore, a hybrid zinc-ion capacitor ($Ti_3C_2T_X$ /NP@NF // Zn) was assembled using the hybrid electrode as the cathode and a zinc plate as the anode. Operating at a voltage of 1 V in 1 M KOH, the device exhibited a specific capacitance of 469.58 mF cm^{-2}, an energy density of 60 μWh cm^{-2}, and a power density of 336 μW cm^{-2}. Notably, the device maintained 93% capacitance retention after 10,000 continuous charge/discharge cycles with nearly 100% coulombic efficiency, underscoring its excellent long-term stability. These results highlight the potential of $Ti_3C_2T_X$ /NP@NF hybrid electrodes for high-performance zinc-ion capacitors in practical energy storage applications.

Keywords: Hybrid MXenes, zinc-ion capacitor, specific capacitance, energy density, power density.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Investigating the performance of lignocellulosic biomass-derived activated carbon for supercapacitor electrode application

Shubham Kumar[1,*], Sandeep Kumar[1], S Parida[2]

[1] Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai 400076, India

[2] Department of Metallurgical Engineering and Material Science , Indian Institute of Technology Bombay, Mumbai 400076, India

* shubhamkr@iitb.ac.in

Abstract

Lignocellulosic biomass is a plant-based material that mainly contains lignin, cellulose and hemicellulose. These materials have potential to produce activated carbon due its natural interconnected pore network. The conversion of lignocellulosic biomass feedstock into porous carbon material for supercapacitor has been increasingly explored by researcher[1]. Lignin, cellulose and hemicellulose have been used as feedstock for producing activated carbon, which is further utilized as an electrode material for supercapacitor application. The carbonizing temperature (700 °C – 950 °C) and chemical treatment methods determine their resulting properties including surface area (500 - 3000 m^2/g) and pore size distribution (0 - 50 nm), which are crucial for fabricating supercapacior electrode material. Moreover, the feedstocks structure composition also affects the morphology and capacitive performance of activated carbon electrode[2]. In this regard, we experimentally charecterize the physicochemical performance of the biomass derived activated carbon using X-ray diffraction, Raman spectroscopy, fourier-transfer infrared spectroscopy, N_2 physisorption, and field emission scanning and transmission electron microscopy. The electrochemical performance is conducted in aqueous electrolyte using technique such as cyclic voltammetry, galvanostatic charge-discharge test and electrochemical impedance spectroscopy. The synthesized electrode demonstrated a maximum specific capacitance of 122 F/g at 1 A/g, highlighting the potential of lignocellulosic-derived activated carbon for supercapacitor applications.

Keywords: Lignocellulosic biomass, Activated carbon, Supercapacitor

References

(1) Jiang, C.; Yakaboylu, G. A.; Yumak, T.; Zondlo, J. W.; Sabolsky, E. M.; Wang, J. Activated Carbons Prepared by Indirect and Direct CO2 Activation of Lignocellulosic Biomass for Supercapacitor Electrodes. *Renew. Energy* 2020, *155*, 38–52. https://doi.org/10.1016/j.renene.2020.03.111.

(2) Mehta, S.; Jha, S.; Liang, H. Lignocellulose Materials for Supercapacitor and Battery Electrodes: A Review. *Renew. Sustain. Energy Rev.* 2020, *134* (October 2019), 110345. https://doi.org/10.1016/j.rser.2020.110345.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Surface-Engineered Pt–Ni Catalysts for Improved Electrochemical Performance in Direct Ammonia Fuel cells

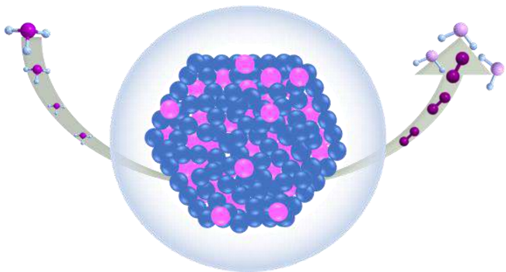
Chaithra Rajeev[12] Vishal M. Dhavale[12,*]

[1] *CSIR-Central Electrochemical Research Institute-Madras Unit, CSIR Madras Complex, Taramani, Chennai, 600113, Tamil Nadu, India.*

[2] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad– 201002, India*

* vishal@cecri.res.in

Abstract



The global transition towards clean and sustainable energy technologies necessitates the exploration of alternative fuels that combine high energy efficiency with minimal environmental impact. Hydrogen has emerged as clean energy carrier owing to its high gravimetric energy density and zero carbon emission upon utilization. However practical challenges associated with hydrogen storage, handling and transportation have driven interest toward ammonia as an alternative energy vector which offers high volumetric energy density and serves as a carbon free and high hydrogen content, making it an attractive fuel for direct ammonia fuel cells (DAFCs).Despite this potential, the practical deployment of DAFCs is significantly limited by the sluggish kinetics of ammonia oxidation(AOR), particularly under low temperature operating conditions. This kinetic limitation is primarily attributed to the formation and accumulation of strongly adsorbed reaction intermediates onto the catalyst surface and hinder catalytic activity. To overcome this challenge, we propose the development of a nanostructured platinum-nickel alloy catalyst featuring a flower-like morphology. This unique structural modification provides an enhanced surface-to-volume ratio and promotes a well- ordered inter/intra-atomic arrangement, which facilitate improved catalytic performance. The tailored Pt-Ni architecture is expected to offer superior resistance to intermediate poisoning and promote efficient low-temperature AOR, thereby advancing the applicability of ammonia-based energy systems.

Keywords : Pt–Ni Alloy Nanostructures, Intermediate Poisoning Resistance,Ammonia oxidation reaction, Direct Ammonia Fuel Cells

References

(1) ACS Sustainable Chem.Eng. 2024, 12, 13030−13047

Interface modulation and redox additive strategies for high-performance solid-state Na^+ ion supercapacitors

Anshuman Dalvi[1,*], Neha[1]

[1] *BITS PILANI, Pilani Campus, India*

* adalvi@pilani.bits-pilani.ac.in

Abstract

This study provides a strategy for improving the performance of Na^+-ion based solid-state supercapacitors (SSCs) via two approaches: (1). interfaces modification by forming a stable thin micro gel layer to ensure optimal utilization of the electrode surface area and (ii). Adding a redox additive, KI, to the composite solid polymer electrolyte enhances ion activity in the electrolyte. The SSCs have been assembled using a Na^+ ion conducting NZSP ($Na_3Zr_2Si_2PO_{12}$) reinforced composite solid polymer electrolyte (CSPE) membrane of room temperature conductivity $\geq 10^{-4} \Omega^{-1} cm^{-1}$ and high surface area (~1800m^2/g) activated carbon-based electrodes. The electrochemical performance parameters dramatically improve when a high-boiling-point organic solvent (DMF) layer is inserted at the electrode-electrolyte interface. Electrochemical investigations reveal that utilizing a nominal amount (≤5μL/cm^2) of such solvent at the interface improves the effective contact area and ionic movement across the interface. The study further explores the role of redox additive addition in the CSPE membrane. The conductivity of CSPE increases to a value of ~3 $\times 10^{-3}$ $\Omega^{-1}cm^{-1}$ at 50 °C when added with a small amount of KI (~0.06g per 1g of CSPE). Results reveal that the utilization of DMF improves the specific capacitance from ~150F-g^{-1} to ~205F-g^{-1}. Also, after the addition of redox additives (KI), the C_S value further rises to ~570F-g^{-1}. Such changes lead to a notable drop in the equivalent series resistance (ESR) of the device and maintain the coulombic efficiency above 95%. The cells exhibit stable electrochemical performance, i.e., ~86% of capacity retention after 2000 cycles of charge-discharge at 1mA/1V (~50% after 10000 cycles). Such SSC combinations demonstrated the remarkable potential of these high-performing supercapacitors by powering 8V LED circuits for at least ~50 minutes during direct discharge.

Keywords: *Electric double-layer supercapacitor; Pseudo capacitance; Interface modification; Solid-state supercapacitor; Solvent-layer approach.*

Synergistic Engineering of Se Vacancy and Heterojunction in $NiSe_2$@FeSe Electrode for Enhanced Ion Transport in High-Performance Flexible Hybrid Supercapacitor and Overall Water Splitting

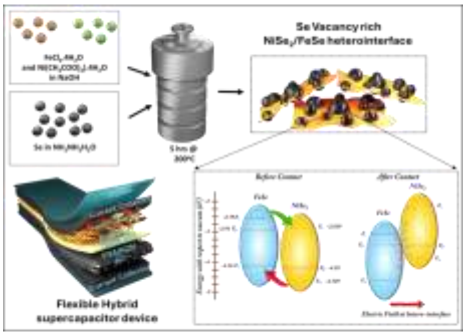
Daya Rani[a], *Harini E M*[a], *Mohd Afshan*[a], *Kaushik Ghosh**[a]

[a]Institute of Nano Science & Technology, Knowledge City, Sector-81, SAS Nagar,140306, Mohali, Punjab, India

***Corresponding Author email: kaushik@inst.ac.in**

Abstract

Flexible hybrid supercapacitors (HSCs) offer great potential for portable, flexible electronics owing to their high-energy storage, stability, mechanical resilience, and eco-friendliness. However, their electrochemical performance is limited by cathode materials. Nickel-based transition metal selenides (TMSs) are promising candidates for cathodes owing to their inherent capacities, yet face challenges such as structural degradation, low electrical conductivity, and sluggish charge transfer, which hinder cycling stability and rate capability. This study employs a synergistic approach by engineering a built-in electric field (BIEF) and Se vacancies in the $NiSe_2$@FeSe heterostructure (VNSFS) through solvothermal method followed by calcination. This synergistic modulation enhances structural integrity during the intercalation/deintercalation of electrolyte ions, boosts ionic and electronic conductivity, improves ion diffusion kinetics, ample electroactive sites, and reduces activation energy supported by theoretical calculations. Consequently, the VNSFS electrode exhibits an impressive specific capacity of 238.89 mAh g^{-1} at 1 A g^{-1}, with excellent rate capability and outstanding cyclic stability, maintaining 98.86% capacitance retention over 12,000 cycles. Additionally, the insertion/deinsertion of OH^- ions in the VNSFS electrode is systematically investigated through a series of in-situ and *ex-situ* characterization techniques. Furthermore, a quasi-solid state VNSFS//AC flexible HSC delivers a high energy density of 94.17 Wh kg^{-1} without compensating power density of 750 W kg^{-1}, prolonged cyclic stability and excellent rate capability. This device advances sustainability by integrating a commercial solar cell module for renewable energy harvesting and storage, capable of powering various electronic devices within 2 mins of charging also supports wireless charging and effective AC filtering. This electrode demonstrates efficient water splitting with self-powered via the HSC. Thus, this work offers a high-safety, flexible energy storage device that supports the development of wearable electronics, replacing bulky capacitors with miniaturized high-performance HSC, promoting eco-friendly energy solutions, and contributing to sustainable development goals.



Strength in Unity: Designing of Hybrid Heterostructure ($NiSe_2$/rGO/PANI) Electrode Towards High Performance, Flexible, Asymmetric Supercapacitor Device for Renewable Energy Storage

Harini E.M. [a], Daya Rani [a,1], Mohd Afshan [a,1], Mansi Pahuja [a], Nikita Chaudhary [a], Seema Rani [a], Shumile Ahmed Siddiqui [a], Subhabrata Das [a], Jyoti [a], Soumyadip Sharangi [a], Rishita Ghosh [a], Sudip Kumar Batabyal [b,c], Kaushik Ghosh [a,*]

a Institute of Nano Science & Technology, Knowledge City, Sector-81, SAS Nagar, 140306 Mohali, Punjab, India

b Department of Physics, Amrita School of Physical Sciences, Amrita Vishwa Vidyapeetham, Coimbatore, 641112 India

c Amrita Centre for Industrial Research & Innovation (ACIRI), Amrita School of Engineering, Amrita Vishwa Vidyapeetham, Coimbatore, 641112 India

***Corresponding Author email:** kaushik@inst.ac.in

Abstract

Heterostructure creation has been an effective strategy to synthesise hybrid supercapacitor electrodes by combining materials of various charge storage mechanisms, leveraging the advantages, and minimising the drawbacks of individual materials as separate entities. Herein, a hybrid supercapacitor electrode has been fabricated producing ternary $NiSe_2$/rGO/PANI heterostructure, through simple hydrothermal followed by in-situ polymerisation techniques. Owing to the synergy between the materials, the electrode decorated on a flexible carbonaceous template exhibits a remarkable capacity of 657.36 Cg^{-1}@1 Ag^{-1} offering excellent stability over 12000 cycles. Subsequently, a hybrid asymmetric supercapacitor (HASC) constructed using $NiSe_2$/rGO/PANI as a positive electrode and AC as a negative electrode possesses a high energy density of 98.82 Wh kg^{-1} at a power density of 750.05 W kg^{-1} with a capacitive retention of 95.04%. Encasing the complete device with Polydimethylsiloxane (PDMS) mould acting as an energy storage band demonstrates an unaltered device performance at various bending angles of 0^{o} to 135^{o}, which refers to its compatibility in flexible electronics. Further, the practical usefulness of the as-designed prototype has been exhibited by powering several devices such as; Light Emitting Diodes (LEDs) of various colours, homemade windmill, Arduino board, and LCD monitor via charging through a commercial silicon solar panel paving the way to bloom renewable energy conversion and storage.

Keywords

$NiSe_2$/rGO/PANI heterostructure, Hybrid supercapacitor, Energy density, Surface passivation, Flexible supercapacitor.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Effect of magnetic field on Manganese Cobalt Phosphide supercapacitor electrode

Anuradha Yadav[1], Manoj Kumar Singh[1,3,*], Chandra Sekhar Rout[2,4,*]

[1] Department of Physics & Astrophysics, Central University of Haryana, Jant-Pali, Mahendergarh-123031, India

[2] Department of Chemical Engineering, Chungbuk National University, Cheongju, Chungbuk 28644, Republic of Korea

[3] School of Engineering and Technology (SOET), Central University of Haryana, Jant-Pali, Mahendergarh-123031, India

[4] Centre for Nano and Material Sciences, Jain (Deemed–to–be University), Jain Global Campus, Kanakapura Road, Bangalore – 562112, Karnataka, India.

[*]Corresponding authors: manojksingh@cuh.ac.in, csrout@gmail.com, r.chandrasekhar@jainuniversity.ac.in

Abstract

As a battery-type material, bimetallic manganese cobalt phosphides (MnCoP) have garnered considerable interest in the domain of energy storage. In this paper, the influence of an external magnetic field on supercapacitor performance was investigated. The electrochemical behavior of the MnCoP electrode was evaluated using a three-electrode configuration. Upon application of a magnetic field, the electrode exhibited a remarkable increase in specific capacitance from 25.9 F/g to 105 F/g at a current density of 5 A/g. The presence of a non-uniform magnetic field created a magnetic gradient force, which enhanced ion transport at the electrolyte/electrode junction, thus thinning the Nernst diffusion layer. Furthermore, the electrode retained a high proportion of its charge storage capability, with values of 72.17% and 84.34% recorded in non-magnetic and magnetic environments, respectively.

Keywords: Supercapacitor, magnetic field, nanorods, battery-type material.

Electrostatically Driven Unidirectional Molecular Flux For High Performance Alkaline Flow Batteries

Bhojkumar Nayak, Ritwik Mondal, and Musthafa Ottakam Thotiyl*

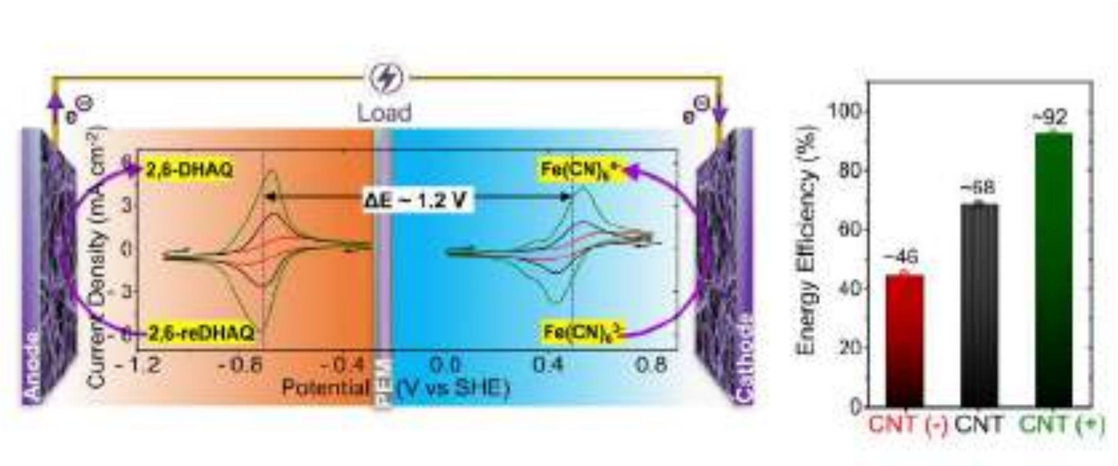
Department of Chemistry, Indian Institute of Science Education and Research (IISER)-Pune,

Dr. Homi Bhabha Road, Pashan, Pune 411008, Maharashtra, India

* musthafa@iiserpune.ac.in

Abstract

To address the discrepancy between energy supply and demand caused by diurnal and seasonal fluctuations, significant efforts focus on storing renewable energy using diverse energy storage technologies. Redox flow batteries are advantageous over traditional types due to their ability to separate energy and power functions. However, critical interfacial processes like mass transport and electron transfer profoundly influence the energy storage and conversion mechanisms of flow batteries. We demonstrate that activation of electrostatic forces at interfaces enables directional molecular flux to and from electrode surfaces, generating concurrent or counteracting electrostatic and diffusion currents. This strategy enhances flow battery volumetric energy density and increases energy efficiency up to approximately 92%, while preserving the redox active species' solubility limit.



Keywords: Redoc Flow Batteries, Electrostatic effect, mass transport.

References

1. *Nanoscale*, 2023,**15**, 14468-14475.

2. *J. Colloid Interface Sci.*, 2024, **662**, 289–297.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Enhanced Solid-State Supercapacitors Using Al^{3+}-Doped Li^{+} Perovskite Electrolyte Integrated with Carbon Aerogel Electrodes

Bhargab Sharma[1,*] and Anshuman Dalvi[1]

[1] *Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Vidya Vihar, Pilani, Rajasthan 333031, India*

* p20220448@pilani.bits-pilani.ac.in

Abstract

We present the development and performance of solid-state ceramic supercapacitors (SSCs) employing a novel composite electrolyte system composed of aluminium-doped lithium lanthanum titanate ($Li_{0.36}La_{0.56}Ti_{0.995}Al_{0.005}O_3$; Al^{3+}-LLTO) and the ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIM BF_4). Structural analysis via Rietveld refinement confirms the retention of the tetragonal perovskite structure post Al^{3+} substitution, while XPS and Raman spectroscopy validate the successful doping without secondary phase formation. Incorporation of ~6 wt.% EMIM BF_4 enhances the ionic conductivity of the composite to ~10^{-3} Ω^{-1} cm^{-1} at room temperature—an increase of nearly three orders of magnitude compared to pristine LLTO. Symmetric SSCs were fabricated by integrating the composite electrolyte between copper electrodes coated with high surface area freeze-dried carbon aerogel (FD-CA), using a cost-effective hot-roll lamination process. The assembled devices demonstrate a high specific capacitance of ~370 F g^{-1} at 1 mA (2 V), excellent cyclic stability (~87% capacitance retention over 15,000 cycles), and high coulombic efficiency (~99%) at 35 °C. The capacitive response is characteristic of ideal electric double-layer behaviour up to 2 V. These findings underscore the promise of Al^{3+}-LLTO/EMIM BF_4 composite electrolytes and FD-CA electrodes for advancing high-performance, safe, and scalable solid-state energy storage technologies.

Keywords : Solid-state supercapacitor; Perovskite; FD-CA; Rietveld refinement; XPS

References

(1) Sharma, B.; Sharma, S.; Kaur, G.; Hardeep; Dalvi, A. High Energy Density Solid State Symmetric Supercapacitors Using Ionic Liquid Dispersed Li + Ion-Perovskites. *RSC Adv* **2025**, *15* (4), 2704–2716. https://doi.org/10.1039/D4RA07417C.

Solid State Supercapacitors with Wide Thermal Stability using Garnet-type $Li_{6.75}Al_{0.25}La_3Zr_2O_{12}$–EMIM BF_4 Composite Electrolyte

Gurpreet Kaur[3*], S.C. Sivasubramanian[1], Anshuman Dalvi[2], Suddhasatwa Basu[3]

[1]*Department of Chemistry, Pilani Campus, Birla Institute of Technology and Science, Pilani, Rajasthan, India, 333031.*

[2]*Department of Physics, Pilani Campus, Birla Institute of Technology and Science, Pilani, Rajasthan, India, 333031.*

[3]*Department of Chemical Engineering, IIT Delhi.*

*gopik3009@gmail.com

Solid-state supercapacitors (SSCs) with composites of Li^+ ion conducting garnet type LALZO ($Li_{6.75}Al_{0.25}La_3Zr_2O_{12}$) with an ionic liquid (EMIM BF_4) as electrolyte are reported. The composite of LALZO with 6 wt% of IL, having high ionic conductivity ≥ 10^{-4} $\Omega^{-1}cm^{-1}$, was used as an electrolyte by compressing between high surface area activated carbon coated copper electrodes, and assembled in 2032 type cell geometry. The SSCs exhibit stable cycling performance for at least ~ 4000 cycles at 1 V operating voltage and 0.57 A/g (1 mA) discharge current with a relatively high coulombic efficiency of ~ 99 %. A typical cell at 35 ^oC exhibits a specific capacitance of ~ 550 F/g at 0.57 A/g (1 mA), and 2 V. The stability of the solid-state converters (SSCs) was tested from 0°C to 100°C. They exhibited consistent performance under these extreme temperature conditions. Supercapacitors performing below an operating voltage of 1.5 V exhibit a pure electric double layer type nature and, in a range of 1.5 V ≤ V ≤2.5 V, a mixed EDLC/pseudo behaviour. At 1.13 A/g (2 mA), a highest specific energy is obtained as ~ 86 Wh/kg. Further, at 5.67 A/g (10 mA), the SSCs exhibited a highest specific power of ~ 2195 W/kg. The results demonstrate that the LALZO-IL composites can potentially be solid-state (ceramic) electrolytes in high-performance supercapacitors. A stack of 4 cells can power two white LEDs (6 V) in series for approximately 30 minutes.

Keywords: solid state supercapacitors; garnet-type Li^+ ion conductors; device stability; ionic liquid-ceramic electrolyte

References:

1. Kwatek, K.; Nowiński, J.L. Electrical properties of $LiTi_2(PO_4)_3$ and $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ solid electrolytes containing ionic liquid. *Solid State Ion.* ***2017***, 302, 54–60.
2. Kaur, G.; Singh, M. D.; Sivasubramanian, S. C.; Dalvi, A. Investigations on enhanced ionic conduction in ionic liquid dispersed sol-gel derived $LiTi_2(PO_4)$. *Materials Research Bulletin* ***2022,*** 145, 111555.
3. Hu, X.; Chen, Y.; Hu, Z.; Li, Y.; Ling, Z. All-Solid-State Supercapacitors Based on a Carbon-Filled Porous/Dense/Porous Layered Ceramic Electrolyte. *Journal of the Electrochemical Society* ***2018,*** 165, A1269-A1274.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Coprecipitation-Hydrothermal Synthesis Method of Conductive Sb-doped SnO_2 for Carbon-free Cathode Catalyst Support of PEMFC

Takeshi Fukuda[1], Yuichi Yoshiyama[1], Naoki Fukumuro[1], Seigo Ito[1]*

[1] *Graduate School of Engineering, University of Hyogo, 2167 Shosha, Himeji, Hyogo 671-2280, Japan*

* itou@eng.u-hyogo.ac.jp

Abstract

To improve the durability of polymer electrolyte fuel cells, carbon-free catalysts are attracting attention. In particular, tin oxide (SnO_2) is fascinating due to its electrical conductivity and chemical stability. It has already been reported that Pt/SnO_2 catalysts using SnO_2 doped with antimony (Sb) and they exhibit high durability [1, 2]. For the practical use of Pt catalysts using Sb-SnO_2 (Pt/Sb-SnO_2) and their large-scale diffusion, it is essential to improve the catalytic activity. Since the catalytic activity of Pt/Sb-SnO_2 depends on the crystallinity, morphology, and conductivity of Sb-SnO_2, it is important to study and optimize the Sb-SnO_2 synthesis method. In this study, we focused on the coprecipitation method and the hydrothermal method to synthesize the Sb-SnO_2 nanoparticles, which have been used as industrial synthesis methods and are also used as laboratory-scale methods. Now, we developed a new synthesis method (coprecipitation-hydrothermal synthesis), and evaluated the prepared Sb-SnO_2 and Pt/Sb-SnO_2.

In the experimental methods, tin fluoride (SnF_2) and antimony chloride ($SbCl_3$) mixed in distilled water. After adding tetramethylammonium (TMAH), the solution stirred for about 3 days, and transferred to a Teflon internal-vessel with stainless-steel-out jacket autoclave. The autoclave was placed in an electric furnace at 240℃. The precipitate was washed 3 times using centrifiguation and dried (named as “coprecipitation-hydrothermal Sb-SnO_2”). Pt catalyst was deposited by the polyol method as “Pt/Sb-SnO_2”. For the “Pt/Sb-SnO_2”, the prepared coprecipitation-hydrothermal Sb-SnO_2 powder was dispersed in a mixed solvent of ethylene glycol and water, then platinum chloride hexahydrate was added. The solution was then heated at 120°C for 2 hours to produce the platinum nanoparticles on the Sb-SnO_2 surface.

The performance of using coprecipitation-hydrothermal Sb-SnO_2 was compared with that of Sb-SnO_2 using the simple coprecipitation (coprecipitation Sb-SnO_2) and hydrothermal methods (hydrothermal Sb-SnO_2). The electrical conductivity of Sb-SnO_2 and the catalytic performance of Pt/Sb-SnO_2 were compared. As a result, coprecipitation-hydrothermal Sb-SnO_2 showed the best results in both cases. This is due to the appropriate doping of Sb by coprecipitation and the improvement of crystallinity by hydrothermal treatment.

Keywords: PEMFCs, carbon-free catalysts, coprecipitation-hydrothermal method, Sb-doped tin oxide

References

(1) K.Kakinuma, *et al., Electrochim. Acta.,* **2013** 110, 316-324.

(2) T. Fukuda, S. Ito, *et al., Crystals,* **2024**, 14, 462.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Mechanism Analysis of Specific Redox Behavior and Durability Evaluation of Pt Catalysts Supported on Sb-Doped SnO_2 for Proton-Exchange-Membrane Fuel Cells

Yuichi Yoshiyama[1], Takeshi Fukuda[1], Seigo Ito[1*]

[1] *Graduate School of Engineering, University of Hyogo, 2167 Shosha, Himeji, Hyogo 671-2280, Japan*

* itou@eng.u-hyogo.ac.jp

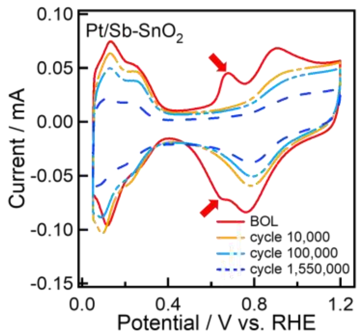
Abstract

Carbon-suported Pt catalyst (Pt/C) are the most widely used for oxygen reduction reaction (ORR) in prton-exchange-membrane fuel cells (PEMFCs) in order to realize a carbon-free hydrogen-energy society. However, the durability of this catalyst is limited by the carbon support, which can cause the degradation. To improve this, metal oxides such as SnO_2 have been investigated as the alternative supporting materials.[1] In our recent study, it was reported that Sb-doped SnO_2 nanoparticles synthesized by an ozone-assisted hydrothermal method exhibit enhanced electrical conductivity and durability.[2] We also reported a unique peak appearing around 0.7 V in cyclic voltammetry (CV) measurements for Pt/Sb-SnO_2 ORR catalysts (Figure 1(a)).[2] Understanding the factors causing this peculiar peak is crucial for the practical application of Pt/Sb-SnO_2. Furthermore, the catalyst performance and particle condition after the peak disappeared must also be clarified.

In this study, electrochemical measurements were conducted to investigate the detailed time-dependent evolution of Pt/Sb-SnO_2 under various operating conditions. Furthermore, a load-cycling durability test using a half-cell was conducted (Figure 1(b)) to confirm the retention rate of catalytic performance. Finally, the catalyst condition after the durability test was evaluated by XPS and STEM-EDX.

Keywords : PEMFC, carbon-free catalyst, Pt/Sb-SnO_2, antimony-doped tin oxide, ozone-assisted hydrothermal method

(a)



(b)

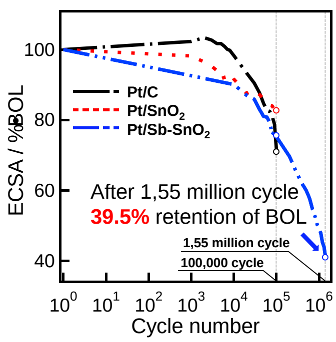


Fig.1 (a)Change in Cyclic Voltammograms, (b)Change in ECSA during durability test

References

(1) K. Kakinuma, et al., *Electrochimica Acta*, 2013, 110, 316–324.

(2) T. Fukuda, et al., *Crystals*, 2024, 14 (5), 462

ACEPS-13, January 11-14, 2026, Bengaluru, India

Electrochemical studies of Pt supported on nitrogen-doped mesoporous carbon in PEFC

Yugo Inagaki[1,] , Tasuku Nakamura[1], Takanobu Ishida[1], Daisuke Ito[1], Yohei Ido[1], Hiroki Kurihara[1*]

[1] *Business Creation Sector R&D Center, 1333-2 Haraichi, Ageo-shi Saitama 362-0021, Japan*

* Corresponding author's email address: hiroki_kurihara@mitsui-kinzoku.com

Pt supported on carbon (Pt/C) has been extensively synthesized and studied due to its high performance in polymer electrolyte fuel cells (PEFCs). The research using porous carbon as a support material for Pt has received considerable attention due to a reduction in ionomer poisoning of the Pt surface. Carbon modification is also an effective method for enhancing catalytic activity. Ref . 1 reported that nitrogen-doped (N-doped) porous carbon increases the interaction between Pt particles and carbon support. We focused on Pt/N-doped mesoporous carbon (MPC) catalyst because we believe that a synergistic effect can be expected from the suppression of ionomer poisoning[2] and the enhancement of the interaction between the Pt particle and carbon support. On the other hand, MPC with a lower nitrogen amount is preferred, as a higher nitrogen amount accelerates water flooding at high current densities. To understand the fuction of low N-doped MPC for cell evaluations at low relative humidity (RH), we compare the electrochemical properties of Pt/5% N-doped MPC [**A**] and Pt/2% N-doped MPC [**B**] to Pt/MPC as a reference material without N-doping.

N-doped mesoporous carbons were produced by heating the MPC with an N-containing compound under an inert atmosphere. Pt loading was carried out by the liquid-phase reduction, obtaining [**A**] and [**B**]. The hydrophilicity by the BET surface areas was in the order of [**A**]>[**B**]>Pt/MPC. Fig. 1 shows a typical polarization curve of the samples under the low RH condition. [**A**] and [**B**] demonstrated higher performance than Pt/MPC (Fig. 1a) across the entire current density range, which can be attributed to the suppression of ionomer poisoning in [**A**] and [**B**]. However, the effect of nitrogen content is evident in the higher current density region. The lower the nitrogen content, the higher the performance, which could be attributed to the reduction of water flooding with low nitrogen content MPC, under low RH conditions (Fig. 1b).

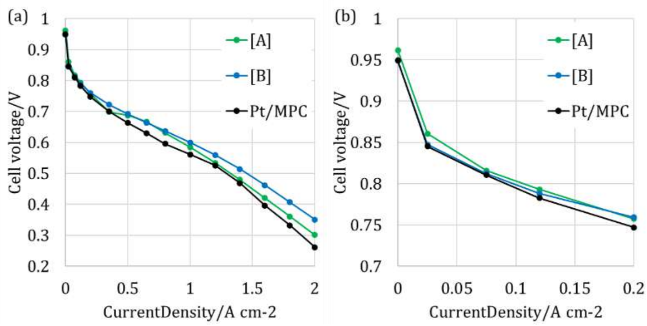


Fig.1. Polarization curves of MEAs.
(a) Overall, (b) Low current density region.

References

(1) Prithi, J.A.; Rajalakshmi, N.; Ranga Rao, G. *Int. J. Hydrog. Energy.* **2018**, 43, 4716-4725

(2) Ott, S.; Orfanidi, A.; Schmies, H.; Anke, B.; Nong, HN.; Hübner, J.; Gernert, U.; Gliech, M.; Lerch, M.; Strasser, P. *Nat. Mater.* **2020**, 19, 77–85

Enhanced supercapacitor performance by the synergistic integration of PANI nanofibers with MXene sheets for high-efficiency electrode development

Nidhi[1], Manoj Kumar Singh[1,2*]

[1]Department of Physics and Astrophysics, Central University of Haryana, Mahendragarh-123031, India

[2]Department of Applied science and Humanities, School of Engineering and Technology (SOET), Central University of Haryana, Mahendragarh-123031, India

*Corresponding authors: *manojksingh@cuh.ac.in*

Abstract

The development of advanced composite materials is essential for enhancing the performance of supercapacitor electrodes in next-generation energy storage devices. In this study, the electrochemical behavior of two-dimensional $Ti_3C_2T_x$ MXene sheets was investigated by integrating them with polyaniline (PANI) nanofibers through a polymerization technique. Electrochemical measurements were carried out using graphite sheets as current collectors. The $Ti_3C_2T_x$/PANI nanocomposite exhibited an impressive specific capacitance of 854 F/g at a current density of 1 A/g in 1 M H_2SO_4 electrolyte. Furthermore, the composite retained 88% of its initial capacitance after 2000 charge–discharge cycles at a high current density of 5 A/g, indicating excellent cyclic stability. Electrochemical impedance spectroscopy (EIS) revealed an ionic conductivity of 48.6 μS/cm and a diffusion coefficient of 196.1×10^{-12} cm^2/s for the $Ti_3C_2T_x$/PANI composite. These results highlight the potential of $Ti_3C_2T_x$/PANI as a promising electrode material for high-performance supercapacitor applications.

Keywords: $Ti_3C_2T_x$/PANI synthesis; mild etching; in situ-polymerization; nanofibers and supercapacitor applications

ACEPS-13, January 11-14, 2026, Bengaluru, India

Dipyridyl dibutyl pyridine (DPDBPy) based extended viologen and $CoMn_2O_4$/Poly 5-cyanoindole (P5CIn) as an Electrochromic Supercapacitor.

Manya Pal[1], Surendra Kumar Martha[2*]

[1] *Department of Chemistry, Indian Institute of Technology, Hyderabad, Kandi, Sangareddy, 502284, India.*

[2] *Department of Chemistry, Indian Institute of Technology, Hyderabad, Kandi, Sangareddy, 502284, India.*

* martha@chy.iith.ac.in

Abstract

Electrochromic supercapacitors (ESCs) merge energy storage with energy saving, offering versatility across applications. Here, we propose a A novel P5CIn/$CoMn_2O_4$//DPDBPy based Electrochromic Supercapacitor (ESC) featuring a 1,1′-dipyridyl dibutyl Pyridine viologen (DPDBPy) gel film and a P5CIn/$CoMn_2O_4$ composite film, containing a 1 M $LiClO_4$ in PC/PMMA gel electrolyte demonstrates impressive characteristics. The pyridine-based extended viologen used here shows electrochromic as well as storage property having a specific capacitance of ~ 11 mF cm^2in three-electrode set up. Featuring a remarkable optical contrast of around 68.5% at 510 nm, this device exhibits exceptional longevity with over 10000 cycles of operation while maintaining minimal transmission modulation loss. Crafted from cost-effective materials, it ensures consistent, reproducible, and reversible color transitions. From a clear pale yellow in its discharged state (0 V), it smoothly transforms into a pinkish-purple when fully charged (1.5 V), highlighting its broad voltage range and vivid contrast. It proves efficient for powering electronic devices by exhibiting a large specific capacitance of around 35.34 mF cm^{-2}, retaining 94 % after 10000 cycles. Additionally, its reasonably rapid switching kinetics (tc = 8 s and tb = 9 s), coupled with its impressive transmission contrast and prolonged operational lifespan across a 4 × 2 cm^2 active area, outperform numerous Electrochromic Supercapacitors (ESCs) documented in existing literature. This establishes the P5CIn/$CoMn_2O_4$//DPDBPy ESC as a premier option for dual-function switchable windows.

Keywords: Supercapacitor, electrochromic, energy storage, viologen.

References

(1) Zhao, X.; Li, Z.; Guo, Q.; Yang, X.; Nie, G. High Performance Organic-Inorganic Hybrid Material with Multi-Color Change and High Energy Storage Capacity for Intelligent Supercapacitor Application. *J. Alloys Compd.* 2021, *855*, 157480.

(2) Guo, Q.; Zhao, X.; Li, Z.; Wang, D.; Nie, G. A Novel Solid-State Electrochromic Supercapacitor with High Energy Storage Capacity and Cycle Stability Based on Poly(5-formylindole)/WO_3 Honeycombed Porous Nanocomposites. *Chem. Eng. J.* 2020, *384*, 123370.

Integration of IL-modified PSK and ATA MOF-based SC to fabricate a Monolithic photo-supercapacitor

Akshay Kumar Ray, Surendra Kumar Martha*

Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, 502284, Telangana, India

Martha@chy.iith.ac.in

Abstract

The integrated photo-supercapacitor (PSC) is a single device where the photovoltaic (PV) layer first converts solar radiation into electrical energy. This energy is immediately conveyed to the storage layers, which store it in the form of charge that can power any electronic device. The PSC is characterised by its ability to self-charge under incident light and self-store the photo-generated current. This removes the need for two separate devices for energy conversion and storage. Deploying a PSC reduces space requirements, cost, and weight [1-3]. In this work, we are trying to develop the Three-electrode monolithic photo-supercapacitor, which requires less space than the conventional photo-supercapacitor. Before integrating the monolithic photo-supercapacitor, an IL-modified HTL-free Perovskite solar cell was prepared with a cell efficiency of > 9 %. Also, we prepared a new material, Ni-ATA MOF, as the cathode material, which gives the capacitance of 820 F g^{-1}, and rGO from the graphite extracted from a spent lithium-ion battery, and it gives 143 F g^{-1} as an anode. An asymmetric supercapacitor was fabricated by sandwiching a KOH-soaked GF/D separator between the cathode and the anode. The asymmetric supercapacitor gives 107 F g^{-1} capacitance in the voltage window of 0-1.5 V. We have integrated the solar cell and asymmetric supercapacitor into a self-charging monolithic photo-supercapacitor.

Photosupercapcitor, Pervoskite, solar cell, supercapacitor, integrated devices.

References

(1) Flores-Diaz, N., De Rossi, F., Das, A., Deepa, M., Brunetti, F. and Freitag, M., 2023. Progress of photocapacitors. *Chemical Reviews*, *123*(15), pp.9327-9355.

(2). Xu, X., Li, S., Zhang, H., Shen, Y., Zakeeruddin, S.M., Graetzel, M., Cheng, Y.B. and Wang, M., 2015. A power pack based on organometallic perovskite solar cell and supercapacitor. *ACS nano*, *9*(2), pp.1782-1787.

(3) Rahman, M.M., 2024. A Comprehensive Review on Perovskite Solar Cells Integrated Photo-supercapacitors and Perovskites-Based Electrochemical Supercapacitors. *The Chemical Record*, *24*(1), p.e202300183.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Efficient $Pt_{3-x}Co_{0.5+\gamma}Ni_{0.5+\gamma}/C$ Electrocatalysts via Single-Step Solid-State Route for PEM Fuel Cell Cathodes

Prateekshita Mukherjee [1*], Akhila Kumar Sahu[1,2*],

[1] ***CSIR Madras Complex, CSIR - Central Electrochemical Research Institute - Madras Unit, Taramani, Chennai 600113, India***

[2] ***Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India***

* Corresponding email: **mprateekshita@gmail.com**

Abstract

The development of cathode catalysts with enhanced oxygen reduction reaction (ORR) activity and long-term durability is critical for advancing polymer electrolyte membrane fuel cells (PEMFCs). While Pt-based alloys are extensively explored, their practical deployment remains challenging due to stability and synthesis limitations. Chemically ordered Pt-alloys have recently gained attention owing to their favorable electronic and geometric structures, which significantly enhance ORR kinetics.

In this work, we report—for the first time—a one-step solid-state synthesis of $Pt_{3-x}Co_{0.5+\gamma}Ni_{0.5+\gamma}/C$ (x = 0, 1, 2; y = 0, 0.5, 1) nanoparticles supported on carbon. Among the series, $Pt_2Co_1Ni_1/C$ emerged as the most promising composition, demonstrating exceptional performance in both half-cell and full-cell configurations. Remarkably, this catalyst achieved a mass activity seven times higher than commercial Pt/C in acidic media, meeting the U.S. DOE 2025 targets. Furthermore, it retained substantial activity after 50,000 potential cycles, underscoring its electrochemical stability.

Under real PEMFC operating conditions, $Pt_2Co_1Ni_1/C$ delivered a peak power density surpassing that of commercial Pt/C, validating its potential for practical application. This study introduces a scalable, single-step route for fabricating high-performing, durable ORR catalysts, offering new perspectives for fuel cell technologies and clean energy research.

Keywords : Platinum ternary alloys, electrocatalyst, oxygen reduction reaction, fuel cell

References

(1) Mukherjee, P.; Patil, I.; Kakade, B.; Das, S.K.; Sahu, A.K.; Swami, A. Methodical designing of Pt3− xCo0. 5+ yNi0. 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. Catalysis Today. 2023, 423, 113963.

Unveiling Charge Dynamics in High-Performance Binder-Free Photo-Rechargeable Supercapacitors

Aadil Rashid Lone [1,2], Sahil Jangra [3], Aditya Sadhanala [4], Kavita Pandey[1,2,*]

[1]Centre for Nano and Soft Matter Sciences, Bangalore (CeNS), 562162, India

[2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India

[3]Department of Applied Science, School of Advanced Engineering, UPES, Dehradun, 248007, India

[4]Centre for Nano Science and Engineering (CeNSE), IISc, Bengaluru, Karnataka, 560012, India

*Corresponding author: kavitapandey@cens.res.in

Abstract

With the growing demand for energy storage from renewable energy sources, photo-rechargeable supercapacitors offer a viable alternative for directly converting and storing solar energy. This will take over the traditional energy solution, which uses a solar cell to convert solar energy and store it in rechargeable batteries. A binder-free nickel-cobalt nanowire arrays with a cubic spinel structure were directly grown on nickel foam via an in-situ hydrothermal process. The resulting one-dimensional nanowires exhibited a uniform morphology and a favourable bandgap of approximately 1.67 eV, making them ideal candidates as electrode materials for photo-assisted supercapacitors. Electronic structure analysis revealed the coexistence of Ni^{2+}/Ni^{3+} and Co^{2+}/Co^{3+} redox pairs, significantly enhancing electrochemical kinetics and facilitating efficient photo-assisted charge storage. Under illumination, we demonstrated a remarkable 54% increase in areal capacitance, attributed to the efficient separation and storage of photo-generated charges driven by surface polarization effects. Density Functional Theory (DFT+U) calculations further confirmed that nickel substitution in the Cobalt matrix significantly reduces the bandgap and enhances magnetic moment, supported by asymmetric spin-resolved density of states and band structure analyses. This research provides valuable insights for developing next-generation photo-assisted energy storage solutions.

Keywords: Photo-rechargeable, Supercapacitors, Cyclic stability, Solar energy,

ACEPS-13, January 11-14, 2026, Bengaluru, India

Hierarchically porous N-doped activated carbon derived from biomass for high voltage EDLC applications

Ajeesh KS[1,3*], Narasimman R[4], Sajitha TS[1], Bibin John[1], Vijayalakshmi KP[2]

[1]*Energy Systems Development Division (ESDD), Vikram Sarabhai Space Centre (VSSC/ISRO), Thiruvananthapuram, Kerala, India*

[2]*Analytical and Spectroscopy Division (ASD), Vikram Sarabhai Space Centre (VSSC/ISRO), Thiruvananthapuram, Kerala, India*

[3]*Faculty of Science, Cochin University of Science and Technology (CUSAT), Cochin, Kerala, India*

[4]*Department of Chemistry, Faculty of Natural Sciences, M S Ramaiah University of Applied Sciences, Bengaluru, India*

* ajeeshks.nk@gmail.com / ks_ajeesh@vssc.gov.in

Abstract

Increased demand for high-capacity and eco-friendly energy storage devices has stimulated intensive research in green electrode materials for electrochemical double-layer capacitors (EDLCs)[1]. In this study, we report the synthesis of a hierarchically porous, N-doped activated carbon derived from a nitrogen rich biomass precursor (cannon ball fruit) via carbonization and chemical activation. Structural and morphological characterization using XRD, SEM-EDS, BET, CHN analysis and Raman spectroscopy, confirmed the formation of a highly porous micro / mesostructure. The activated carbon exhibited N content of 1.4 % and a surface area of 1483 m^2g^{-1}. Electrochemical performance was evaluated in a symmetric two-electrode pouch cell configuration (1.0 F-3.0 V) using high voltage non-aqueous electrolyte ($SBPBF_4$ in acetonitrile). The material exhibited superior double layer capacitive behaviour with a specific capacitance of 75 F/g at 1 A/g with excellent cycling stability (> 95% retention over 10000 cycles). The hierarchical porous structure combined with N doping contributed to efficient ion transport and increased specific capacitance. This sustainable synthesis route eliminate the need for external dopants and offers a scalable and environmentally friendly approach towards advanced electrode materials for next generation supercapacitors.

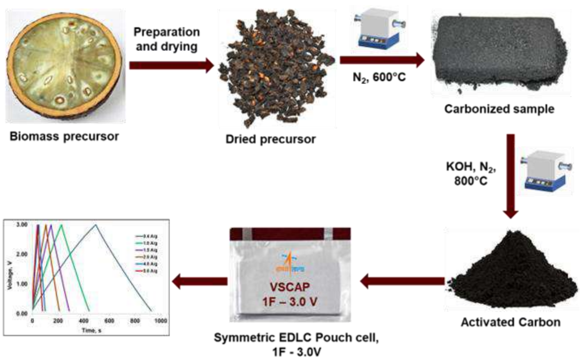


Figure 1: Schematic representation of synthesis of cannon ball fruit derived AC

Keywords: Activated carbon, Biomass, EDLC, High-voltage electrolyte

References

(1) Venkatesan, Natesan.; Kesavan, Thangaian.; Raja, Murugan.; Ramanujam, Kothandaraman.; Fathima, Nishter Nishad. Efficient electrochemical performance of nitrogen-doped porous activated carbon for high energy symmetric pouch cell supercapacitors. *Journal of Energy Storage.* **2022**, 55, No. 105698.

Liquid Crystal MXene Stabilized Cationic Naphthalene Diimide Charge Host for Ammonium ion Storage

Narendra Kurra[1]*, Kotagiri Venkata Rao[1]*, Rituprava Dash[1], Shubham Bhoi[1], Soujanya H. Goudar[1]

Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana State, 502284, India

Email id: narendra@chy.iith.ac.in, kvrao@chy.iith.ac.in

Abstract

The current trend of past pace development of aqueous energy storage devices which utilize non-metallic ammonium ions (NH_4^+) as charge carriers, owing to their sustainability, suitability for grid scale energy storage[1]. Unlike traditional metallic charge carriers such as Li^+, Na^+, Zn^{2+} and Mg^{2+} ions; NH_4^+ ions exhibit fast diffusivity due to small ionic size and light molar mass. The selection of appropriate electrode materials possess significant challenges. Functional organic materials are gaining interest as efficient candidates for processing of electrodes due to sustainability, low-cost and environmental friendliness. However, dissolution of the organic materials in aqueous medium is a major obstacle which leads to capacity fading of the device. In this work, we have demonstrated the incorporation of $Ti_3C_2T_x$ MXene sediment into the cationic naphthalene diimide (*c*NDI) organic imide group to form a hybrid structure known as *c*NDI@LC-$Ti_3C_2T_x$. Non-covalent H-bonding interactions are the key driving force for these organic-inorganic hetero structures which has been investigated using FTIR and UV-visible study[2]. *c*NDI@LC-$Ti_3C_2T_x$ hybrid electrode showed pseudocapacitive behavior in aqueous NH_4^+ ion electrolyte. Due to the hydrophilicity nature and high electronic conductivity of MXene, this MXene-organic hybrid electrode improves the specific capacitance and rate performance for non-metallic ammonium ion storage devices.

Keywords: Cationic naphthalene diimides, Liquid crystal MXenes, Pseudocapacitance, Ammonium ion electrolytes, Polarized microscopy.

References

(1) Bao, Z.; Lu, C.; Liu, Q.; Ye, F.; Li, W.; Zhou, Y.; Pan, L.; Duan, L.; Tang, H.; Wu, Y.; Hu, L.; Sun, Z. An Acetate Electrolyte for Enhanced Pseudocapacitve Capacity in Aqueous Ammonium Ion Batteries. *Nat. Commun.* **2024**, *15* (1), 1934.

(2) Bhoi, S.; Goudar, S. H.; Rao, K. V.; Kurra, N. Extrinsic Pseudocapacitance of $Ti_3C_2T_x$ MXenes in Divalent Metal-Ion Electrolytes after Assembly with Perylene Diimides. *Cell Reports Phys. Sci.* **2024**, *5* (10), 102229.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Ionic Liquid in NASICON: Impact on All-Solid-State Na^+ Supercapacitors

Hardeep *, **and Anshuman Dalvi**

[1]*Department of Physics, Birla Institute of Technology & Science, Pilani-333031*

*p20230082@pilani.bits-pilani.ac.in

Abstract

The present investigation delves into the ionic transport studies of EMIM-BF_4 ionic liquid reinforced into nano-crystallites of $Na_{3.45}Zr_2Si_2PO_{12.225}$ (NZSP) and reveals their possible application as a solid-state electrolyte, particularly in supercapacitors. NZSP has been prepared by a conventional solid-state reaction route, and Rietveld refinement confirms the formation of NZSP. Highest conductivity of ~10^{-3} $\Omega^{-1}cm^{-1}$ is achieved by the incorporation of ~12wt% EMIMBF_4 in NZSP. Increasing the content of ionic liquid tends to reduce the grain boundary resistance of NZSP crystallites. Further, all solid-state supercapacitors have been prepared in a sandwich geometry in hot roll lamination operated at 100 °C with activated carbon electrodes of surface area ~1800m^2-g^{-1}. Ionic liquid content in NZSP matrix tends to enhance the overall device performance. The supercapacitors are stable with CV and galvanostatic charge-discharge cycling, exhibiting a specific capacitance of ~ 225F-g^{-1} at an operating voltage of ~2V with ~1mA discharge current. The device has excellent cycle stability(~80% capacitance retention over 15,000 cycles) and high coulombic efficiency. These findings promise that the composite NZSP/EMIMBF_4 with AC electrodes has significant potential in the field of energy storage and can be scaled to solid-state energy storage technologies.

Keywords: Solid-State Supercapacitor, NASICON, Ionic liquid.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Interface-Engineered Telluride@MXene Heterostructures for High-Performance Binder-Free Solid-State Hybrid Supercapacitors

Antra Choubey[1,*], Ashish Yadav[1]

[1] *Indian Institute of Technology Roorkee, India*

* ashish@ch.iitr.ac.in

Abstract

The implementation of a stratified architecture in electrode design offers a promising approach to enhance the energy density of supercapacitors without compromising their power density. Additionally, interface engineering within heterostructured electrodes serves as a highly efficient method for modulating their physical and chemical properties, thereby boosting their charge storage capability. This study presents the synthesis of a $Ti_3C_2T_x$ MXene–nickel manganese telluride (NMTe) composite, achieved via acid etching followed by a simple one-step in situ hydrothermal method, wherein lychee-like NMTe structures are embedded within multilayered $Ti_3C_2T_x$ sheets. Notably, the binder-free NMTe@$Ti_3C_2T_x$ electrode outperforms its individual components—NMTe and $Ti_3C_2T_x$—owing to the synergistic interaction between the two materials and a unique structural design that enhances electrode–electrolyte interfacial dynamics. The composite structure successfully suppressed the restacking of $Ti_3C_2T_x$ layers and the aggregation of NMTe particles. As a result, the NMTe@$Ti_3C_2T_x$ battery-type electrode exhibited a remarkable specific capacitance of 2139.1 F g^{-1} at 1 A g^{-1} and excellent cycling stability, retaining 96.5% of its performance over 10,000 cycles with only minor changes in surface morphology. Mechanistic insights revealed a deeper understanding of interfacial charge transport modulation and the reorganization of electronic states during the charge storage process. Mechanistic insights revealed a deeper understanding of interfacial charge transport modulation and the reorganization of electronic states during the charge storage process. To assess device-level performance, symmetric and asymmetric supercapacitors were assembled using binder-free NMTe@$Ti_3C_2T_x$ electrodes. The asymmetric device, in particular, exhibited an expanded voltage window of 1.6 V and achieved a high energy density of 114.2 Wh kg^{-1} at a power density of 756.8 W kg^{-1}. These outcomes underscore the potential of telluride/MXene-based architectures for advanced energy storage applications.

Keywords: MXene, transition metal telluride, supercapacitor, energy density, power density

ACEPS-13, January 11-14, 2026, Bengaluru, India

High-Temperature PEM Fuel Cell Membranes Reinforced with MOFs for Sustainable Hydrogen Energy.

Akshay Sharma[1,*], Amit C Bhosale[1], Bhaskar Jyoti Deka[2,3]

[1] Green Hydrogen Lab, Department of Hydro and Renewable Energy, Indian Institute of Technology Roorkee, Haridwar, Uttarakhand, India 247667

[2] Advanced Membrane Research Lab, Department of Hydrology, Indian Institute of Technology Roorkee, Haridwar, Uttarakhand 247667, India

[3] Centre for Nanotechnology, Indian Institute of Technology Roorkee, Haridwar, Uttarakhand 247667, India

* bhaskar.deka@hy.iitr.ac.in

Abstract

The increasing global demand for clean and sustainable energy has intensified interest in Proton Exchange Membrane Fuel Cells (PEMFCs), which generate electricity with water as the only byproduct. High-Temperature PEMFCs (HT-PEMFCs), operating in the range of 100–200 °C, offer several advantages over conventional low-temperature PEMFCs, including reduced catalyst poisoning and elimination of cathode flooding [1]. However, the commercialization of HT-PEMFCs is hindered by the lack of proton exchange membranes (PEMs) that are thermally stable, cost-effective, and exhibit high proton conductivity under anhydrous conditions. To address this challenge, nanocomposite membranes incorporating metal–organic framework (MOF)-based nanofillers have been investigated to improve the mechanical and proton-conducting properties of phosphoric acid (PA)-doped membranes. MOFs are crystalline porous materials consisting of metal ions coordinated to organic ligands, known for their high surface area and excellent chemical and thermal stability [2].

In this study, we fabricated a dense, defect-free nanocomposite membrane by incorporating zirconium-based MOF UiO-66 into a polyvinylpyrrolidone–polyether sulfone (PES–PVP) polymer matrix to form a UiO-66/PES–PVP composite membrane. The UiO-66 nanofillers were homogeneously distributed within the membrane, significantly enhancing its mechanical properties. Various UiO-66 loadings (1–5 wt%) were explored to determine the optimal concentration, with strong UiO-66–PA interactions confirmed via Fourier Transform Infrared (FTIR) spectroscopy. Thermogravimetric Analysis (TGA) indicated high thermal stability, showing negligible weight loss up to 200 °C. The composite membrane exhibited improved PA uptake, reaching up to 2.14 mol of PA per monomer unit of PVP. The optimal composition (3 wt% UiO-66) demonstrated a low ohmic resistance and achieved a proton conductivity of 50 mS/cm under anhydrous conditions. Furthermore, the PES–PVP–3 wt% UiO-66 membrane exhibited superior chemical stability, as validated by Fenton's test, and demonstrated higher power density compared to the pristine PES–PVP membrane. These findings confirm that the UiO-66/PES–PVP nanocomposite membrane is a promising candidate for high-performance and durable HT-PEMFC applications.

Keywords: Proton Exchange membrane, Fuel cell, metal-organic framework, Proton conductivity, Hydrogen Energy.

References

(1) Wang, A.-L.; Ji, W.-X.; Li, J.; Wu, J.-N.; Zhang, L.-G.; Zhang, T.-Y. The Research Progress of Phosphoric Acid Doped Polybenizimidazole Based High-Temperature Proton Exchange Membrane. *Polym. Bull 37*(2), 137–149. https://doi.org/10.14028/j.cnki.1003-3726.2024.23.165.

(2) Tran, M. H.; Jheng, L. C.; Zhao, Z. L.; Ko, W. C.; Ho, K. S.; Liao, T. C. Polybenzimidazole Nanocomposite Membranes Containing Imidazole-Functionalized UiO-66 Nanocrystals with Optimal Interfacial Compatibility for High-Temperature Proton Exchange Membrane Fuel Cells. *Int J Hydrogen Energy* 2024, *77*, 1375–1386. https://doi.org/10.1016/j.ijhydene.2024.06.252.

"Hybrid Polymer Composites infused with Li^+ ion Garnet for all Solid-State Supercapacitors"

Kamaldeep Bisht[1], Anshuman Dalvi[1*]

[1]Department of Physics, Birla Institute of Technology & Science, Pilani, Rajasthan, India (333031)

[1*]Email - adalvi@pilani.bits-pilani.ac.in

Abstract

This work focuses on the fabrication of hybrid polymer composites incorporating lithium garnets. It has been found that the ionic conductivity of pristine Polyethylene oxide (PEO) is very low, in the range of 10^{-7} to 10^{-8} $\Omega^{-1}cm^{-1}$. Several measures are considered to enhance the thin polymer electrolyte's overall ionic conductivity and ion transport, including suitable ionic salt and specific additives. The additive used in this study is Lithium garnet incorporated with Niobium, specifically $Li_{6.75}La_3Zr_{1.75}Nb_{0.25}O_{12}$ (LLZNO), prepared via the sol-gel method. The LLZNO fused with polymer has a reported ionic conductivity range of 10^{-3} to 10^{-4} $\Omega^{-1}cm^{-1}$ at room temperature. The hybrid polymer composite is synthesized by optimizing the salt concentration and varying the ratios of garnet to polymer in polymer-in-ceramic and ceramic-in-polymer configurations. This optimization is expected to enhance the ionic conductivity by promoting the formation of more prominent grains and reducing grain boundary resistance. However, it is also observed that the ionic conductivity decreases beyond a specific concentration of garnet and polymer, which is due to the crowding of ions that results in the ion path blocking.

Keywords – LLZNO, Hybrid Supercapacitor, Garnet

References

1. Swathi Pandurangan, Karthik Kaliyappan, Arun Prasath Ramaswamy, Murugan Ramaswamy, Polymer-garnet composite electrolyte based on comb-like structured polymer for lithium-metal batteries, Materials Today Energy, 2021, 21, 100836.
2. Chen, Yue & Luo, Jing & Guo, Xiangxin & Sun, Xueliang.. Rational Design of Hierarchical "Ceramic-in-Polymer" and "Polymer-in-Ceramic" Electrolytes for Dendrite-Free Solid-State Batteries, Advanced Energy Materials, 2019, 9(17).
3. Yuta Shimonishi, Akiharu Toda, Tao Zhang, Atsushi Hirano, Nobuyuki Imanishi, Osamu Yamamoto, Yasuo Takeda, Synthesis of garnet-type Li7−xLa3Zr2O12−1/2x and its stability in aqueous solutions, Solid State Ionics, 2011, 183(1), 48-53.
4. Long Chen, Yutao Li, Shuai-Peng Li, Li-Zhen Fan, Ce-Wen Nan, John B. Goodenough, PEO/garnet composite electrolytes for solid-state lithium batteries: From "ceramic-in-polymer" to "polymer-in-ceramic", Nano Energy, 2018, 46, 176-184.
5. Tianhang Zhang, Yangai Liu, Timothy Daniel Christopher, Saifang Huang, Tilo Söhnel, Xin Song, Wei Gao, Peng Cao, The effect of water vapor on structure and electrochemical performance of an aluminum-free niobium-doped garnet electrolyte, Ceramics International, 2020, 46(3), 3889-3895.

ACEPS-13, January 11-14, 2026, Bengaluru, India

CVD-Grown MoO_3 flakes anchored on Stainless Steel Mesh for High-Performance Structural Supercapacitors

Neeraj Yadav[1], Nitika Arya[1], Yadu Chandran[1] Bhumit Luhar[2], Viswanath Balakrishnan[1,*]

[1] Nanoscale Materials and Devices Laboratory, School of Mechanical & Materials Engineering, Indian Institute of Technology Mandi, Mandi, Himachal Pradesh-175005, INDIA

[2] School of Physical Sciences, Indian Institute of Technology Mandi, Mandi, Himachal Pradesh-175005, INDIA

* viswa@iitmandi.ac.in

Abstract

The development of multifunctional materials that merge mechanical strength with energy storage capabilities is essential for progressing lightweight and integrated technologies in aerospace, automotive, and wearable systems. This study introduces an innovative method for the fabrication of structural supercapacitor electrodes through the growth of molybdenum trioxide (MoO_3) nanostructures on stainless steel (SS) mesh using chemical vapor deposition (CVD), followed by O_2 and Ar plasma treatment to improve their properties. The application of plasma markedly boosts surface activation, enhances film adhesion, and facilitates surface modification. The morphological and structural characterizations conducted through SEM, XRD, and Raman spectroscopy validate the formation of uniform, vertically aligned MoO_3 with optimized oxidation states. Electrochemical testing demonstrates improved areal capacitance, outstanding rate performance, and remarkable cycling stability. Furthermore, mechanical testing under bending shows that the electrode preserves its structural integrity and electrochemical functionality, confirming its potential application in structural energy storage. Fabrication of supercapacitor devices in serial and parallel architectures is also demonstrated for the various portable device applications. This approach provides an effective method for producing high-performance structural supercapacitors, showcasing a promising avenue for multifunctional material systems in future engineering applications.

Keywords: Molybdenum trioxide, Chemical vapour deposition, plasma treatment, Structural Supercapacitors.

References

(1) Kundu, M.; Mondal, D.; Mondal, I.; Baral, A.; Halder, P.; Biswas, S.; Paul, B. K.; Bose, N.; Basu, R.; Das, S. A Rational Preparation Strategy of Phase Tuned MoO3 Nanostructures for High-Performance All-Solid Asymmetric Supercapacitor. *Journal of Energy Chemistry* 2023, *87*, 192–206. https://doi.org/10.1016/j.jechem.2023.08.014.

Temperature-Dependent Performance of Ink-Processed VO_2 Supercapacitors

Rohini Kakunuri[1,*], Neeraj Yadav[1], Viswanath Balakrishnan[*]

[1] *Nanoscale Materials and Devices Lab., School of Mechanical and Materials Engineering, Indian Institute of Technology, Mandi, Himachal Pradesh,17505, India*

* viswa@iitmandi.ac.in

Abstract

Metal-insulator transition near 68 °C in Vanadium dioxide (VO_2), provides a unique platform for thermally adjustable energy storage devices. VO_2 nanostructures, synthesized using hydrothermal methods are used to prepare stable ink for direct application on nickel foam, carbon fiber paper, and stainless steel mesh. The ink-based method allows for the development of cost-effective, VO_2 coating on on rigid and flexible substrates.Using each substrate design, two-electrode symmetric supercapacitor cells were built and tested for electrochemical performance using CV, GCD, and EIS. Measurements were taken at ambient temperature and above the VO_2 phase transition temperature to examine how the metal–insulator transition affects capacitive performance. Specific capacitance, charge transfer resistance, and rate capability varied across the temperature range, with improved performance at the phase transition due to increased electrical conductivity and ion mobility.

This study shows that ink-processed VO_2 can be used for temperature-responsive supercapacitors and underlines the influence of substrate architecture on device performance. This can inform the design of future thermally adaptive energy storage devices for various applications.

Keywords: VO_2, MIT, Supercapacitor, Ink, rigid & flexible substrates

References

(1) Alhebshi, N. A.; Vaseem, M.; Minyawi, B. A.; AlAmri, A. M.; Shamim, A. Single and Double Layer of Monoclinic VO2 Ink-Based Printed and Interdigitated Supercapacitors. Energy Technol. 2022, 10, 2200432.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Sb-Ta-codoped SnO_2 with High Durability for Catalysts of Proton-Exchange-Membrane Fuel Cells

Haruto Futatsuya[1], Takeshi Fukuda[1], Kassim Jose Mendoza Pena[1], Seigo Ito[1,*]

[1] *Department of Materials and Synchrotron Radiation Engineering, Graduate School of Engineering, University of Hyogo, 2167 Shosha, Himeji, Hyogo 671-2280, Japan*

* ito@eng.u-hyogo.ac.jp

Abstract

Proton-exchange-membrane fuel cells (PEMFCs) are expected to be widely used as clean energy devices that do not emit greenhouse gases. Improving the durability of catalysts is essential for the large-scale adoption of these devices. The research using metal oxides is actively being conducted to improve durability. However, their low conductivity results in low catalytic activity. To address this, the SnO_2 has been doped with Sb or Ta.[1,2] To realize the catalyst which has the high activity and durability, we synthesized the Sb-Ta co-doping SnO_2 as the Pt catalyst support. We prepared the Pt/Sb-Ta-SnO_2, and evaluated the catalyst activity and durability.

SnO_2 and Sb-SnO_2 were prepared by ozone-assisted hydrothermal method as previously reported.[3] Furthermore, Sb-Ta-codoped SnO_2 samples were obtained by applying a second co-doping process to Sb-doped SnO_2. This second co-doping was carried out using two methods: one at room temperature (Sb-Ta-SnO_2_RT) and another under hydrothermal conditions (Sb-Ta-SnO_2_HT).

Platinum was supported on SnO_2 as a catalyst, and electrochemical measurements and durability tests were conducted using a half cell. Compared to conventional catalysts (Pt/C), the degradation ratio relative to the maximum value of electrochemical surface area (ECSA) was mitigated(Fig 1), and the mass activity retention rate after durability testing was more than four times higher. This is thought to be due to the interaction between Pt and Ta.

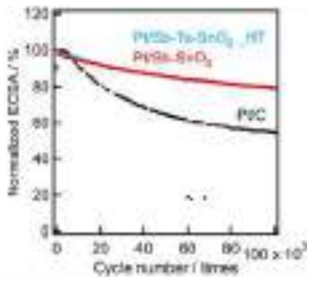


Figure 1. Transition during durability testing of ESCA retention rate of Pt/C, Pt/Sb-SnO_2, Pt/Sb-Ta-SnO_2_HT

Keywords : PEMFCs, co-doped SnO_2, ozone-hydrothermal method, carbon-free catalysts

References

(1) M. Inaba; *et al.*, *Applied Materials & Interfaces* **2024,** 16 (8), 10295-10306.

(2) Y. Senoo; *et al.*, *Electrochem. Commun.* **2015,** 51, 37-40.

(3) T. Fukuda; *et al., Crystals.* **2024**, *14*, 462.

ACEPS-13, January 11-14, 2026, Bengaluru, India

Development of MOF-303/SPEEK Mixed Matrix Membrane for Anhydrous Proton Exchange Membrane Fuel Cells

Rahul Patel[1], Yogesh Sharma[2,3,*]

[1] *Centre for Nanotechnology, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

[2] *Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

[3] *Centre for Sustainable Energy, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

* Corresponding author's email address: yogesh.sharma@ph.iitr.ac.in

Abstract

In this work, we report the synthesis and application of MOF-303, an aluminium-based metal-organic framework constructed from Al^{3+} and 1H-pyrazole-3,5-dicarboxylic acid (H_2PZDC), for the development of a composite proton exchange membrane. The successful formation of MOF-303 was confirmed by X-ray diffraction (XRD), showing high phase purity and crystallinity consistent with reported structures. MOF-303 exhibits outstanding water adsorption capacity, with a steep uptake at low relative humidity and strong water retention due to its polar pyrazole-NH functionalities and open pore structure[1]. These properties make it highly suitable for enhancing water management in proton-conducting systems. We incorporated MOF-303 into sulfonated poly(ether ether ketone) (SPEEK) to fabricate a mixed matrix membrane (MMM) aimed at anhydrous or low-humidity operation in proton exchange membrane fuel cells (PEMFCs). The target is to provide additional hydrogen bonding sites and promote stable proton conduction under dry conditions by retaining water within the pores of MOF-303. The composite membrane is expected to exhibit enhanced conductivity, mechanical stability, and operational resilience at elevated temperatures without external humidification. The MMM properties and its PEMFC performance will be shown at the conference.

Keywords (max 5): MOF-303, SPEEK, mixed-matrix membrane, proton conduction, PEMFC

References

(1) Hanikel, N.; Pei, X.; Chheda, S.; Lyu, H.; Jeong, W.; Sauer, J.; Gagliardi, L.; Yaghi, O. M. Evolution of Water Structures in Metal-Organic Frameworks for Improved Atmospheric Water Harvesting. *Science* **2021**, *374* (6566), 454–459. https://doi.org/10.1126/science.abj0890.

Ceria-based Electrodes for High Temperature solid oxide fuel cell: Effects of CO_2 and O_2 concentration on ORR performance

Shivam[1], Chinmoy Ranjan[1,*]

[1] *Department of Inorganic and Physical Chemistry, Division of Chemical Sciences, Indian Institute of Science, Bengaluru 560012, Karnataka, India*

*E-Mail: ranjan@iisc.ac.in

Abstract

In solid oxide fuel cells (SOFCs), the oxygen reduction reaction (ORR) is a crucial electrochemical process and is often the rate-limiting step affecting overall fuel cell performance. Therefore, enhancing ORR activity is critical for the efficient operation of intermediate temperature solid oxide cells (SOCs). In this work, we have selected ceria as the ORR catalyst over other well-known options due to its favorable chemical and mechanical stability, as well as its operability at intermediate temperatures[1]. Ceria was synthesized using the glycine nitrate combustion method. The formation of a pure phase was confirmed by powder X-ray diffraction (PXRD), and characteristic peaks were identified in the Raman spectrum of the synthesized material. Ceria ink was prepared using optimized concentrations of additional components. The cell was operated at 800 °C and tested under varying concentrations of O_2 and CO_2. Performance was evaluated using electroanalytical techniques, online mass spectrometry, and operando Raman spectroscopy.

An increase in O_2 concentration led to improved electrode performance. Similarly, applying a higher bias enhanced the electrode's electronic conductivity and reaction kinetics. Mass spectrometry results showed consistent and reproducible cell behavior. Operando Raman spectroscopy, conducted under different gas concentrations and applied biases, revealed no significant changes in the Raman spectra—indicating that CeO_x remains stable even under higher bias and in the presence of O_2 and CO_2. These results demonstrate that ceria exhibits promising behavior as an ORR catalyst in SOC applications.

Keywords: Solid oxide cells (SOCs), Oxygen reduction reaction (ORR), ECO_2RR, Ceria Catalyst, Operando Raman Spectroscopy

References

(1) J.A. Kilner, M. Burriel, 2014, Annual Review of Materials Research, 44, 365–393.

Sustainable Recovery of Cobalt as Co_3O_4 from Spent LIBs for High-Performance Supercapacitor Applications

Yash Srivastava[1,*], Prasenjit Mondal[1]

[1] *Department of Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee*

[2] [1]*Department of Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee*

* *prasenjit.mondal@ch.iitr.ac.in

Abstract

The rapid expansion of lithium-ion battery (LIB) usage has led to significant amount of spent batteries, posing both environmental challenges and opportunities for resource recovery. In this study, cobalt was selectively recovered from the leaching residue of waste LIBs and converted into cobalt oxide (Co_3O_4) via a controlled thermal decomposition process followed by co-precipitation. The synthesized Co_3O_4 was systematically characterized using XRD, SEM, and BET to confirm its phase purity, morphology, and surface area. The recovered Co_3O_4 was subsequently employed as an active electrode material for supercapacitor applications. Electrochemical performance was evaluated through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The material exhibited promising pseudocapacitive behavior with a high specific capacitance and excellent cycling stability, demonstrating its potential as a sustainable electrode material. This work not only promotes the circular economy by recovering valuable metals from e-waste but also advances the development of eco-friendly energy storage devices.[1,2]

Waste lithium-ion batteries, Cobalt oxide, Supercapacitor, Co-precipitation

References

(1) Yasa, S.; Birol, B.; Donmez, K. B.; Gencten, M. Recovery of Cobalt Based Materials from Spent Li-Ion Batteries and Their Use as Electrode Material for Supercapacitor. *J Energy Storage* **2024**, *81*. https://doi.org/10.1016/j.est.2023.110291.

(2) Yang, S.; Yang, G.; Zou, J.; Liu, W.; Lei, A.; Lan, M.; Zhang, X.; Liu, K.; Li, Q.; Lai, F. Selective Recovery of Metals from Spent Batteries by Carbonthermic Reduction Simultaneously Catalyzing High-Performance Carbon Anode. *Sep Purif Technol* **2025**, *352*. https://doi.org/10.1016/j.seppur.2024.128161.

Synthesis and Characterization of Carbonized Polymer-MoS_2/SnS_2 based Composite Material for Asymmetric Supercapacitors

Fatma Parween*, Ganesh Chandra Nayak

Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, Jharkhand, India-826004

*Corresponding author, Email: 23dr0057@iitism.ac.in

Abstract

Supercapacitors (SCs) are known for their application in areas that need fast, stable, and high energy throughput serving as a bridge between batteries and conventional capacitors. The capacitive property of a SC is influenced by parameters such as assembling technology, selection of electrolyte, potential window, and most importantly, electrode materials. This study reports the synthesis of carbonised polyaniline (C@PANI) using mesoporous silica (MCM) as the removable scaffold to develop a porous conducting structure. Composites using the carbonised polyaniline with transition metal dichalcogenides (TMDC), named C@PANI/MoS_2 and C@PANI/SnS_2, were subsequently fabricated to enhance the pseudocapacitance. Spectroscopic (PXRD, FT-IR, Raman) and microscopic (FE-SEM, HRTEM) characterisations were employed to verify the porous polyaniline structure along with formation of nanosheets of MoS_2 and SnS_2. Subsequently, the application of synthesized materials was assessed by fabricating asymmetric supercapacitor (ASC) devices with synthesized material as anode, MnO_2 as cathode, and 1 M $TEABF_4$ in acetonitrile as the electrolyte. Electrochemical analysis revealed that the synergic effect of TMDC integration led to enhanced electrochemical performance of the final composites compared to porous carbonized polyaniline.

Keywords: Asymmetric supercapacitor; polyaniline; pseudocapacitance; energy storage.

References

(1) Wang, Y.; Song, Y.; Zhao, X.; Sun, Y. MoS2/polyaniline/functionalized carbon cloth electrode materials for excellent supercapacitor performance. *RSC Adv.* 2021, *11*, 10941–10950. **https://doi.org/10.1039/D0RA09126J**