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

Towards a Mechanistic Understanding of Dendrite Growth in Solid State Batteries

Naga Phani Babu Aetukuri[1,*]

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

* phani@iisc.ac.in

Abstract

In this talk, we will discuss our work on Solid State Li-ion batteries with garnet-based electrolytes. First, we will discuss the broad mechanisms that underpin lithium filamentary growth in solid-state Li-ion batteries followed by some of our early work on refractory metal interlayers. We will then discuss the role of impurities in solid state electrolytes in dictating critical densities for lithium filamentary growth; the impedance modeling approach for accurate determination of impurities and the correlation with critical current densities. Time permitting, we will touch upon expected charge transfer resistances at 'clean' solid-solid electrode/electrolyte interfaces and its implication for solid state batteries.

Keywords (max 5): Interlayers, solid electrolytes, garnets, charge transfer, DRT analysis

References

(1) Raj, V.; Venturi, V.; Kankanallu, V. R.; Kuiri, B.; Viswanathan, V.; Aetukuri, N. P. B. Direct Correlation between Void Formation and Lithium Dendrite Growth in Solid-State Electrolytes with Interlayers. *Nature Materials* ***2022*** *21*, 1050-1056

Invited Lecture-2

All-solid-state batteries using low-temperature-sintered $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$

Hirotoshi Yamada*

[1] *1-14, Bunkyo-machi, Nagasaki 8528521, Japan*

* h-yama@nagasaki-u.ac.jp

Abstract

All-solid-state batteries (ASSBs) are one of the next-generation batteries towards carbon neutral societies. While sulfide-based ASSBs are on the stage for their practical application, oxide-based ones are still under the feasibility studies, mainly because of their interfacial issues: interphases and/or contact areas that would limit the energy and the power of the ASSBs. These issues are more severe for the full-inorganic ASSBs without any organic electrolytes, although they would would extend the application fields of the next-generation batteries: high voltage batteries and batteries for severer environment (vacuum, high temperature, etc.). In this study, materials and processes of NASICON-type solid electrolytes are developed to prepare the electrochemically active interfaces between the solid electrolytes and the active materials.

For the NASICON-based ASSBs, a precursor of $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$ (LAGP) was prepared by a solution method using oxalic acid as a chelate, which was sintered and crystallized at 600°C. LAGP obtained by sintering the precursor at 600°C exhibited rather high total conductivity of 2×10^{-5} S/cm. The hot press fascilitated the ionic conductivity to 1×10^{-4} S/cm that is comparable with LAGP prepared by solid state sintering at 800°C or a higher temperature. A 3 V-class ASSBs without any organic components was fabricated with TiO_2 anode and $LiCoPO_4$ cathode, which exhibited an initial discharge capacity of 66 mAh/g (0.17 mAh/cm^2) at 25°C. The performance could be further improved by optimizing materials, processes, and architectures, some of which will be shown and discussed in the talk.

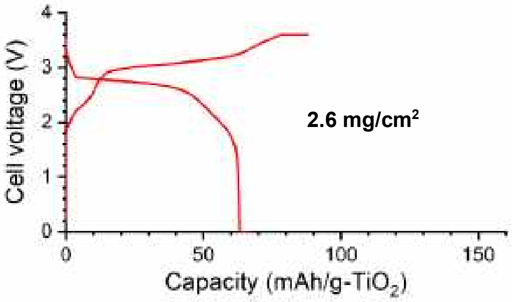


Figure 1. Charge/discharge curves of a full-inorganic ASSB in the TiO_2 | LAGP | $LiCoPO_4$ system. The battery was operated at 25°C, 0.01 C.

Keywords: Solid-state batteries, NASICON, LAGP

Suppressing surface and bulk degradation of single-crystal cathodes for lithium-ion batteries

Sooyeon Choi, Dong-hee Lee, Minkyung Kim,*

Department of Electronic Materials Engineering, Kwangwoon University, 60 Gwangun-ro 1-gil, Nowon-gu, Seoul, Republic of Korea 01897, Republic of Korea

* minkyungkim@kw.ac.kr

Abstract

Stable cathode materials for lithium-ion batteries are essential to meet increasing performance demands. Single-crystal cathodes have attracted significant attention, as they effectively enhance stability by eliminating intergranular cracks. However, single-crystal cathodes still suffer from degradation mechanisms distinct from those in polycrystalline counterparts, leading to limited cycle stability. Therefore, it is crucial to investigate the degradation behavior of single-crystal cathodes.

In this study, we examined the degradation of single-crystal cathodes with a focus on their surface and interfacial chemistry. The surface properties of single-crystal cathodes are critical not only for maintaining surface stability but also for preserving bulk structural integrity.

This presentation will discuss the impact of surface chemistry on the electrochemical performance of single-crystal Ni-rich layered oxide cathodes. Surface modifications with both amorphous and crystalline phases were employed, which revealed distinct phase transition behaviors while both approaches improved cycling stability. Furthermore, the formation of cathode–electrolyte interphase (CEI) layers significantly influenced degradation behavior. These findings provide insights into the importance of surface stabilization in achieving superior cycle life for single-crystal cathodes.

Keywords (max 5): Single-Crystal Cathodes, Surface chemistry, Cathode-electrolyte Interface, Single crystal degradation, Long-cycle performance

Suppressing Thermal Runaway of High-Energy Lithium-ion Battery Using Nonflammable Liquid Electrolyte

Yen Hai Thi Tran[1], Kihun An[1], Chilhoon Doh[2,*], Seung-Wan Song[1,*]

[1] *Department of Chemical Engineering & Applied Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea*

[2] *Next-Generation Battery Research Center, Korea Electrotechnology Research Institute, Changwon 51543, Republic of Korea*

* swsong@cnu.ac.kr

Abstract

Safety hazard issue is a weakness of state-of-the-art Li-ion batteries (LIB), and LIB-powered EV, aviation and ESS. Advancement of liquid electrolyte is urgently needed, aiming at the attainment of battery safety without the loss of energy density and cycle life. Replacement of highly flammable LIB electrolyte with a nonflammable liquid electrolyte is a critical step to reduce or prevent the risk of thermal runaway (TR) and fire events. The solid electrolyte interphase (SEI; interface) stabilization technology on graphite-based anode is a must for dendrite-free safe LIBs. I will present that well-designed nonflammable liquid electrolyte enables TR suppression and long-cycled high energy LIBs.(1)

Keywords (max 5): Battery safety, Thermal runaway, Nonflammable liquid electtrolyte, Solid electrolyte interphase

Reference

(1) Tran, Y. H. T.; An, K.; Lim, G.; Kim, D.; Lee, Y. J.; Doh, C.; Song, S.-W. Mater. Sci. & Eng. R-Reports **2025**, *164*, 100980.

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

Thermo-Electrochemical Activation of V_2O_5 to ZnV_3O_8 for Ultra-Stable Zinc-Ion Batteries

Rahuldeb Roy[1], Prince Sharma[2], Prashant Singh[2], Ashutosh K. Singh*[,1]

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

[2]*Ames National Laboratory, U.S. Department of Energy, Iowa State University, Ames, Iowa, 50011, USA*

*Corresponding author and e-mail addresses: Dr. Ashutosh K. Singh (aksingh@cens.res.in)

Abstract

Zinc-ion batteries (ZIBs) are promising energy storage systems due to their safety, cost-effectiveness, and abundant resources. However, their practical application is hindered by the lack of stable, high-performance cathode materials. Vanadium-based compounds offer potential due to their structural versatility and multivalent redox chemistry, yet they suffer from sluggish ion kinetics and poor electronic conductivity. Here, we present a novel thermo-electrochemical activation strategy that transforms V_2O_5 into defect-rich ZnV_3O_8, significantly enhancing electrochemical performance. The activated cathode delivers an exceptional specific capacity of 302 mAh/g at 0.1 A/g (up from 73 mAh/g) and demonstrates ultralong cycling stability over 4500 cycles at 2 A/g. Electrochemical analysis reveals accelerated Zn^{2+} diffusion, while first-principles calculations emphasize the stabilizing effect of hydrogen intercalation. The activation process triggers a thermodynamically favorable phase transition to ZnV_3O_8, enabling improved ion storage, lower activation energy, and enhanced structural integrity. Ex-situ studies provide insights into the material's evolution during cycling. This work highlights thermo-electrochemical activation as a simple yet effective method for optimizing vanadium oxide cathodes, paving the way for high-performance ZIBs with superior energy density and cycling durability..

Keywords: Rechargeable Zinc-Ion Batteries, Vanadium Cathodes, Thermo-Electrochemical Activation Engineering, DFT, Sustainable Energy Storage Technologies

References

(1) Roy, R.; Mahendra, G.; Singh, A. K. Photo-assisted self-chargeable aqueous Zn-Ion energy storage device, *Chemical Engineering Journal* **2024**, *500*, 156870.

(2) Roy, R.; Greeshma, R.; Basith, A.; Banerjee, R.; Singh, A. K. Self-rechargeable aqueous Zn^{2+}/K^{+} electrochromic energy storage device via scalable spray-coating integrated with Marangoni flow, *Energy Storage Materials* **2024**, *71*, 103680.

(3) Mahendra, G.; Roy, R.; Singh, A. K. $VO_2 \cdot xH_2O$ nanoribbons as high-capacity cathode material for aqueous zinc-ion batteries: Electrolyte selection and performance optimization, *Journal of Power Sources* **2024**, *64*, 235515.

Developing the Value-added Reaction-assisted Zn-air Battery *via* 2e⁻ Oxygen Reduction Reaction

Min-Hsin Yeh[1,2*]

[1] *Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan*

[2] *Sustainable Electrochemical Energy Development Center, National Taiwan University of Science and Technology, Taipei 10607 Taiwan*

* mhyeh@mail.ntust.edu.tw

Abstract

Zinc–air batteries (ZABs) are regarded as potential alternatives for storing energy cause by their considerable theoretical energy density, economical, and security. Nonetheless, their practical application remains restricted by a large charge–discharge potential gap and low round-trip efficiency, primarily due to the sluggish kinetics and high overpotentials of conventional four-electron oxygen reduction reactions ($4e^-$ ORR). To address these challenges, we successfully proposed the value-added reaction-assisted ZABs (VAR-ZABs) with hydrogen peroxide formation *via* the $2e^-$ pathway of ORR. The electrochemical two-electron oxygen reduction reaction ($2e^-$ ORR) offers a sustainable and energy-efficient alternative to the conventional anthraquinone process for H_2O_2 production. We proposed several kinds of functional quantum dots to boost the efficiency and selectivity. For example, we report the rational design of oxygen-rich CNQDs decorated on graphene frameworks (CNQDs/Gr), enabling the precise tailoring of active sites to promote the $2e^-$ ORR pathway. The rich C–O–C moieties within CNQDs effectively address the oxygen-deficient sites in Gr, serving as key active sites for selective $2e^-$ ORR for H_2O_2 generation. Furthermore, the interaction between the C atoms in Gr and neighboring N atoms in CNQDs facilitates π–π stacking, which stabilizes the *OOH intermediate and thereby promotes selective H_2O_2 formation. These synergistic effects result in the CNQDs/Gr with outstanding H_2O_2 selectivity of 96.5% at 0.6 V vs.. RHE in 0.1 M KOH. Furthermore, the CNQDs/Gr demonstrates outstanding performance in a VAR-ZAB, achieving an impressive capacity of 768.58 mAh g^{-1} with a high H_2O_2 production rate of 136 mmol g^{-1} h^{-1}.

Keywords: Zinc–air batteries, two-electron oxygen reduction reactions, H_2O_2, graphene quantum dots

References

(1) S. Aulia, L. Y. Chang, H. H. Su, M. Rinawati, P. C. Shi, M. H. Lin, W. H. Huang, H. Setyawan, B. J. Hwang, and **M. H. Yeh***, *"Core-Shell Architected Active Sites from Prussian Blue Analogue Enable Bifunctional Oxygen Electrocatalysis for High-Performance Rechargeable Zinc-Air Batteries," ACS Applied Energy Materials,* 2025, 8, 7283–7292.

Addressing Issues in Next Generation Electrochemical Energy Storage Devices

Aditi Halder1,*

[1]*School of Chemical Sciences, Indian Institute of Technology Mandi, Himachal Pradesh 175005.*

** Corresponding author's email address:aditi@iitmandi.ac.in*

Abstract

Successful integration of renewable energy into the mainstream energy utilization requires the development of efficient and cheaper energy storage devices. While, lithium-ion batteries are effective for the same, they face critical limitations such as restricted resource availability, environmental concerns, and safety risks. To address the growing energy demands, it is crucial to develop high-performance, eco-friendly beyond lithium energy storage systems, especially metal-air batteries. In this talk, we will discuss the strategic development of three major components of flexible zinc air battery(ZAB): cathode, anode and membrane. Our research groups have developed many transition metal oxides-based cathode materials for flexible ZAB with the properties of good bi-functionality as oxygen electrode. The major constraints that limit the performance of zinc air batteries are the sluggish kinetics of oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). Different strategies like doping, hetero-junction formation etc have been adopted to improve the performances of these reactions. We have also successfully developed few gel-electrolyte based membrane and evaluated their performance. Our experimental observations led to this conclusion that, the development of a flexible solid electrolyte focuses on achieving an optimal balance between high ionic conductivity and robust mechanical strength—both critical for practical and durable energy storage.

Keywords: metal-air battery, membrane, oxygen electrode, oxides, thiospinel

References

(1) Ravinder Sharma, Arkaj Singh, Aditi Halder; Synergistic effect of lattice strain, oxygen vacancy and morphology in Mo doped $NiCo_2O_4$ for high-performance zinc air batteries, J. of Energy Storage. 2025,107,114918

(2) Arkaj Singh, Ravinder Sharma, Aditi Halder; Flexible solid-state Zn–air battery based on polymer-oxygen-functionalized gC_3N_4 composite membrane.Nanoscale,2024, 16,8,4157-4169

(3) Ankita Mathur; Kumari, Sonu; Singh, Arkaj; Mitra, Rahul; Sharma, Ravinder; Biswas, Krishanu; Aditi Halder; Surface engineering of 2D layered MnO_2 with co-doping of Ni and Fe for rechargeable zinc-air battery, J. of Energy Storage. 2023, 74, 109350,

A rechargeable Zn-ion battery

Arindam Sarkar*[1],

[1] *Department of Chemical Engineeering, IIT Bombay, Mumbai 400076, India*

* a.sarkar@iitb.ac.in

Abstract

Rechargeable zinc-ion batteries (ZIBs) have emerged as a promising alternative for energy storage, primarily owing to the abundance, low cost, and environmental friendliness of zinc-based materials. However, several critical challenges must be overcome to realize their full potential. These include dendrite formation, which can lead to short circuits and compromise battery safety; thermodynamic limitations of aqueous electrolytes, which restrict the operational voltage window to approximately 1.23 V due to water decomposition; and the lack of an ideal host material capable of facilitating the reversible insertion and extraction of Zn^{2+} ions with high capacity and long cycle life.

The talk will highlight recent research efforts aimed at improving the performance of zinc-ion batteries. One promising strategy involves the use of glycol-based electrolytes containing both Zn^{2+} and K^+ ions, paired with a Prussian blue analogue (PBA) cathode. In such systems, potassium ions (K^+) preferentially intercalate into the cathode framework during initial cycles, which facilitates more reversible zinc plating and stripping at the anode. Additionally, K^+ ions contribute to enhancing the physicochemical properties of the electrolyte, improving ion transport kinetics. This dual-ion approach leads to better charge/discharge stability and overall enhancement in battery efficiency. This work underscores the critical role of electrolyte composition and ion management strategies in addressing fundamental limitations of zinc-based batteries. By tailoring the electrolyte environment and leveraging synergistic ion interactions, it becomes possible to enhance electrochemical performance, ultimately paving the way for more durable, efficient, and potentially higher-voltage zinc-ion energy storage systems.

Keywords: ZIBs, Glycol, Dual ion, Prussian blue Analogues

Advanced Electrolyte and Interface Engineering for Next-Generation Sodium Batteries

Manjusha Shelke

CSIR-National Chemical Lboratory, Dr. Homi Bhabha Road, Pune-411008, MH, India

* mv.shelke.ncl@csir.res.in

Abstract

Sodium-based battery technologies, particularly sodium-ion and sodium metal systems, are rapidly advancing toward broader commercial relevance. Major manufacturers are planning mass production lines, signaling accelerating adoption in electric vehicles and stationary storage applications.

Despite these gains, fundamental challenges such as sluggish ion transport at low temperatures, unstable electrode-electrolyte interfaces and uncontrolled sodium metal deposition, have constrained performance and limited deployment in demanding environments. This talk discusses our recent breakthroughs that can widen the practical scope of sodium-based batteries by directly addressing these bottlenecks through electrolyte and interface engineering. Together, these studies reveal how electrolyte chemistry, solvation structure and engineered interlayers synergistically control SEI formation and sodium metal nucleation dynamics. The talk concludes by outlining a unified interface-centric design strategy for next-generation sodium batteries, bridging fundamental interfacial chemistry with practical requirements such as low-temperature operability, higher specific energy and safety.

Keyword: Sodium batteries, metal anode, anode-less, interfacial layers, electrolyte engineering

References

(1) Kundan Wasnik, Poonam Yadav, Manuj Ahuja, Vinay Mirzapure, Priya Johari*, Manjusha Shelke*, Investigations into the Nucleation Dynamics of the Stable Na-metal Anode: Revealing the Role of Tin-infused Carbon Nanofiber Interlayer, ACS Applied Materials & Interfaces, 17, 12281 - 12290 (2025)

(2) Kundan Wasnik, Rajesh Bhatt, Manjusha Shelke*, Enhanced Stability of Sodium Metal Anodes in Covalent Triazine Frameworks via Progressive Nucleation with Optimized Conducting Composite Matrix, Small, 21, 2502636 (2025)

(3) Soohwan Kim, Vinay Mirzapure, Rasha Atwi, Heramba V. S. R. M. Koppisetti, Kundan Wasnik, Nav Nidhi Rajput, Manjusha Shelke*, Vilas G. Pol*, Insights into Electrolyte-Solvent Interactions and SEI Formation for Sustainable Sodium-Ion Battery Operation at Low Temperatures, Small Methods, 9, e02142, (2025)

Advancements and challenges in sodium-ion battery technology: from novel cathode materials to full-cell systems

Annigere S. Prakash*

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

* prakash.as@gmail.com; asprakash.cecri@csir.res.in

Abstract

Sodium-ion batteries (SIBs) have emerged as strong contenders in the race for next-generation energy storage, offering strategic advantages in terms of resource abundance, cost-effectiveness, and environmental sustainability. This talk will present recent advancements in the development of high-performance electrode materials, with a particular emphasis on novel cathode chemistries, including layered transition metal oxides and polyanionic compounds as well as engineered hard carbon anodes tailored for reversible sodium-ion storage.[1] Strategies for improving sodium-ion intercalation kinetics, structural stability, and cycle life through material and interface design will be discussed in detail. In addition, the talk will highlight the evolving landscape of electrolyte systems and their role in stabilizing electrode interfaces and enhancing ion transport. Emphasis will be placed on translating material innovations into practical full-cell configurations, addressing key challenges such as energy density limitations, degradation mechanisms, and scale-up potential. Finally, future directions for enabling commercially viable SIB technologies will be outlined, focusing on integrative approaches that connect fundamental materials research with system-level performance and manufacturability.

Keywords: Sodium-ion batteries, Cathodes, Anodes, Electrolytes, Battery manufacturing.

References

(1) Gaoyue Zhang *Energy & Fuels* **2024** *38* (9), 8326-8336

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

Exploring NASICON Frameworks for Rechargable Sodium-ion Batteries

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

[†]New Chemistry Unit, [‡]International Centre for Materials Science, [§]School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore-560064, Karnataka, India.

* prem@jncasr.ac.in

Abstract

Li-ion battteries have become as the prominent energy storage solution for portable electronics and electric vechicles market. However, their expansion to large-scale storage raises concerns over the cost, availability and geopolitical accessibility of lithium and cobalt sources. In response to these concerns, a wide range of alternative battery chemistries have been explored over the past decade. The present Na-ion batteries utilize a wide range of cathodes including layered oxides, Prussian blue analogues and polyanionc compounds. Among them, vanadium-based NASICON cathodes are interesting due to their higher voltage insertion, structural, chemical and cycling stabilities and superior Na-ion diffusivity. However their storage capacities are limited to 100 mAh g^{-1}. To overcome this issue, multi-electron reactions (e.g., $Na_4VMn(PO_4)_3$, $Na_3VCr(PO_4)_3$, etc.). Similarly, Nb-based NASICON anodes were also developed to deliver reversible capacities as high as 180 mAh g^{-1} with extrondiary cycling stability and rate performances. In this talk, we will discuss how chemical tuning approaches impact structural and electrochemcial properties of NASICON frameworks.

Keywords: Sodium-ion batteries; NASICON; electrodes

References

(1) Ghosh, S.; Jose, N.; Senthilkumar, B.; Amonpattaratkit, P.; Senguttuvan, P. Multi-Redox ($V^{5+}/V^{4+}/V^{3+}/V^{2+}$) Driven Asymmetric Sodium (De)Intercalation Reactions in NASICON-$Na_3VIn(PO_4)_3$ Cathode. *J. Electrochem. Soc.* **2021**, *168*, 050534 .

(2) Ghosh, S.; Barman, N.; Gonzalez-Correa, E.; Mazumder, M.; Zaveri, A.; Giovine, R.; Manche, A.; Pati, S. K.; Clément, R. J.; Senguttuvan, P. Elucidating the Impact of Mg Substitution on the Properties of NASICON-$Na_{3+y}V_{2-y}Mg_y(PO_4)_3$ Cathodes. *Adv. Funct. Mater.* **2021**, *31*, 2105463.

(3) Patra, B.; Kumar, K.; Mazumder. M..; Pati, S. K.; Senguttuvan, P. Tailoring High-Performance Ternary Transition Metal-Based NASICON-$Na_{(9-2x-3y-4z)}Mn_xV_yZr_z(PO4)_3$ Cathodes via Combinatorial Chemical Substitutions. *Chem. Mater.* **2024**, 36, 3107.

Role of Cationic Sublattice Configuration for Designing Low-Cost Li^+ Superionic Halospinel

Susmita Bera,[1] Selva Chandrasekaran Selvaraj,[3], Lily Mandal,[1] Ripan K. Biswas,[1] Amit Kumar,[4,5] S. M. Yusuf,[4,5] Jagjit Nanda,[6,7] Zhao Chen[8], Aditya Rawal[9], Maxim Avdeev[10-11], Amreen Bano[1,2], Neeraj Sharma[8], Anh T. Ngo[3] and Abhik Banerjee*[1,2]

[1]*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*

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

[3]*Department of Chemical Engineering, University of Illinois Chicago, Chicago, Illinois 60608, United States of America*

[4]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*

[5]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, 400094, India*

[6]*Applied Energy Division, SLAC National Laboratory, 2575, Sand Hill Road, Menlo Park, 94025, USA*

[7]*Materials Science and Engineering, Stanford University, Stanford, CA, 94035, USA*

[8] *School of Chemistry, UNSW Australia, Sydney, NSW 2052, Australia*

[9]*Mark Wainwright Analytical Centre, University of New South Wales, Kensington, NSW, 2052, Australia*

[10] *Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, NSW 2234, Australia*

[11] *School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia*

* Abhik.banerjee@tcgcrest.org

Abstract

Recent environmental concerns have driven the major research focus towards efficient and economically viable strategies for clean energy harvesting, storage and conservation. Batteries represent a unique device system of critical interest for the modern electrically driven world and attempts are now being made to move towards all solid-state battery (ASSB) for safety and efficiency, as they replace flammable liquid electrolytes with solid electrolytes and Li metal anode, having much higher capacity compared to conventional graphite anode.

Halide Solid Electrolytes (HSEs) have gained significant attention for the development of ASSB due to their high oxidation stability and favorable mechanical properties. The HSEs studied in recent decades are typically contain expensive metals such as Y, In, Sc, Er, Ho, and Hf (excluding Zr), which presents challenges for commercial viability [1,2]. As an alternative, spinel-based HSEs incorporate more affordable elements like Mn and Mg. However, in many spinels, the lithium occupancy is either fully saturated or exhibits limited disorder at elevated temperatures, resulting in lower ionic conductivity and a higher activation barrier [3,4]. To address these issues, we introduced aliovalent substitution of Al^{3+}, Fe^{3+},

Zr^{4+} into $Li_2Mn(Mg)Cl_4$, which results in a dramatic enhancement in ionic conductivity, reaching conductivity up to ~2 $mScm^{-1}$ at room temperature (RT). Refinement of the structure using neutron and synchrotron diffraction, followed by, pair distribution function (PDF) analysis and machine-learning based large-scale molecular dynamics, we infer that, aliovalent substitution creates new octahedral and tetrahedral Li sites in the structure along with Li vacancy, enabling facile Li transport via interstitial and vacancy hoping mechanism. The optimized composition shows high oxidative stability and compatibility with high-voltage cathode, and an ASSB assembled with this SE as catholyte delivers an initial discharge capacity of 155 $mAhg^{-1}$ at 4.3V.

Keywords: Superionic conductor, Halospinel, Solid State Battery, Diffusion, NMC cathode

References

(1) Wang, Q., Zhou, Y., Wang, X., Guo, H., Gong, S., Yao, Z., Wu, F., Wang, J., Ganapathy, S., Bai, X. and Li, B., 2024. Designing lithium halide solid electrolytes. *Nature Communications*, *15*(1), p.1050.

(2) Tao, B., Zhong, D., Li, H., Wang, G., & Chang, H. (2023). Halide solid-state electrolytes for all-solid-state batteries: structural design, synthesis, environmental stability, interface optimization and challenges. *Chemical Science*, *14*(33), 8693-8722.

(3) Rom, C. L., Yox, P., Cardoza, A. M., Smaha, R. W., Phan, M. Q., Martin, T. R., & Maughan, A. E. (2024). Expanding the Phase Space for Halide-Based Solid Electrolytes: Li–Mg–Zr–Cl Spinels. *Chemistry of Materials*, *36*(15), 7283-7291.

(4) Yu, Y., Huang, Y., Xu, Z., Wu, Z., Wang, Z., & Shao, G. (2024). A High-Voltage Solid State Electrolyte Based on Spinel-Like Chloride Made of Low-Cost and Abundant Resources. *Advanced Functional Materials*, *34*(24), 2315512.

Computational insights for designing frameworks of intercalation devices for energy storage systems

Swapan K Pati[,*], Mayank Sharma, M. Mazumder

Theoretical Sciences Unit

School of Advanced Materials (SAMat)

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)

Jakkur Campus, Bangalore 560064, India

E-mail: pati@jncasr.ac.in and swapan.jnc@gmail.com

Abstract

After a brief introduction to the working principles of Li and Na ion battery, I shall discuss at length the computational modelling approach. I shall discuss then the high Na content fluorophosphate skeleton, $Na_5M(PO_4)_2F_2$, with M being V and Cr as cathode material. We have computed the voltages for both the transition metal ions and these are 4.77 V and 4.56 V for Cr and V systems, respectively, which are distinctly high among previously reported voltages obtained in Sodium Ion Batteries. We have also probed the trajectories for Na ion migration and identified a minimum energy route, which leads to high ionic conductivity through low hopping barriers [1]. I shall then discuss our theoretical attempt on finding a stable, efficient, and superior 5V-solid electrolyte and present a work on the modeling of oxygen deficient perovskite material, $Na_3MnV_2O_{7.5}$ as cathode material for battery application [2, 3].

References

(1) M. Mazumder, S. K Pati, J. Phys. Chem. **C 125**, 19593 (2021).

(2) M. Sharma, S. K Pati (Submitted 2025).

(3) 4. M. Sharma, S. K Pati to be submitted.

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

"Liquid" and "Solid" Therapeutic Approaches for Overcoming Interfacial Challenges in LLZO-Based Solid-State Lithium Metal Batteries

Kuntal Ghosh, 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: mwraja.cgcri@csir.res.in

Abstract

Since its inception Lithium-ion Battery (LIB) technology achieved tremendous commercial success relying upon liquid or polymer electrolytes, but in expense of reduced energy density, power density and safety. The reason despite of its high theoretical capacity of 3860 $mAhg^{-1}$, Li metal was never been used as an anode,[1]therefore, focus is now shifted to develop solid inorganic electrolytes which offer opportunity to use Li metal as high capacity anode. Varieties of Li-ion conducting inorganic oxides were explored having ionic conductivity in the range of 10^{-2}-10^{-3} S/cm. Nevertheless, a workable All Solid-State Lithium Metal Batteries (ASSLMBs) is still far from its practical realization. The critical bottleneck arises at the solid electrolytes-electrode interfaces which become detrimental for its cycling performance and safety. Therefore, an effective cell configuration is required using solid electrolytes to achieve high performance SSLMBs.

In this present contribution, we aimed to develop engineered Ga-LLZO ($Li_{6.25}La_3Ga_{0.25}Zr_2O_{12}$) solid inorganic electrolyte scaffold infused with solvated ionic liquid (SIL). The SIL thus infused in solid Ga-LLZO matrix was used as a liquid therapeutic agent which resulted in enhanced Li-ion transport properties and superior Li-metal compatibility.[2] Furthermore, the solid electrolyte was microstructurally engineered to develop interconnected Ga-LLZO to achieve high Li-ion mobility across the grains. Exhaustive characterizations were performed and compared with conventionally prepared Ga-LLZO to check its superiority. The developed configuration proved to be advantageous in terms of cell performance, high-rate capability (0.1-3.0 mA/cm^2), long term cyclability (>500 Cycles) and high coulombic efficiency (>98%) while in operation in SSLMBs. In a similar approach, Thus, the compiled data suggested that engineered solid electrolyte infused with SIL could be an innovative approach for developing practical lithium metal batteries.

Keywords: Solid State Electrolyte, Lithium Metal Batteries, LLZO electrolyte, engineered microstructure, Interfacial Impedance

References

1. Wang, J.; Ge, B.; Li, H.; Yang, M.; Wang, J.; Liu, D.; Fernandez, C.; Chen, X.; Peng, Q. Challenges and Progresses of Lithium-Metal Batteries. *Chemical Engineering Journal,* **2021**, *420*, 129739. https://doi.org/10.1016/J.CEJ.2021.129739.
2. Ghosh, K.; Raja, M.W.; Facile Li-ion transport in microstructurally engineered hybrid LLZOelectrolyte for application in pseudo-solid state lithium metal batteries.*Chemical Engineering Journal,* **2024**,*480*,148200. https://doi.org/10.1016/j.cej.2023.148200

Polymer Membranes for the use in Fuel Cell

Tushar Jana[1*]

[1] *School of Chemistry, University of Hyderabad, India*

* tusharjana@uohyd.ac.in

Abstract

The demand of alternate source of energy with environmental-friendly fuels has increased dramatically in recent years amid global warming, climate change and various geo-political crisis. Among various new energy technologies, hydrogen-based energy solution is getting maximum attention as this offers numerous advantages. In order to utilize hydrogen as alternative energy, the overall technology development process must be carried out in an integrated manner in three verticals namely production, storage and use of hydrogen gas. Various kinds of materials are needed for the development of above three verticals. Interestingly, polymer-based materials especially polymer ion exchange membrane is a common thread among these various stages of hydrogen technology development. Ion exchange membrane (IEM) is the heart of the water electrolyzer to produce green hydrogen by water hydrolysis and similarly IEM is the main component in a fuel cell for the generation of electrical energy from the hydrogen gas. Therefore, research and development efforts for the search of efficient IEM has been given a priority in recent times.

Past 15 years, in our group, we are pursuing the efforts of developing polybenzimidazole (PBI) based IEM by adopting various approaches. Over the years, we have made significant contributions in this area, recently, we have focused our attention towards a new class of pyridine bridged PBI materials/membranes and also developed PBI based IEM for the use in microbial fuel cell to generate green energy from the waste. In my talk, I will discuss on these aspects with few representative examples from our recent results.

Keywords: Fuel Cell, Polymer Membrane, Polybenzimidazole,

References

1. Subhadarshini, S.; Sravan, J. S.; Sarkar, O.; Venkata Mohan, S.; Roy, T. K.; Jana, T. *ACS Appl. Energy Mater.* **2023**, *6*, 1422-1438.
2. Harilal, Shukla, A.; Ghosh, P. C.; Jana, T. *Euro. Polym. J.* **2022**, *177*, 111445.
3. Harilal, Bhattacharyya, R.; Shukla, A.; Ghosh, P. C.; Jana, T. *J. Mater. Chem. A* **2022**, *10*, 11074-11091.
4. Harilal, Shukla, A.; Ghosh, P. C.; Jana, T. ACS Appl. Energy Mater. **2021**, *4*, 1644-1656.

Electricity from Acid Base Reaction

Musthafa Ottakam Thotiyl[1,*]

[1] *Professor, Department of Chemistry, Indian Institute of Science Education and Research, Pune, Maharashtra, India*

* musthafa@iiserpune.ac.in

Abstract

Proton exchange membrane fuel cells are promising zero-emission technologies, but challenges with hydrogen storage, safety, and transport hinder widespread adoption. Using alcohols as liquid hydrogen carriers offers a solution, but current reforming methods require high temperatures (>200℃) and pressures (>25 bar), producing hydrogen with excess carbonization unsuitable for fuel cells. We introduce a method that harnesses neutralization energy to generate hydrogen and electricity under ambient conditions. This approach enables spontaneous hydrogen production, simultaneous desalination of saline water, and fuel purification. The electrochemical neutralization process operates efficiently without high temperatures or pressures and holds potential for organic synthesis, waste heat recovery, and hydrocarbon reforming, enhancing energy storage and contributing to climate change mitigation (1-5).

Keywords: Fuel cells, Energy of neutralization, Alcohol reformation, Fuel purification, Desalination

References

(1) Mondal, R.; Shyaam, S. Y.; Nayak, B.; Pradhan, H.; Musthafa. O. T. A non-isothermal water formation cell for electrochemical heat recovery. *Chem, Sci.,* **2025,** *16,* 7751.

(2) Mondal, R.; Nayak, B.; Musthafa. O. T. A Spontaneous Heavy Hydrogen Generator via a Protium Redox. *J. Phys. Chem. Lett.* **2024,** *15,* 6866.

(3) Mondal, R.; Thimmappa, R.; Nayak, B.; Dewan, A.; Devendrachari, M. C.; Chen, Q.; Wen, Z.; Musthafa. O. T. A spontaneous hydrogen fuel purifier under truly ambient weather conditions**.** *Energy Environ. Sci.*, **2023,** *16,* 3860.

(4) Bhat, Z. M.; Thimmappa, R.; Dargily, N. C.; Raafik, A.; Kottaichamy, A. R.; Devendarachari, M. C.; Kotresh, H. M. N.; Fruenbuerger, S.; Musthafa. O. T. Ambient Condition Alcohol Reforming to Hydrogen with Electricity Output. *ACS Sustain. Chem. Eng.*, **2022,** *10,* 10781.

(5) Bhat, Z. M.; Pandit, D;. Ardo, S;. Thimmappa, R.; Kottaichamy, A. R.; Dargily, N. C.; Devendrachari, M. C.; Musthafa. O. T. An Electrochemical Neutralization Cell for Spontaneous Water Desalination. *Joule* **2020,** *4,* 1730.

Cell Performance of Pt Catalyst Supported on Mesoporous Carbon

H. Daimon[1*], N. Kuroda[1], K. Yamada[1], J. Manabe[1], T. Doi[1], H. Inoue[2], and M. Inaba[1]

[1]Faculty of Science and Engineering, Doshisha University, 1-3 Tatara-Miyakodani, Kyotanabe, Kyoto, Japan 610-0321

[2]ISHIFUKU Metal Industry Co., Ltd., 2-12-30 Aoyagi, Soka, Saitama, 340-0002 Japan

*jt-ksi08@mail.doshisha.ac.jp

Abstract

In Japan, extremely high cell performance is required in PEFCs applied to FCEVs after 2030 as depicted in Figure 1 (1). One strategy to achieve the high cell performance is to use mesoporous carbon (MPC) supports for the Pt and Pt-based catalysts. We selected CNovel® MH-18 (pristine CNovel® was bead-milled to 800 nm) as the MPC support, and Pt/MPC (800 nm) catalyst with a Pt loading of 50 wt.% was synthesized *via* impregnation/thermal reduction method. Cross-sectional TEM observation of the catalyst revealed that Pt NPs (2.5 nm in size) were uniformly dispersed in the MPC support, and half-cell measurements showed that ECSA and MA of the catalyst were 96 m^2/g and 741 A/g@0.9 V *vs.* RHE, respectively. 3D-TEM analysis of the MPC support demonstrated that well-interconnected mesopores (2-6 nm) and macropores (> 50 nm) coexist in the MPC support, and thus the MPC support has a high oxygen diffusivity and the Pt/MPC catalyst exhibited a higher cell performance than the Pt catalyst supported on a conventional porous carbon support of Ketjen Black EC-600JD (KB-600JD) under 80°C 75% RH standard conditions (2). However, the cell performance was significantly declined under a high humidity condition of 80°C 95% RH as shown in Figure 2. It was supposed that ionomer agglomerates formed between the large MPC supports (800 nm) swelled in the high humidity conditions, blocking the gas flow paths and increasing the diffusion overpotential, which caused the cell voltage drop. To mitigate the formation of the ionomer agglomerates, Pt-unsupported KB-600JD (50 wt.% of the MPC support) was added in the cathode catalyst layer, which suppressed the increase in the diffusion overpotential and increased the cell voltage under the high humidity condition as shown in Figure 2. The addition of the Pt-unsupported KB-600JD is simple and low-cost method to improve the cell performance of the Pt/MPC (800 nm) under the high humidity conditions.

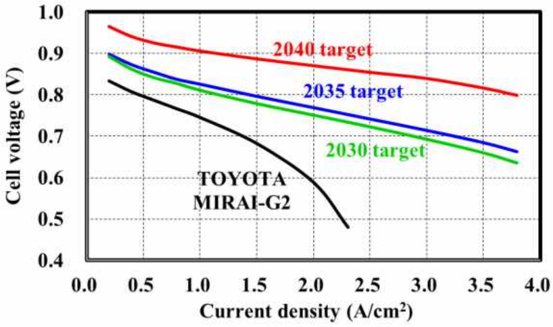


Fig. 1. Cell performance of PEFCs targeted by 2030-2040.

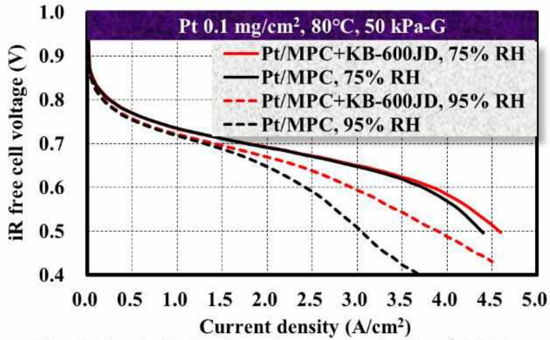


Fig. 2. H_2-air fuel cell performance of 1.0 cm^2 MEAs.

References

(1) https://www.nedo.go.jp/content/800020391.pdf

(2) H. Daimon *et al.*, *J. Electrochem. Soc.*, 2025, **172**, 34503.

Molecularly Engineered Ion Exchange Membranes for Fuel Cells

Farsa Ram[1,*], Rikta Das[1]

[1] *Interdisciplinary Centre for Energy Research, Indian Institute of Science, Bengaluru - 560012, India*

* ramf@iisc.ac.in

Abstract

Clean energy generation using electrochemical power sources is becoming more common and affordable due to the focus of various countries around the globe on the hydrogen economy. Fuel cells such as proton exchange membrane fuel cell (PEMFC) that can convert chemical energy into electricity are promising clean energy sources, which are used for both stationary and transport applications [1], [2]. One of the bottleneck components in the fuel cell is the membrane, which is known as the heart of the fuel cell that selectively transports the ionic species across the electrodes. Currently, perfluorosulfonated acid membranes like Nafion® are costly and suffer from several issues, such as thermo-mechanical and chemical stability, reduced proton conductivity at elevated temperature and low humidity, etc. One strategy to solve these issues is to add suitable filler to tailor the membrane property as required (3). Contrary to common methods of tailoring one kind of membrane property at a time, we addressed several PEM issues simultaneously using a molecularly engineered biopolymer filler (4). Another strategy is to move beyond PEM to the anion exchange membranes (AEM), where AEM FCs can be operated at ~1/3 the cost of the PEMFCs with the use of non-noble metal catalysts, and relatively cheaper AEMs. Here, we are trying to create molecularly engineered membranes for high hydroxide ion conductivity with high mechanical properties that could lead to the durable AEM FC operation.

Keywords: Fuel Cells, Hydrogen Economy, Proton Exchange, Anion Exchange, Membranes

References

(1) Onecore Energy's fuel cell-based MicroGrid for Residential applications - https://oncoreenergy.com/hydrogen-microgrid/. Accessed on July 05, 2025.
(2) Toyota's fuel cell-based car - https://www.toyota.com/mirai/. Accessed on July 05, 2025.
(3) Cele, N.; and Ray, S. S. *Macromol. Mater. Eng.* **2009***, 11,* 719-738.
(4) Ram, F.; Velayutham, P.; Sahu, A. K.; Lele, A. K.; Shanmuganathan, K. A*CS Appl. Energy Mater.* **2020***, 3*, 1988-1999.

Nano-crystalline $Fe_3V_3O_8$ Material as an Efficient Advanced Anode for Energy Storage Applications

Rasu Muruganantham, Jun-Ying Huang and Wei-Ren Liu*

Department of Chemical Engineering, Chung Yuan Christian University, 200 Chung Pei Road, Chung Li District, Taoyuan City-32023, Taiwan

* Corresponding author's email address: WRLiu1203@gmail.com

Abstract

Sodium-ion battery (SIB) is a rapidly developing electrochemically rechargeable storage device and a direct substitute for Li-ion batteries. Therefore, identifying novel materials for sodium-ion storage applications is important. Efficient electrodes are particularly desirable for enhancing storage performance in battery applications. In this study, we fabricated a novel $Fe_3V_3O_8$ (FVO) anode material for Na/Li-ion storage using hydrothermal technology for the first time. The electrochemical results indicated that the initial sodiation capacity of the FVO anode is as high as 805 mA h g^{-1} at 100 mA g^{-1}, and a reversible sodiation capacity of 540 mA h g^{-1} is maintained over 200 cycles at 500 mA g^{-1}, which is more than 1.8 times the commercial hard carbon of ~300 mA h g^{-1}(1). In addition, the oxidation states of the chemical compound and the corresponding sodium reaction mechanism are predicted using X-ray absorption spectroscopy (XAS), X-ray photoelectron spectroscopy (XPS), and in-situ/ex-situ X-ray diffraction (XRD) analysis. Overall, the FVO material exhibited significantly higher electrochemical performance, demonstrating promising suitability for sodium-ion storage.

Keywords: Anode, Sodium ion batteries, Tranision metal oxides

Reference

(1) Rasu Muruganantham, Jun-Ying Huang, Pei-June Wu, Liang-Yin Kuo, Chun-Chuen Yang, Yan-Gu Lin, Ju Li and Wei-Ren Liu,* "Nano-crystalline $Fe_3V_3O_8$ Material as an Efficient Advanced Anode for Energy Storage Applications," J. Power Sources, 613 (2024) 234947.

Self-Healing Liquid Gallium Alloy Composite Anode for High-Performance Sodium-Ion Storage

Thangavelu Palaniselvam*

[1] *Assistant Professor, Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India.*

* Email: palaniselvam@iitm.ac.in

Abstract

Lithium-ion batteries (LIB) have proven to be promising energy storage for transport and stationary applications. Significant advancements have occurred in LIB production over the last few decades. However, the limited availability of certain elements, including Li, Ni, and Co, combined with geopolitical factors, critically hampers their widespread growth. Similar to LIBs, alternative cell chemistries utilizing other alkali or alkaline earth metal ions have gained high attention. Among these, sodium-ion battery (SIB) presents a promising alternative for LIB, as both exhibit similar electrochemical behaviors. Considering cathodes, significant progress has already been made in enhancing capacity. Anode materials are also being equally investigated for SIBs. However, finding an anode with a suitable Na^+ storage voltage (0.0–2.0 V vs Na/Na^+), large reversible capacity, high structural stability, and minimal volume change poses a significant challenge. Here, the development of a self-healable GaSb alloy featuring a confined Sn (core-shell) structure is reported for stable Na^+ storage. The core-shell architecture of GaSb@Sn has been validated through HAADF-STEM paired with EELS analysis. The GaSb@Sn/C electrode has delivered specific capacity of 560 mAh $g_{electrode}^{-1}$ at 50 mA g^{-1} with 89% retention capacity after 1200 cycles. The GaSb@Sn/C electrode stores Na^+ by forming Na-Sn, Na-Sb-O, and Na-Ga-O intermetallic compounds, as confirmed by operando XRD studies. Operando electrochemical dilatometry studies reveal that the self-healable electrode expands by 33% at the electrode level during Na^+ insertion, significantly lower than the theoretically predicted expansion of Sn, which is 420%. The weaker interaction between diglyme and GaSb@Sn could be responsible for the thinner SEI formation on the edges of GaSb@Sn, thereby resulting in the high initial coulombic efficiency (GaSb@Sn- 81%, Bulk Sn-62%) and stable cycle life.

Keywords : Batteries, liquid alloys, operando charecterizations, self-healing, sodium storage

References

(1) Deori, D.; Buragohain, M.; Son, Y.; Kunnikuruvan, S.; Nanjundan A. K.; Adelhelm, P.; Palaniselvam, T. Self-Healing, Ga-Sb Alloy Confined Sn Anode for StableNa-Ion Storage in Glyme Based Electrolytes, *Small* **2025**, 2504185.

(2) Palaniselvam, T. et.al., Sodium Storage and Electrode Dynamics of Tin–CarbonComposite Electrodes from Bulk Precursors for Sodium-IonBatteries, *Adv. Funct. Mater.* **2019**, 29, 1900790.

Design of Localized High Concentration Electrolytes for High-Voltage Anode-Free Lithium Metal Batteries

Wei-Nien Su[1,3*], Mei-Ru Lai[2], Jyh-Chiang Jiang[2,3], Bing-Joe Hwang[2,3]

[1] *Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, 43 Keelung Road, Section 4, Taipei 106, Taiwan*

[2] *Department of Chemical Engineering, National Taiwan University of Science and Technology, 43 Keelung Road, Section 4, Taipei 106, Taiwan*

[3] *Sustainable Electrochemical Engergy Development (SEED) Center, National Taiwan University of Science and Technology, 43 Keelung Road, Section 1, Taipei 106, Taiwan*

* wsu@mail.ntust.edu.tw

Abstract

Anode-free lithium-metal batteries (AFLMBs) offer high energy density but suffer from unstable SEI formation and lithium dendrite growth, particularly when using conventional carbonate-based electrolytes. To address these challenges, we developed a dual-salt localized high-concentration electrolyte (LHCE) comprising $LiPF_6$ and LiTFSI in EC/EMC with fluorinated co-solvents and multiple additives. This formulation tailors solvent coordination, reduces side reactions, and stabilizes the electrode interface. Ab initio molecular dynamics (AIMD) simulations and DFT calculations reveal that aggregate formation in LHCE minimizes free solvent content, while TTE modulates viscosity and solvation structures. FEC is introduced to replace excess TTE, and additives like LiDFOB and $LiNO_3$ help form a robust SEI and mitigate cathode corrosion.

Keywords : Dual salt electrolytes, localized high-concentration electrolyte, high-voltage cathode; Anode-free; diluent

References

(1) Semaw Kebede Merso, Teshager Mekonnen Tekaligne, Misganaw Adigo Weret, et al. Multiple protective layers for suppressing Li dendrite growth and improving the cycle life of anode-free lithium metal batteries. Chemical Engineering Journal, **2024**, 485, 149547, https://doi.org/10.1016/j.cej.2024.149547.

(2) Teklay Mezgebe Hagos, Hailemariam Kassa Bezabh, Chen-Jui Huang, Shi-Kai Jiang, Wei-Nien Su, Bing Joe Hwang. A Powerful Protocol Based on Anode-Free Cells Combined with Various Analytical Techniques. Accounts of chemical research, **2021**, 54, 24, 4474–4485.

What happens to Li-rich Layered oxides when we cation disorder them?

Susim Sabuj Sarkar[a], Subham Ghosh[a], Urmimala Maitra[a]*

School of Materials Sciences, Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Jadavpur, Kolkata, India

**Correspondence email: urmimala.maitra@iacs.res.in*

Abstract

Successful integration of renewable energy into the mainstream energy utilization requires the development of efficient and cheaper energy storage devices. While, lithium-ion batteries are effective for the same, they face critical limitations such as restricted resource availability, environmental concerns, and safety risks. To address the growing energy demands, it is crucial to develop high-performance, eco-friendly beyond lithium energy storage systems, especially metal-air batteries. In this talk, we will discuss the strategic development of three major components of flexible zinc air battery(ZAB): cathode, anode and membrane. Our research groups have developed many transition metal oxides-based cathode materials for flexible ZAB with the properties of good bi-functionality as oxygen electrode. The major constraints that limit the performance of zinc air batteries are the sluggish kinetics of oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). Different strategies like doping, hetero-junction formation etc have been adopted to improve the performances of these reactions. We have also successfully developed few gel-electrolyte based membrane and evaluated their performance. Our experimental observations led to this conclusion that, the development of a flexible solid electrolyte focuses on achieving an optimal balance between high ionic conductivity and robust mechanical strength—both critical for practical and durable energy storage.

Keywords: metal-air battery, membrane, oxygen electrode, oxides, thiospinel

References

(1) Ravinder Sharma, Arkaj Singh, Aditi Halder; Synergistic effect of lattice strain, oxygen vacancy and morphology in Mo doped NiCo2O4 for high-performance zinc air batteries, J. of Energy Storage. 2025,107,114918

(2) Arkaj Singh, Ravinder Sharma, Aditi Halder; Flexible solid-state Zn–air battery based on polymer-oxygen-functionalized gC3N4 composite membrane.Nanoscale,2024, 16,8,4157-4169

(3) Ankita Mathur; Kumari, Sonu; Singh, Arkaj; Mitra, Rahul; Sharma, Ravinder; Biswas, Krishanu; Aditi Halder; Surface engineering of 2D layered MnO2 with co-doping of Ni and Fe for rechargeable zinc-air battery, J. of Energy Storage. 2023, 74, 109350,

All-Solid Polymer Electrolyte System Enabling Li-metal Batteries

Sirin Kamarulzaman[1,*], Dorsasadat Safanama[1], Shermin Goh[1*], Derrick Fam[1,2*]

[1] *Institute of Materials Research and Engineering, A*STAR, 2 Fusionopolis Way, Singapore 138634*

[2] *School of Materials Science and Engineering, NTU, #01-30, 50 Nanyang Ave, Blk N4.1, Singapore 639798*

* Corresponding author's email address

Abstract

Solid Polymer Electrolytes (SPEs) have good manufacturability and can form good electrode-electrolyte interfaces. However, they often suffer from low ionic conductivities ($<10^{-5}$ S cm^{-1}) in its solid state and poor electrochemical stabilities. In addition, polymer-in-salt systems typically have low Li^+ transference numbers (<0.4) resulting in steep ion concentration gradients and lower cyclability. The low ionic conductivity in solid-polymer systems is due in part to crystallinity[1]- the polymer-in-salt forms either pure polymer or complex crystals which reduces cationic movement resulting in poor ionic conductivities and transference numbers. In this work, an amorphous dynamically crosslinked solid-polymer (DSPE) electrolyte system synthesised in a one-pot process is presented. The DSPE exhibits a practical conductivity of 10^{-4} S cm^{-1} and a transference number of ~0.8 was measured in all solid-state, without any addition of any liquids or small molecules, which surpasses the performance of commercial SPEs. It also displays reformability upon mechanical damage. The DSPE has also been applied to a solid-state Li|$LiFePO_4$ cell, showing stable charge-discharge profiles over 200 cycles with an average Coulombic efficiency of 99.6 %.

Keywords (max 5): All solid-state batteries, solid polymer electrolytes, polyethylene oxide, Li-metal

References

(1) Ning D et. Al. Revealing Phase Transitions in Poly (Ethylene Oxide)-Based Electrolyte for Room-Temperature Solid-State Batteries, Advanced Energy Materials 2024 14 (40), 2470172. DOI: **doi.org/10.1002/aenm.202402986**

Functional Quasi-Solid-State Electrolyte Based on an Ionic MOF for Enhanced Sodium Metal Battery Stability

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

Sodium metal is a promising anode for next-generation batteries due to its natural abundance, low cost, and favorable electrochemical potential (−2.71 V vs. SHE); however, its practical implementation is hindered by dendritic growth and unstable interfacial layers (SEI and CEI) in conventional liquid electrolytes. These issues result in the formation of electronically isolated "dead sodium," leading to capacity fading and poor cycling stability. We report a quasi-solid-state electrolyte (QSSE) comprising an ionic metal–organic framework (MOF) embedded in a PVDF-HFP matrix to address these limitations. The MOF introduces a highly porous structure and a cationic framework, which enhances sodium-ion accommodation and promotes effective ion dissociation via localized electric fields, thus enabling fast ion transport.[1,2] The resulting QSSE achieves a high ionic conductivity of 0.42 mS cm^{-1} at room temperature, a low activation energy of 0.15 eV, and a sodium-ion transference number of 0.87. Long-term symmetric cell testing demonstrates stable sodium plating/stripping for over 1500 hours at 0.02 mA cm^{-2} with minimal polarization growth. Moreover, the electrolyte exhibits a wide electrochemical stability window up to 4.8 V. When integrated into a full cell with $Na_3V_2(PO_4)_3$ (NVP) as the cathode (NVP|QSSE|Na), the system delivers 110 mAh g^{-1} at 0.2 C, retains 65 mAh g^{-1} at 5 C, and maintains 95% of its initial capacity over 500 cycles, achieving a high energy density of 350 Wh kg^{-1}, thereby underscoring the potential of MOF-based QSSEs for high-performance sodium metal batteries.

Keywords: Metal organic framework, Cationic framework, solid state electrolyte, ionic conductivity, sodium metal battery.

References

(1) Hou, T.; Xu, W.; Pei, X.; Jiang, L.; Yaghi, O. M.; Persson, K. A. Ionic Conduction Mechanism and Design of Metal–Organic Framework Based Quasi-Solid-State Electrolytes. J. Am. Chem. Soc. 2022, 144 (30), 13446–13450. https://doi.org/10.1021/jacs.2c03710.

(2) Xue, W.; Sewell, C. D.; Zhou, Q.; Lin, Z. Metal–Organic Frameworks for Ion Conduction. Angew. Chemie Int. Ed. 2022, 61 (34). https://doi.org/10.1002/anie.20220651.

Pseudocapacitive Charge Storage of MXene-Organic Hybrids in Divalent Metal-ion Electrolytes

Priyaranjan Sahoo, Shubham Bhoi, Suman Yadav and Narendra Kurra

Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi-502284, Sangareddy, Telangana State, India

Email: narendra@chy.iith.ac.in

Abstract

By the virtue of abundancy and sustainability, organic materials are an emerging class of charge storage hosts for the development of low-cost multivalent metal-ion-based electrochemical energy storage devices in the era of post-lithium-ion batteries. However, poor electronic conductivity, dissolution and mechanical instability hamper the long-term cycling stability. MXenes are a large family of two-dimensional (2D) transition metal carbides, nitrides and carbonitrides, with rare combination of properties of metallic conductivity and hydrophilicity. Solution processability enables the formation of hybrids of organic materials via non-covalent interactions. $Ti_3C_2T_x$ MXene- perylene diimide hybrid electrodes demonstrated reversible electrochemical storage of Mn^{2+}, $Zn^{2+,}$ and Ca^{2+} ions with three-fold enhancement in charge storage capacities over pristine $Ti_3C_2T_x$. *In situ* Ultraviolet-Visible spectroscopy studies confirm the potential dependent reversible formation of radical anions and dianions of *c*PDI at -0.3 and -0.6 V vs. Ag wire, respectively. Moreover, 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 research paves the way for developing MXene-organic hybrid electrodes towards development of high-capacity, high-rate multivalent metal-ion storage devices.

Keywords: MXenes, Organic materials, pseudocapacitance, multivalent metals, in-situ spectroscopy

References

(1) 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.

(2) S Goudar, S. H.; Bhoi, S.; Sahoo, S. K.; Rao, K. V.; Kurra, N. Supramolecular Engineering of $Ti_3C_2T_x$ MXene -Perylene Diimide Hybrid Electrodes for the Pseudocapacitive Electrochemical Storage of Calcium Ions. *Small* **2024**, *20* (26), 2309905.

(3) 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*, 102229.

(4) Yadav, S.; Kurra, N. Diffusion Kinetics of Ionic Charge Carriers across $Ti_3C_2T_x$ MXene-Aqueous Electrochemical Interfaces. *Energy Storage Mater.* **2024**, *65*, 103094.

Toward Sustainable Lithium-Ion Batteries: Advances in Low- and Zero-Cobalt Electrode Materials

Surendra K. Martha

Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, 502284, TS, India. Tel: +91-7989729379; *martha@chy.iith.ac.in

Abstract

The Indian transport ministry has announced of going 30% electric mobility (Hybrid and Electric vehicles-HEV and EVs) by 2030s to be at par with the rest of the world. The heart of EVs is energy storage, i.e. Rechargeable lithium-ion batteries (LIBs). LIBs have dominated the market due to their high energy density (150-250 Wh kg^{-1}), operating voltage (>3.7 V), and long cycle life (> 1000 cycles). Commercial cathodes in use are $LiCoO_2$ (LCO), $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA), $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC), and $LiFePO_4$. Cobalt plays a leading role in commercialized LIBs because of its high voltage, structural stability, and good diffusivity of Li^+ ions during the charge-discharge. However, experts doubt that the scarcity of cobalt will stop the growth of LIB manufacturing shortly. Besides, Ni-rich layered oxides, such as NCA, $Li_{1.2}Mn_{0.55}Ni_{0.15}Co_{0.1}O_2$, and $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$, are gaining popularity as cathode materials for EVs due to their enhanced capacity (~200 mAh g^{-1}) compare to LCO (~150 mAh g^{-1}). Though the redox activity of nickel occurs at a higher potential *vs.* Li^+/Li, resulting in high energy density, the issues of storage (formation of residual lithium compounds inhibits the performance), structural instability at high voltages, and thermal and cycle stability have limited their application. Additionally, no cobalt-based cathodes, such as LMFP ($LiMn_{0.8}Fe_{0.2}PO_4$, 4.1 V) and LNMO ($LiNi_{0.5}Mn_{1.5}PO_4$, 4.7 V), are proposed as ideal cathodes for next-generation LIBs and Solid-state Lithium batteries. Ni-Rich, Co-Less layered/spinel oxide-based, high voltage olivine cathodes could meet the demand for next-generation LIBs with a high energy density beyond >250 Wh kg^{-1}. Besides, dual carbon (ion) batteries find a space for the next generation of LIBs. Given these developments, alternative applications of graphite in energy storage systems is vital for maintaining its relevance and fostering circularity. A particularly promising avenue is its use as a cathode in dual-ion batteries (DIBs), where graphite can intercalate anions, resulting in high voltage, enhanced safety, and sustainability.

The presentation will focus on the development of the current Li-based rechargeable batteries development in our laboratory and the prospects of LIBs.

Keywords: Ni-rich NMC, LMFP, LNMO, Cathodes, Li-ion batteries

References

1. S. Ghosh, U. Bhattacharjee, S. Patchiyappan, J. Nanda, N. J. Dudney, and **S. K. Martha***, ***Advanced Energy Materials***, 11 (17) (2021) 2100135.
2. J. Dutta, S. Ghosh, and **S. K. Martha***. ***ACS Appl. Mater. Interfaces*** 2024, 16, 15, 19720–19729.
3. J. Dutta, S. Ghosh, K. K. Garlapati, **S.K. Martha***, ***J. Power Sources*** 587(2023) 233717.
4. J. Dutta, S. Ghosh, Vilas G. Pol and **S. K. Martha***, DOI: 10.1039/D5TA03286E, J. Mater. Chem. A, 2025.
5. G. Kiran Kumar, S. Ghosh, J. Dutta, B. B. Panigrahi, **S. K. Martha***, Adv. Energy Mater. 2025, 2500501 https://doi.org/10.1002/aenm.202500501.

Enhancing Rate and Cycling Stability of $Na_4MnV(PO_4)_3$-Carbon Dots Composite Cathode for Sodium-Ion Batteries

Sujeera Pleuksachata[1], Nattha Chaiyapo[1], Komsak Aranmala[1], Phongsit Krabao[1], Natthapong Kamma[1], Songyoot Kaewmala[1,2], Jeffrey Nash[2], Wanwisa Limphirat[3], Yujeong Jeong[4], Myong Yong Choi[4], and Nonglak Meethong[1,2]*

[1]*Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

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

[3]*Synchrotron Light Research Institute (SLRI), Nakhon Ratchasima 30000, Thailand*

[4]*Core-Facility Center for Photochemistry & Nanomaterials, Department of Chemistry (BK21 FOUR), Research Institute of Natural Sciences, Gyeongsang National University, Jinju 52828, Republic of Korea1Department,*

*Email: nonmee@kku.ac.th

Abstract

NASICON-structured $Na_4MnV(PO_4)_3$ (NMVP) has attracted considerable interest due to its notable characteristics, including a high theoretical capacity of 110 mAh/g, good ionic conductivity, and structural stability. NMVP, achieved through suitable manganese (Mn) substitution for vanadium (V), not only exhibits reduced toxicity, but also minimizes the use of expensive V. However, NMVP suffers from low electronic conductivity, leading to unsatisfactory rate and cycle performance. In this work, we address a critical limitation by employing two key strategies: carbon coating and morphology control. NMVP/C-Carbon dots (NMVP/C-CDs) was prepared via a scalable spray-drying method to control morphology, utilizing citric acid (C) and activated carbon derived from coconut shell chars (AC) as carbon sources. Notably, our process enables the in-situ formation of CDs from AC, significantly enhancing the material's conductivity. Compared to NMVP/C, NMVP/C-CDs exhibited outstanding rate performance, especially at high C-rates. It also demonstrated excellent cycling stability, retaining more than 80% of its capacity at a 1C rate over 1,000 cycles. CDs serve as a conductive carbon source, improving electron transport and strengthening the structural integrity of the carbon matrix. These findings highlight NMVP/C-CDs as a promising cathode material for sodium-ion batteries (SIBs), effectively addressing the challenge of poor electronic conductivity through the incorporation of CDs and providing a practical and scalable solution with strong potential for large-scale commercialization.

Keywords: Sodium ion battery, Cathode $Na_4MnV(PO_4)_3$, Carbon dots, Scalable Spray-Drying Synthesis

Vacuum-Processable Additive for Controlling Growth of Perovskite Crystals in Vacuum Processed Perovskite Solar Cell

Kyungkon Kim[1,*]

[1] *Department of Chemistry and Nano Science, Ewha Womans University, Seoul 03760, Republic of Korea*

* Corresponding author's email address: kimkk@ewha.ac.kr

Abstract

In this study, we present a novel method for controlling the growth of perovskite crystals in a vacuum thermal evaporation process by utilizing a vacuum-processable additive, propylene urea (PU). By co-evaporating perovskite precursors with PU to form the perovskite layer, PU, acting as a Lewis base additive, retards the direct reaction between the perovskite precursors. This facilitates larger domain size and reduced defect density. Following the removal of the residual additive, the perovskite layer, exhibiting improved crystallinity, demonstrates reduced charge recombination, as confirmed by time-resolved microwave conductivity analysis. Consequently, there is a notable enhancement in open-circuit voltage and power conversion efficiency, increasing from 1.05 V to 1.15 V and from 17.17% to 18.31%, respectively. The incorporation of a vacuum-processable and removable Lewis's base additive into the fabrication of vacuum-processed perovskite solar cells offers new avenues for optimizing these devices.

Keywords: Solar cells, Perovskite solar cells, vacuum processed perovskite solar cells

Advancement of Surface Engineered Semiconductor heterostructures in Photoelectrochemical devices for solar water splitting

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

Photoelectrochemical (PEC) water splitting is a solar-driven approach to hydrogen generation from water.[1] Despite its considerable potential, the widespread application of PEC water splitting remains hindered by limitations such as low efficiency, which arises from charge carrier recombination, and sluggish reaction kinetics. The integration of cocatalyst decoration with complementary enhancement strategies has shown promise in overcoming these challenges, offering improved efficiency and stability. A promising class of next-generation photocatalysts, conjugated polymer nanostructures (CPNs) exhibit a distinctive capacity to hybridize with other nanomaterials to form heterostructures.[2,3] Notably, femtosecond transient absorption spectroscopy has revealed that the incorporation of metal oxide and polymer nanostructures substantially enhances the separation and transfer of photoinduced charge carriers.[3] For instance, embedding polypyrrole (PPy) nanofibers within Bi_2WO_6 has been shown to markedly increase conductivity and catalytic performance, while maintaining activity through multiple operational cycles. Furthermore, an indigenous prototype device incorporating a photocatalyst layer within tandem PEC cells has been developed, underscoring practical advancements in this field. A deeper understanding of the photoelectrochemical behavior of emerging carbon-based nanostructures, along with elucidation of their underlying mechanisms and associated challenges, holds significant potential for scaling up solar fuel production technologies.

Keywords: Conjugated polymer nanostructures, Heterostructures, Surface engineering, S-scheme heterojunction, Photoelectrochemical water splitting

References

(1) Song, H.; Luo, S.; Huang, H.; Deng, B.; Ye, J. Solar-Driven Hydrogen Production: Recent Advances, Challenges, and Future Perspectives. *ACS Energy Lett.* **2022**, *7*, 1043–1065.

(2) Ghosh, S.; Natalie, K. A.; Ramos, L.; Remita, S.; Dazzi, A.; Besseau, A. D.; Goubard, F.; Aubert P.-H.; Remita, H. Conducting polymer nanostructures for photocatalysis under visible light. *Natur. Mater.* **2015**, *14*, 505–511.

(3) Pal, S.; Das, P. S.; Naskar, M. K.; Ghosh, S. Metal oxide nanocrystals embedded polypyrrole nanohybrid: Exploring role of interface in photocatalytic hydrogen generation. *Mater. Today Sustainability* **2024**, *25,* 100610.

(4) 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.

Photo-Rechargeable Sodium-Ion Batteries

Rajendra Kumar Singh, Vikash Yadav, Anupam Patel, Shitanshu Pratap Singh, Samriddhi, Tanya Jaiswal

Department of Physics, Banaras Hindu University, Varanasi 221005, India

email:rajendrasingh.bhu@gmail.com

Abstract

The growing demand for sustainable and efficient energy storage solutions has intensified interest in next-generation battery technologies that can directly integrate renewable energy harvesting and storage. Photo-rechargeable sodium-ion batteries (PR-SIBs) represent a novel class of energy storage devices that combine the abundance and low cost of sodium with the capability of solar energy conversion, enabling direct sunlight-driven battery charging without the need for separate photovoltaic and storage units. This talk will explore the fundamental principles, material innovations, and recent advancements in PR-SIBs, with a particular focus on dual-functional photoelectrodes, interfacial charge dynamics, and strategies to overcome key challenges such as low photovoltage, poor charge separation, and material degradation. Emphasis will be placed on the design of layered transition metal dichalcogenides and heterostructured nanocomposites for enhanced photo-induced Na^+ deintercalation and improved cycling stability. The presentation will also discuss potential applications in off-grid energy systems and integrated solar energy storage platforms, highlighting the future scope and interdisciplinary opportunities in this emerging field.

Electrocatalyst and Electrolyte Engineering for Energy Applications

Vishal M. Dhavale[1,*]

[1]*CSIR-Central Electrochemical Research Institute (CSIR-CECRI), CSIR Madras Complex, Taramani, Chennai – 600 113, Tamil Nadu*

* vishal@cecri.res.in

Abstract

The development of advanced PGM, non-PGM-based electrocatalysts for polymer electrolyte membrane fuel cells (PEMFCs) and the engineering of aqueous electrolytes for improved charge storability in aqueous Zn-ion battery (AZIBs) are crucial for the next-generation energy storage and conversion technologies. The multifaceted investigation into two distinct but related areas will be focused.

First, the beneficial role of a CoNi-alloy in facilitating the formation of N-doped bamboo knotted tube morphology via a tip-in growth mechanism. This unique structure establishes the CoNi-alloy as a highly promising Pt-free cathode electrocatalyst for anion exchange membrane fuel cells, addressing the need for efficient and cost-effective noble-metal alternatives.

Second, a revolutionary reverse dual-ion battery design that leverages a low-redox potential anode and a cation-deficient cathode to fundamentally alter ion de(insertion) chemistry within a $ZnCl_2$ water-in-salt electrolyte (WiSE). This innovative sequencing of ion-born chemistry represents a significant leap forward, showcasing groundbreaking potential for advancements in aqueous energy storage technology. Complementary to this, we provide molecular insights into the behaviour of methanol as an antisolvent in $ZnCl_2$ WiSE and experimentally evaluate its impact on the performance and efficiency of AZIBs. Understanding these interactions is vital for optimizing electrolyte formulations and enhancing battery longevity and capacity.

Lastly, the glimpse of design, development and demonstration (D^3) of CECRI's PEMFC technologies in the stationary and automotive sectors will be discussed.

Keywords: PGM and Non-PGM Electrocatalyst, Dual-ion Battery, Antisolvets, PEMFCs

References

(1) Anil Kumar U., Vishal M. Dhavale, J. Mater. Chem. A, 2024, 12, 22820-22831

(2) Asis Sethi, Anil Kumar U., Vishal M. Dhavale, ChemPhysChem 2023, 24, e202300098

(3) Asis Sethi, C Rajeev, Anil Kumar U., P Sharma, AP Sunda, Vishal M. Dhavale, J. Mater. Chem. A, 2024, 12, 23049-23058

Three-Dimensionally Connected Nanoparticles for Advanced Oxygen Reduction Catalysts in PEFCs

Hidenori Kuroki[1,*]

[1] *Laboratory for Chemistry and Life Science, Institute of Science Tokyo (Former Tokyo Institute of Technology), R1-17, 4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa 226-8501, Japan*

* kuroki@cls.iir.isct.ac.jp

Abstract

We are developing a connected Pt-based nanoparticle catalyst for oxygen reduction reaction (ORR) in polymer electrolyte fuel cells (PEFCs).[1,2] As shown in Figure 1, this catalyst consists of a three-dimentional (3D) nanonetwork formed by the connection of Pt-based nanoparticles with high electrical conductivity. Connected Pt-alloy nanoparticles demonstrate an ORR specific activity about 10 times higher than a conventional Pt/C catalyst. Additionally, we have developed connected core-shell nanoparticle catalysts with a higher surface area. These connected nanoparticle catalysts improve the durability against start/stop and load cycle operations. In this presentation, the ORR activity and durability of 3D connected nanoparticles, as well as the fuel cell performance of the membrane–electrode assemblies using the connected catalysts will be introduced.

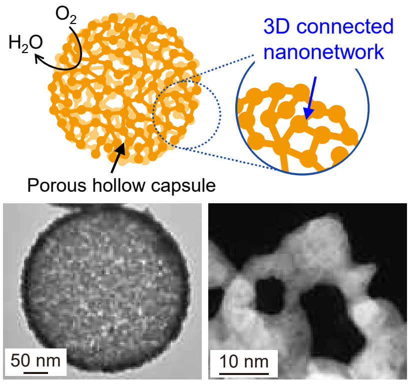


Figure 1. Illustration and TEM/STEM images for a 3D connected nanoparticle catalyst with a porous, hollow-capsule structure.

Keywords: Electrocatalyst, Oxygen Reduction Reaction, Fuel Cell

References

(1) Tamaki, T.; Kuroki, H.; Ogura, S.; Fuchigami, T.; Kitamoto, Y.; Yamaguchi, T. Connected Nanoparticle Catalysts Possessing a Porous, Hollow Capsule Structure as Carbon-Free Electrocatalysts for Oxygen Reduction in Polymer Electrolyte Fuel Cells. Energy Environ. Sci. 2015, 8 (12), 3545–3549, DOI: 10.1039/C5EE02450A

(2) Sudheer, A. C.; Anilkumar, G. M.; Kuroki, H.; Yamaguchi, T. Support-free, Connected Core-shell Nanoparticle Catalysts Synthesized via a Low-temperature Process for Advanced Oxygen Reduction Performances. Adv. Sci. 2025, 12, 2408614, DOI: 10.1002/advs.202408614

Solid oxide electrolysis of CO_2: Power to X

Vipin Kamboj[1,*], Soham Raychowdhury[1], Shivam[1], Chinmoy Ranjan[1]*

[1] *Indian Institute of Science, Bengaluru, 560012, India*

ranjan@iisc.ac.in

Abstract

CO_2 electro-reduction using solid oxide electrodes is one of the most promising technologies for converting CO_2 to fuels (Power to X). CO_2 reducing cathodes such as Ni-YSZ and $MCeO_{2-\delta}$ -YSZ have shown promise in converting CO_2 to CO. In the presence of H_2, these systems are prone to reverse water gas shift reactions and at 800 degrees both electrochemical and thermochemical reactions compete.

Our operando studies will report on Ni-YSZ and Ceria -YSZ based electrodes. $CeO_{2-\delta}$ electrodes perform well in both CO_2 and CO_2 (+H_2) environments. The CO yield increases with increasing negative bias concomitant with increase in the number of Ce^{3+} sites. Our studies will uncouple production of CO by both thermochemical and electrochemical means and how they are correlated through similar active sites. The studies will highlight mechanistic aspects of both CO production and coking. Nature of the active site will be discussed. Unlike purely thermochemical systems, electrochemical systems present an opportunity to control CO and H2 ratios in syngas using simply bias.

Keywords: CO_2 electrolysis, solid oxide electrolysis, operando spectroscopy

References

(1) Enabling pure CO_2 reduction on Ni {Cu} x-YSZ electrode via an oxide-mediated mechanism V Kamboj, S Raychowdhury, C Ranjan, Applied Catalysis B: Environment and Energy 344, 123631

(2) Operando studies on solid oxide ceria electrodes during CO_2 electroreduction V Kamboj, S Raychowdhury, C Ranjan, Applied Catalysis B: Environment and Energy 365, 124880

(3) Cu infiltrated Ni-YSZ cathode in CO2 (+H_2) stream: Reverse water gas shift vs. CO_2 electrolysis V Kamboj, Chinmoy Ranjan, Journal of Power Sources 614 (15), 234985

Modified Current Collectors for Stable Anode-less Lithium/Sodium Metal Batteries

R. Rajasekharan,[1,2] Nilesh Pandey[1], M. M. Shaijumon[1,2*]

[1]*School of Physics, Indian Institute of Science Education & Research Thiruvananthapuram, Maruthamala P. O., Kerala, India, 695 551*
[2]*Centre for Advanced Materials Research with International Engagement (CAMRIE), Indian Institute of Science Education & Research Thiruvananthapuram, Maruthamala P. O., Kerala, India, 695551*
* Email: shaiju@iisertvm.ac.in

Abstract

Lithium/Sodium metal batteries offer great promise towards realizing high energy density devices. However, challenges such as lithium/sodium metal degradation and dendrite growth remain critical, especially when using lean metal anodes. We present some of our recent effrots in exploring efficient strategies toward modifying the current collectors for stable anode-less Li/Na metal batteries. For example, a thin layer of copper selenide grown on commercial Cu foil via chemical vapor deposition and subsequently lithiated to form a Li_2Se matrix with interspersed Cu particles serves an efficient current colletor. During lithium plating, the electroplated lithium is encapsulated within the Cu-Li_2Se matrix in a protective configuration, contrasting the exposed and dendritic lithium deposition observed on bare copper current collectors. This beneficial interface layer facilitates the guided migration of lithium ions toward the base Cu substrate, driven by its negative potential, thereby minimizing direct lithium metal exposure to the corrosive electrolyte. Full cell studies carrie out using LFP cathodes, and carbonate-based electrolytes (without additives) demonstrate superior cycling stability. We further address similar issues in sodium metal batteries through a simple yet effective surface modification using an indium oxychloride coating on the current collector. Formation of an artificial SEI hybrid layer composed of NaIn and sodium oxychloride (Na3OCl) results in enhanced ion diffusion, improved interfacial stability, and space charge regulation to enable uniform dendrite-free sodium deposition. These studies provide insights into interfacial engineering strategies for future solid-state battery designs.

Keywords (max 5): Anode-less batteries, Metal batteries, Current collector modification, Li/Na batteries,

References

(1) Lin, D., Liu, Y. & Cui, Y. Reviving the lithium metal anode for high-energy batteries. Nature Nanotechnology 12, 194–206 2017).
(2) Liu, B., Zhang, J. G. & Xu, W. Advancing Lithium Metal Batteries. Joule 2, 833–845 (2018).
(3) Rajasekharan, Nadarajan, Das, S, Kumar, H., Shaijumon, M. M. Bifunctional Current Collectors for Lean-Lithium Metal Batteries. Adv. Funct. Mater. 2502473 (2025).

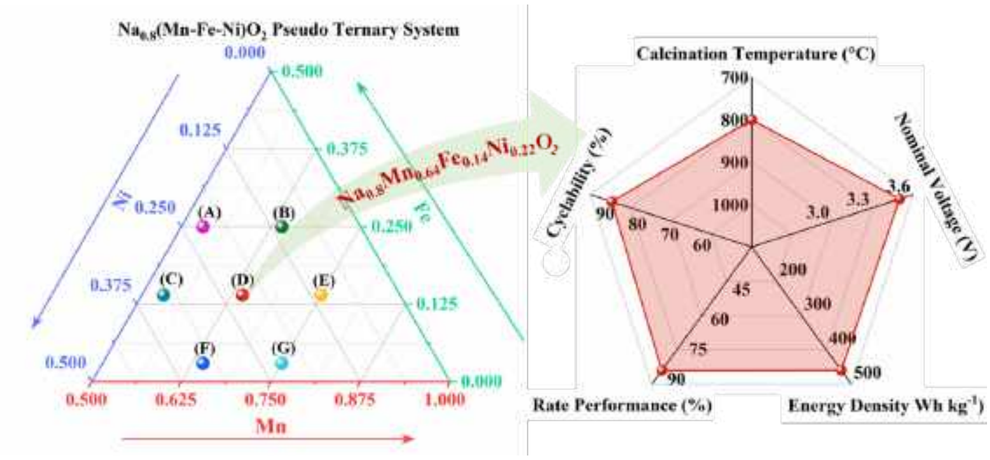
Composition Tuning Effects on the Phase Formation and Electrochemical Performance of $Na_x(Mn\text{-}Fe\text{-}Ni)O_2$ Cathodes

Sunil Kumar[1,*], Samriddhi Saxena[1], Neha Dagar[1], Hari Narayanan Vasavan[1]

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

* sunil@iiti.ac.in

Developing high-performance cathode materials remains a key challenge for cost-effective sodium-ion batteries, especially in achieving high energy density and cycling stability. $Na_x(Mn\text{-}Fe\text{-}Ni)O_2$ system is a promising cathode candidate due to its structural tunability and high voltage redox activity. This talk focuses on the effects of calcination temperature and transition metal composition on the structural, morphological, and electrochemical properties of $Na_x(Mn\text{-}Fe\text{-}Ni)O_2$ layered oxides.[1,2] Samples calcined at different temperatures display diverse phase compositions, including P- and O-type structures. XRD analysis indicates increased Mn content induces biphasic P2/O3 behavior, while Ni-rich compositions have a contracted *c* parameter. The P2/O3-type $Na_{0.8}Mn_{0.53}Fe_{0.14}Ni_{0.33}O_2$, calcined at 900 °C, achieves the highest specific discharge capacity (~139 mAh g^{-1}). $NaMn_{0.500}Fe_{0.125}Ni_{0.375}O_2$ achieves a high specific capacity of ~149 mAh g^{-1}, while $NaMn_{0.500}Fe_{0.250}Ni_{0.250}O_2$ exhibits superior rate capability (85.7% capacity at 1C and 69.7% at 3C, compared to 0.1C). The biphasic $NaMn_{0.625}Fe_{0.125}Ni_{0.250}O_2$ (MFN-512) retains 93% of its initial capacity after 100 cycles and delivers a specific capacity of ~92 mAh g^{-1} and a nominal voltage of ~2.9 V at a 0.1C in a full-cell with hard carbon anode, highlighting its practical applicability. *Operando* Synchrotron XRD further reveals reversible phase transformations in MFN-512.



Optimized composition in $Na_{0.8}(Mn\text{-}Fe\text{-}Ni)O_2$ system yields superior properties

Keywords: Na-ion Battery Cathodes, Layered Oxides, Electrochemical Behavior

References

(1) S. Saxena et al., Battery Energy, e70018 (2025)

(2) S. Saxena et al., Journal of Power Sources, 644: 237115 (2025)

Effect of particle morphology of as prepared sulfur on the electrochemical performance of Li-S batteries

Subhasish Basu Majumder[1], Debayan Chatterjee[2], Udita U. Ghosh[3]

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

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

[3] *Affication-2, Department of Chemical Engineering & Technology, Indian Institute of Technology (BHU) Varanasi*

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

Lithium-sulfur batteries are identified as one of the most promising rechargeable energy systems due to their high theoretical capacity (1675 mAh/g), high gravimetric energy density (2600 Wh/Kg), low cost and low environmental impact. 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.). Keeping all this points in consideration we are proposing an efficient, cost-effective measure to prepare CTAB (a cationic surfactant)-assisted submicrometer-sized sulfur particle. Suitability of CTAB as a surfactant in this process is assessed prior to this via sessile droplet contact angle measurements with myriad surfactants (CTAB, PVP, TWEEN 20 etc.) representing anionic, cationic and non-ionic groups. A correlation between the synthesized sulphur particle morphology with the employed surfactant range is also attempted and CTAB is found to exhibit the highest reduction in contact angle and thereof is chosen as the suitable surfactant for this study. This as synthesized sulfur particles are mixed with super P conductive carbon black and an aqueous binder to form a slurry which is to be 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 poly sulfides (Li_2S_n, $4 \leq n \leq 8$) which improves the cyclability, rate performance, above all helps to extinguish the polysulfide shuttle effect. 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, CTAB, E/S ratio, cathodes

Design and Development of Electrode Materials for Li- and Na-ion Batteries: From Lab-Scale Innovation to Demonstration

Srinivasan Anandan
Centre for Advanced Materials & Batteries, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Balapur, Hyderabad, Telangana, India.
Email: anandan@arci.res.in

Translational research plays a crucial role in moving scientific innovations from the laboratory to real-world applications, particularly in strategic sectors such as energy storage. With India's rapidly expanding electric mobility and renewable energy landscape, the demand for indigenous, scalable, and commercially viable energy storage technologies has never been greater. This presentation highlights ARCI's efforts for the development, demonstration, and technology transfer of lithium-ion batteries (LIBs) and Na-ion batteries (NIB) materials. The first part of the presentation highlights ARCI's development of indigenous electrode material technologies for domestic LIB manufacturing. Lithium iron phosphate (LFP) is a preferred cathode chemistry owing to its intrinsic safety and strong thermal stability arising from robust P–O bonding, which prevents self-oxidation and thermal runaway. ARCI has developed a cost-effective high-energy milling process for synthesizing in-situ carbon-modified LFP (C-LFP), with 15–20 kg batch-scale production successfully demonstrated and validated at the cell level. Patents have been filed in India and internationally, and the technology has been transferred to M/s. Allox Minerals (India) and M/s. ALTMIN (Global & India). A 250 kg/day pilot plant has been established by M/s. ALTMIN at the ARCI incubator. Additionally, M/s. ALTMIN laid the foundation for its new plant recently, and the facility is expected to begin operations by Q4 2026, producing 20,000 MTPA of LFP CAM & meeting about 20% of India's projected LFP cell demand by 2028.

The second part of the presentation highlights ARCI's development of NVP and hard carbon materials for Na-ion batteries. $Na_3V_2(PO_4)_3$ (NVP) is a NASICON-type cathode for sodium-ion batteries, featuring a stable 3D framework with fast Na^+ diffusion. It operates at ~3.4 V (V^{3+}/V^{4+} redox) with a theoretical capacity of ~117 mAh g^{-1}, offering excellent cycling stability and safety. NVP synthesized by high energy milling using N,V, and P precursors at 1kg batch and subsequently calcined at 800oC under inert atm. The resulting pure NVP material delivers specific capacity of 110-115mAh/g with good rate capability and excellent cyclic stability retention (>80%) after 200 cycles. Currently, the up-scaling of the process for 20 kg batch is in progress and validation of material at pouch cell level is in progress. Hard carbon is considered a promising anode material for sodium-ion batteries due to its larger interlayer spacing (>0.35 nm), tunable microstructure, low specific surface area, and hierarchical porosity, which collectively facilitate efficient Na^+ storage and diffusion [1]. Further, ARCI also focus on synthesis of hard carbon (HC) using coconut husk biomass by . high-temperature carbonization at 1400 °C for 2 h under an inert atmosphere. The electrochemical performance is evaluated in a half-cell configuration vs. Na/Na^+ using 1 M $NaClO_4$ in EC:PC (1:1 vol%) electrolyte. Galvanostatic charge–discharge studies demonstrate specific capacities of 233, 142, 101, 48, and 33 mAh g^{-1} at current densities of 20, 50, 100, 500, and 1000 mA g^{-1}, respectively. Furthermore, the electrode exhibits good cycling stability with >80% capacity retention after 50 cycles at 50 mA g^{-1}. Further insights and technical details will be presented during the talk.

Development of Sodium-ion batteries for energy storage

Rajendra S. Dhaka

Department of Physics, Indian Institute Technology Delhi,
Hauz Khas, New Delhi-110016, India

* Corresponding author's email address: rsdhaka@physics.iitd.ac.in

Abstract

In recent years, energy storage devices especially rechargeable batteries have become part of our daily life in portable electronic devices like mobiles, laptops as well as being used at large scale in electrical vehicles (EV), etc. Among various types of batteries, the only commercially established and feasible technology is based on Li-ion intercalation, mainly due to the advantage of its high energy density, good rate kinetics and light weight. However, the main concern comes from the limited availability and uneven distribution of Li in the earth crust. This motivates researchers to search for alternative avenue, and the Na-ion batteries are one of the potential candidates particularly for grid level storage due to its low cost and abundance on the globe, and therefore extensive research has been started in this field over past few years [1]. In this direction, it is vital to find suitable and high-performance electrode materials. However, there are many challenges due the larger size of the Na-ion as compared to the Li. Therefore, constant efforts are going on to search new electrode materials (negative as well as positive) for improving the electrochemistry. Recently, we have developed few cathode and anode materials and tested their electrochemical performance to understand the diffusion kinetics, stability, rate capability and coulombic efficiency in sodium ion batteries [2-10]. In the talk, I will present some of our effort towards development of cost-effective/high-performance sodium-ion batteries for energy storage applications.

References

[1] S. K. Sapra, J. Pati, P. K. Dwivedi, Suddhasatwa Basu, J.-K. Chang, and **R. S. Dhaka***, WIREs Energy and Environment **10**, e400 (2021).

[2] P. K. Dwivedi, S. K. Sapra, Jayashree Pati, and **R. S. Dhaka***, ACS Appl. Energy Materials **4**, 8076 (2021).

[3] J. Pati, Hari Raj, S. K. Sapra, Anita Dhaka, A. K. Bera, S. M. Yusuf, and **R. S. Dhaka***, Journal of Materials Chemistry A **10**, 15460 (2022).

[4] M. K. Singh, J. Pati, D. Seth, J. Prasad, M. Agrawal, M. Ali Haider, J.-K. Chang, & **R. S. Dhaka*** Chemical Engineering Journal **454**, 140140 (2023).

[5] Jayashree Pati, and **R. S. Dhaka***, Journal of Power Sources **609**, 234646 (2024).

[6] S. K. Sapra, J.-K. Chang, and **R. S. Dhaka***, ACS Appl. Mater. Interfaces **16**, 43535 (2024).

[7] S. K. Sapra, M. Das, M. W. Raja, J. -K. Chang, and **R. S. Dhaka***, J. of Materials Chem. A **13**, 1996 (2025).

[8] Madhav Sharma, Riya Gulati, and **R. S. Dhaka***, Coord. Chem. Rev. **543**, 216912 (2025).

[9] S. K. Sapra, J.-K. Chang*, and **R. S. Dhaka***, Energy Storage Materials xx, xxxx (2025) accepted.

[10] Madhav Sharma and **R. S. Dhaka***, Small **21**, 2505200 (2025).

Reactive Interfaces for Ambient Pressure Anodeless Solid-state Batteries

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

[1] *Department of Chemistry, Indian Institute of Technology Bombay, Powai, India*

* srini@chem.iitb.ac.in

Abstract

Solid-state Li batteries are considered as promising advancements to Li-ion batteries due to their superior energy density and safety. Moreover, these batteries in the 'anodeless' configuration can further boost volumetric energy density by minimizing dead volume in the cell. The application of NASICON type ceramics ($Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$/ $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$) as the solid electrolyte (SE) is preferred over oxide-based ceramics such as LLZO due to the higher ionic conductivity at ambient conditions of the former. However, their practical implementation in SSBs presents challenges due to their anodic instability against reduction by Li metal. Herein, we present a surface engineering approach for the Cu current collector by introducing a porous reactive layer through a simple solution based chemical etching protocol. Over successive Li plating/stripping cycles this reactive layer forms a passivating film by reacting with the deposited Li in an anodeless solid-state configuration. The post cycling characterization showed that the Li plating/stripping cycles leads to an Li_2O and LiF rich surface, which results in a significant boost in Coulombic efficiency and cycling performance at ambient pressure and temperature.

Keywords: Solid-state batteries, Interfacial Passivation, Anodeless,

References

(1) Pahari, P; Ramakrishnan, S; 10.26434/chemrxiv-2025-7jc1f

Reinforcing a Lithium-ion Battery Cathode (NCA) with Mn Doping

Swati Panigrahi[1], Kothandaraman Ramanujam[1,2,*]

[1] *Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036*

[2] *Adjunct Faculty, University of Southern Queensland, Australia*

* rkraman@iitm.ac.in

Abstract

Nickel-rich layered oxide cathodes have emerged as one of the leaders for next-generation lithium-ion batteries (LIBs), offering high energy density and a relatively lower cobalt content. However, challenges such as cation mixing, structural degradation, and poor cycle retention persist. In this study, we systematically investigate the effect of controlled manganese (Mn) substitution in a NCA cathode materials synthesized via a solid-state route, targeting enhanced structural and electrochemical stability. XRD, Rietveld and TEM analyses confirm single-phase layered α-$NaFeO_2$-type structures with decreasing phase purity and increasing c/a ratios at high Mn content ($x \geq 0.2$), indicating an increased cation disorder in the samples with increasing Mn contents. Mn introduction affects oxidation states of both Ni and Co leading to defects in the structure. Besides, due to Jahn-Teller distortion, particles undergo pulverization with the introduction of Mn. The presence of excess of Mn on the particle surface is confirmed with EELS. The sample with $x = 0.1$ (NMCA-1) demonstrated the optimal balance, exhibiting minimal lattice strain (0.0004%), the smallest crystallite size (~50 nm), and comparable structural integrity with an I(003)/I(104) ratio of 1.25. Electrochemically, NMCA-1 delivered the highest capacity retention (~85% after 100 cycles at 0.2C), outperforming both undoped NCA (~70%) and fully Mn-substituted NMA (~45%). Despite a slight reduction in initial capacity (137 mAh g^{-1}), NMCA-1 exhibited superior rate capability (77 mAh g^{-1} at 2C) and reduced overpotential growth, confirmed by CV and EIS analyses. Our findings highlight the synergistic effect of Mn and Al co-doping in optimizing cathode performance by tuning structural strain, mitigating phase degradation, and enhancing long-term cycling behaviour. This approach offers a cost-effective and scalable strategy to engineer high-performance cathode materials for future LIB applications.

Keywords: NCA cathode, Li-ion battery, Anti-site defect, Covalency enhancement

References:

(1) Wan, D. Y.; Fan, Z. Y.; Dong, Y. X.; Baasanjav, E.; Jun, H.-B.; Jin, B.; Jin, E. M.; Jeong, S. M. Effect of Metal (Mn, Ti) Doping on NCA Cathode Materials for Lithium Ion Batteries. *Journal of Nanomaterials* **2018**, *2018*, 1–9. https://doi.org/10.1155/2018/8082502.

(2) Wang, B.; Zhang, F.; Zhou, X.; Wang, P.; Wang, J.; Ding, H.; Dong, H.; Liang, W.; Zhang, N.; Li, S. Which of the Nickel-Rich NCM and NCA Is Structurally Superior as a Cathode Material for Lithium-Ion Batteries? *J. Mater. Chem. A* **2021**, *9* (23), 13540–13551. https://doi.org/10.1039/D1TA01128F

Solvation Thermodynamics and its Impact on Electrolyte Properties and Lithium Battery Performance

Sang Cheol Kim[1*]

[1] *Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore 117585, Singapore*

* Corresponding author's email address: sckim@nus.edu.sg

Abstract

The electrolyte plays a critical role in lithium batteries. In particular, Li ion solvation critically impacts electrolyte properties and the battery performance. Solvation thermodynamics is at the foundation of solvation phenomena, but our understanding of it and how it impacts solvation structure, electrolyte properties and the battery performance remains elusive. In this talk, I will begin by introducing experimental methods to probe solvation free energy and solvation entropy. Then I will discuss our recent works on how solvation free energy impacts important electrolyte properties and battery performance metrics in two important next-generation battery systems: lithium metal batteries and lithium-sulfur batteries. We find that solvation free energy impacts the voltage profile and polysulfide solubility in Li-S batteries. We also find correlations between solvation free energy and ion transport properties of Li metal battery electrolytes. I will conclude by summarizing the relationships between solvation thermodynamics, solvation structure and electrolyte properties for Li battery electrolytes.

Keywords: Battery, electrolytes, solvation, thermodynamics

References

(1) Kim, S. C., Pan, J.-A., Shah, A., Chen, Y., Park, H., Yang, Y., Zhang, W., Greenburg, L. C., Sogade, T., Chen, A., Qin, J., Bao, Z. & Cui, Y. Correlating Solvation Free Energy to Electrolyte Properties for Lithium Metal Batteries. Nano Letters 25, 4673-4680 (2025).

(2) Kim, S. C., Gao, X., Liao, S.-L., Su, H., Chen, Y., Zhang, W., Greenburg, L. C., Pan, J.-A., Zheng, X., Ye, Y., Kim, M. S., Sayavong, P., Brest, A., Qin, J., Bao, Z. & Cui, Y. Solvation-property relationship of lithium-sulphur battery electrolytes. Nature Communications 15, 1268 (2024).

(3) Kim, S. C., Kong, X., Vilá, R. A., Huang, W., Chen, Y., Boyle, D. T., Yu, Z., Wang, H., Bao, Z., Qin, J. & Cui, Y. Potentiometric Measurement to Probe Solvation Energy and Its Correlation to Lithium Battery Cyclability. Journal of the American Chemical Society 143, 10301-10308 (2021).

Predicting migration barriers in battery materials

Sai Gautam Gopalakrishnan[1,*], Reshma Devi[1], Keith T. Butler[2]

[1] *Department of Materials Engineering, Indian Institute of Science, Bengaluru 560012, India*

[2] *Department of Chemistry, University College London, London WC1E 6BT, United Kingdom*

* saigautamg@iisc.ac.in

Abstract

The rate performance of a given material that is used as an electrode or a solid electrolyte in a battery is a critical metric determining the commercial viability of the corresponding battery technology. In turn, rate performance in solids is significantly influenced by the activation energy required for ion migration (E_m) between crystallographic sites. Traditional computational methods for estimating E_m, such as density functional theory based nudged elastic band calculations or ab-initio molecular dynamics simulations, are typically constrained by computational challenges, including convergence issues and the demands associated with sampling larger length/longer time scales, respectively. To mitigate these limitations, we introduce a graph neural network based machine learning (ML) approach designed to efficiently and accurately predict E_m, leveraging the framework of transfer learning. Specifically, we fine-tune (FT) a model that has been simultaneously pre-trained on seven distinct bulk material properties across a wide range of materials, on a manually curated dataset comprising 619 E_m values from literature. Our FT model demonstrates substantial improvements in prediction accuracy compared to traditional statistical ML methods and models trained from scratch (i.e., without any pre-training), and is able to effectively distinguish multiple migration pathways within a given structure. Ultimately, we expect our FT model to accelerate material screening efforts, particularly for the discovery of novel electrode and electrolyte materials for advanced batteries.

Keywords: Electrodes, Solid electrolytes, Migration barrier, Machine learning, Transfer learning

Tuning Ion Transport and Host Interactions in Beyond-Lithium Ion Storage: Insights from First-Principles Simulations

Swastika Banerjee,*, Shweta Choudhary, Vikas Singh Thakur
Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand 247667, India
* *swastika.banerjee@cy.iitr.ac.in*

Abstract

As the demand for scalable and sustainable energy storage grows, beyond-Li chemistries such as sodium, potassium, and magnesium are gaining momentum due to their abundance and complementary electrochemical properties. In this work, we leverage first-principles simulations to uncover fundamental mechanisms that govern ion transport and storage in non-Li systems. In complex borohydride-based solid electrolytes, we reveal that Na^+ and K^+ migration is highly sensitive to the local coordination geometry and steric constraints, offering a design lever through cation–framework interactions. For sodium-ion anodes, we demonstrate that graphullerene frameworks support efficient electron injection and stable NaC_2 cluster formation, yielding reversible and high-capacity storage—a distinct mechanism compared to intercalation or alloying. For multivalent systems, we design layered Mg-hosts with enhanced rigidity using linker engineering, which significantly lowers Mg^{2+} diffusion barriers and improves insertion thermodynamics. These findings collectively showcase how chemical design, orbital interactions, and host lattice control can enable effective Na^+, K^+, and Mg^{2+} transport, pushing the frontier of next-generation, post-Li energy storage materials.

Keywords: Beyond-Li storage, Sodium-ion battery, Potassium transport, Magnesium mobility, Computational design

References

(1) Choudhary, S.; Banerjee, S. *Commun. Chem.* 2025, 8, 123.
(2) Banerjee, S.; Tkatchenko, A. *Nat. Commun.* 2025, 16, 1672.
(3) Choudhary, S.; Saroha, R.; Banerjee, S. *ACS Appl. Mater. Interfaces* 2024, 16(38), 50859–50869.
(4) Thakur, V. S.; Banerjee, S. *J. Phys. Chem. C* 2024, 128(19), 7865–7875.

Designing Cathode Materials for Li-Ion and Na-Ion Batteries Using Advanced Computational Methods

Mudit Dixit[1,*]

[1] *CSIR-Central Leather Research Institute (CSIR-CLRI), Sardar Patel Road, Adyar, Chennai 600020, India*

* muditdixit@clri.res.in, dixitmuditk@gmail.com

Abstract

In this talk, I will present our recent efforts to stabilize and understand layered metal oxide cathodes for Li-and Na-ion batteries, with a particular focus on anionic redox and the inherent trade-offs between structural stability and capacity. Guided by first-principles calculations, we validate our predictions through targeted experiments in collaboration with experimental groups, offering key insights into phase stability under cycling conditions. I will also highlight the use of Machine Learning Interatomic Potentials (MLIPs) as a powerful tool for accelerating materials discovery. We critically evaluate their application in single-atom catalysis and Li–S batteries, especially in modeling polysulfide binding, while also discussing the limitations and failure modes of MLIPs when extrapolating beyond their training domains. Shifting focus to sodium-ion batteries, I will present the design of a series of layered transition metal oxide cathodes where anionic redox mechanisms hold the promise of achieving high capacities. Through electronic structure engineering, our goal is to develop materials that not only exhibit reversible anionic redox activity but are also stable in air and moisture, including novel multi-component compositions. Our findings contribute to a deeper fundamental understanding and provide valuable guidance for experimental efforts aimed at enhancing existing materials and designing next-generation cathode materials

Keywords: Cathode materials, Li-ion battteries, DFT, Computational modeling, Li-S chemistry

References

1. Singh, P.; Dixit, M. *J. Phys. Chem. C* 2024, 128 (22), 8883–8893
2. Singh, P.; K R, A. M.; Dixit, M. *ACS Appl. Electron. Mater.* 2024, *6* (10), 7065–7074
3. Singh, P.; Dixit, M. Langmuir 2023, 39 (1), 28–36.

Atomistic Understanding of Electrode Materials for High-Performance Alkali-Ion Batteries

Zubair Nabi[1], Priya Johari[1*]

[1] *Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Greater Noida, Gautam Buddha Nagar, Uttar Pradesh – 201314 India;*

* priya.johari@snu.edu.in

Abstract

The development of computational resources and methodologies has become a cornerstone in the quest to reliably predict promising electrode materials for rechargeable batteries, offering a cost-effective and time-efficient alternative to traditional experimental methods. These advancements provide valuable insights for experimentalists, guiding efforts to enhance battery performance and pave the way for next-generation, energy-efficient batteries with improved electrochemical behaviour, crucial for grid storage and electric vehicles. In this context, we employ first-principles density functional theory and evolutionary algorithms to conduct a comprehensive investigation of promising materials. Our aim is to gain an atomistic-level understanding of the reaction mechanism and identify efficient electrode materials for alkali-ion batteries, contributing to the evolution of cutting-edge energy storage technologies.

Keywords (max 5): first-principles calculations, electrode materials, next-generation alkali-ion batteries, electrochemical analysis

Plating Dynamics in Sodium Metal Anodes: Linking Molecular Interactions to Macroscopic Stability

Kingshuk Roy[1,*],

[1] *aResearch Institute for Sustainable Energy, TCG Centres for Research and Education in Science and Technology, Salt Lake, Kolkata 700091, West Bengal, India*

email address: kingshuk.roy@tcgcrest.org

Abstract

The promise of sodium metal batteries, particularly anode-less configurations, rests on mastering one deceptively simple event: the first nucleation of sodium on a bare substrate. Yet, this event is governed by a complex web of interfacial kinetics, solvation chemistry, nucleation energetics, and evolving interphases. This talk will present a ground-up exploration of sodium metal anode stability, integrating molecular-level electrolyte behavior, current collector surface chemistry, and spatially modulated ion flux. This talk will begin with probing the interfacial charge transfer kinetics and solvation-desolvation dynamics using fast-scan voltammetry, capturing transient plating behavior in real time. By combining variable-temperature nuclear magnetic resonance, Raman spectroscopy, and several other fundamental material and electrochemical characterization techniques across length and time scales, this talk will help uncover how solvation asymmetry and mobility dictate desolvation energetics and SEI evolution. These insights are distilled into mechanistic descriptors that quantify electrolyte efficacy. Building on this, the talk will also demonstrate how spatially engineered sodiophilic domains engineer sodium ion flux and stabilize deposition morphology. Various degrees of post-cycling in-situ measurements will reveal that edge-localized electric fields and chemical defects can guide uniform plating and suppress dendrites. Together, these findings reframe the problem of Na metal stability; not as a materials limitation, but as an interfacial design challenge, solvable through a unified, multiscale strategy linking molecules to morphology.

Keywords: Sodium Metal Anode, Interfacial Kinetics, Desolvation Dynamics, Spatial Ion Flux Engineering, Multiscale Characterization

Li–Organopolysulfide Batteries: Opening New Avenues in Battery Chemistry

Dr. Sattwick Haldar[1*], Prof. Xinliang Feng[2], Prof. Stefan Kaskel[1*]

[1] *IIT Tirupati, Chemistry Department, Andhra Pradesh, India*

[2] *Technical University Dresden, Inorganic Chemistry Department, Bergstr. 66, Dresden, Germany*

*Email Id: sattwick07@iittp.ac.in

Abstract

Chalcogenide electrodes—particularly those based on the highly abundant and low-cost sulfur—hold immense promise for developing lightweight, high-energy batteries suited for next-generation aviation technologies. Yet, this class of batteries still faces practical challenges, primarily due to slow charging rates caused by poor conductivity and degradation from the solubility of sulfur in the electrolyte, limiting their durability and cycle performance. Among several strategies explored, using conducting host materials to trap sulfur has shown notable success, but this often comes at the cost of reduced practical energy density, as the inactive mass of the host adds to the overall weight of the battery. To address this, we developed a smart approach by covalently integrating charge-storing sulfur directly into charge-storing host materials, enabling the host to compensate for theoretical energy loss. Our design transforms the traditionally inactive host into an electrochemically active component. This enhances charge transport and enables fast charging through efficient electronic communication between insulating sulfur and semiconducting or conducting polymers. We realized this advantage with novel sulfur-linked organic polymers, and verified the underlying mechanism using a custom operando Raman setup. The resulting cell, assembled with a lithium counter electrode, significantly outperformed conventional Li–S batteries—earning the name Li-Organopolysulfide battery. This innovation paves the way for a new class of various Metal–Organopoylchalcogenide batteries, such as Li-Organopoylselenide and Na–Organopolysulfide systems, with viable device-level performance. We are now actively working to scale this lab-level breakthrough toward industrial relevance, with ongoing studies to evaluate and mitigate the system's limitations.

Keywords: Sulfur, Metals, Organopolysulfides, Battery, Mechanism.

References

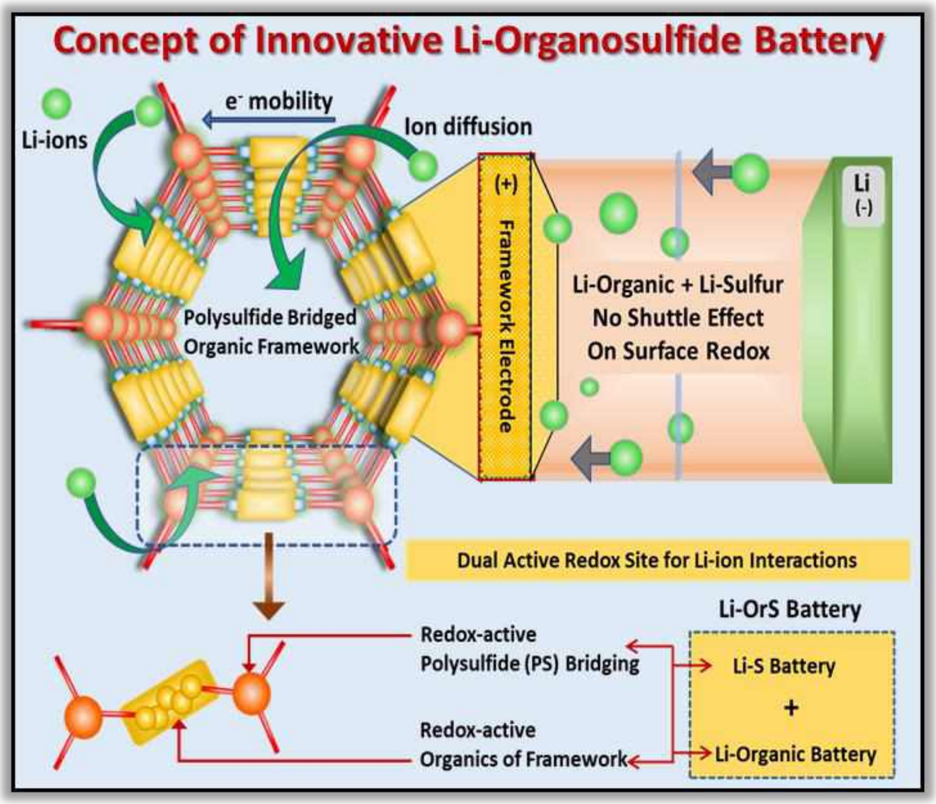
(1) Haldar, S.; Waentig, A. L.; Ramuglia, A. R.; Bhauriyal, P.; Khan, A. H.; Pastoetter, D. L.; Isaacs, M. A.; De, A.; Brunner, E.; Wang, M.; Heine, T.; Weidinger, I. M.; Feng, X.; Schneemann, A.; Kaskel, S. Covalent Trapping of Cyclic-Polysulfides in Perfluorinated Vinylene-Linked Frameworks for Designing Lithium-Organosulfide Batteries. *ACS Energy Lett.* **2023**, 8 (12), 5098–5106. https://doi.org/10.1021/acsenergylett.3c01548.

(2) Haldar, S.; Bhauriyal, P.; Ramuglia, A. R.; Khan, A. H.; Kock, S. D.; Hazra, A.; Bon, V.; Pastoetter, D. L.; Kirchhoff, S.; Shupletsov, L.; De, A.; Isaacs, M. A.; Feng, X.; Walter, M.; Brunner, E.; Weidinger, I. M.; Heine, T.; Schneemann, A.; Kaskel, S. Sulfide-Bridged Covalent Quinoxaline Frameworks for Lithium-Organo-Sulfide Battery. Adv. Mater. **2023**, 35, 2210151. https://doi.org/10.1002/adma.202210151.

(3) Haldar, S.; Schneemann, A.; Kaskel, S. Covalent-Organic Frameworks as Model Materials for Fundamental and Mechanistic Understanding of Organic Battery Design Principles*. J. Am. Chem. Soc.* **2023**, 145 (25), 13494–13513. https://doi.org/10.1021/jacs.3c01131.

(4) Haldar, S.; Wang, M.; Bhauriyal, P.; Hazra, A.; Khan, A. H.; Bon, V.; Isaacs, M. A.; De, A.; Shupletsov, L.; Boenke, T.; Grothe, J.; Heine, T.; Brunner, E.; Feng, X.; Dong, R.; Schneemann, A.; Kaskel, S. Porous Dithiine-Linked Covalent Organic Framework as a Dynamic Platform for Covalent Polysulfide Anchoring in Lithium–Sulfur Battery Cathodes. *J. Am. Chem. Soc.* **2022**, 144 (20), 9101–9112. https://doi.org/10.1021/jacs.2c02346.

(5) Haldar, S.; Khan, A. H.; De, A.; Reichmayr, F.; Morag, A.; Yu, M.; Schneemann, A.; Kaskel, S. Fluorinated Benzimidazole-Linked 2D-Conjugated Polymer Enabling Covalent Polysulfide Anchoring for Stable Sulfur Batteries. *Chem. Eur. J.* **2024**, 30, e202302779. https://doi.org/10.1002/chem.202302779.



$Fe–N_4–O_2$ and $Mn–N_4–C≡N$ Single-Atom Incorporated Anodes for Sodium-Ion Storage and Transport with Hollow Diffusion Sites

Saikat Dutta[1,*], Anubha Yadav[1]

[1] Electrochemical Energy & Sensor Research Laboratory
Amity Institute of Click Chemistry Research & Studies
Amity University Uttar Pradesh, Noida, India, E-mail: sdutta2@amity.edu

Abstract

Sluggish diffusion kinetics of Na^+-ion drastically restrain the rate capability and capacitance of anode for sodium-ion batteries (SIBs). Herein, we report a unique process to access a single-Fe-atom incorporated anode material $Fe–N_4$-O_2–WNC from delignified wood for coin cell SIBs to address the above challenges. The charging Na^+-ion through $Fe–N_4–O_2$–WNC anode was revealed by electrochemical capacitive and charge-discharge studies to establish a reversible conversion and diffusion of Na^+-ion supported by theoretical calculation of Na^+-ion migration energy (eV) against the diffusion path. $Fe–N_4–O_2$–WNC anode, assembled with sodium foil as counter electrodes in coin cell, exhibits the discharge-specific capacity of 140 $mAhg^{-1}$ at a current density of 100 mAg^{-1}. The diffusive behavior of $Fe–N_4–O_2$–WNC reveals a diffusion coefficient 10^{-8} to 10^{-10} cm^2 s^{-1} within a 0.01–3.0 V voltage. The GITT profile, EIS, and post-cycling analysis support the role of Fe–N bonding in modulating the electronic environment of Na^+-ion diffusion sites. The incorporation of $Fe–N_4–O_2$ in WNC results 1) faster Na^+-ion diffusion through hollow (H) sites, 2) stretching of Fe–N bond during discharge cycles supported by the DFT analysis. In addition, $Fe–N_4–O_2$–WNC anode promises for manufacturing of advanced SIBs from a renewable material, and thereby enhancing investigation of sodiophilic Fe–N sites, and factors suppressing the Na-dendrite formation. $Mn–N_4–C≡N$ single-Atom incorporated anode also exhibits interesting Na^+/electron transport features based on the $Mn–N_4$ and -C≡N sites. We will reveal the role of isolated single metal-atoms and diffusion sites based on X-rab absorption spectra, electrochemical performance in coin-cells and densty functional theory (DFT) for pushing the discharge-specific capacity and rate capability of our coin-cell SIBs.

Keywords (max 5): Single $Fe–N_4–O_2$, Na^+-ion diffusion path, Na^+-intercalated hollow sites, Mn-single-atom, SIB coin-cell.

References

(1) Wang, Y.; Yi, Z.; Xie, L.; Mao, Y.; Ji, W.; Liu, Z.; Wei, X.; Su, F.; Chen, C.-M. *Adv. Mater.* **2024**, *36*, 2401249.

(2) Liu, P.; Miao, L.; Sun, Z.; Chen, X.; Jiao, L. *Adv. Mater.* **2024**, *36*, 2406058.

(3) Patil, R.; Wu, K.; Salunkhe, R.; Dutta, S.* et al. 2025 (unpublished results, submitted).

(4) Yadav, A.; Wu, K.; Dutta, S.* et al. (unpublished results, submitted).

From Unstoppable Electrons in Unlikely Alloys to Hydrogen Harmony

Sayan Bhattacharyya*

Department of Chemical Sciences, and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur - 741246, India

*Email address: sayanb@iiserkol.ac.in

The recent literature is abundant with earth-abundant electrocatalysts that have shown the ability to surpass the noble metal benchmark for driving the redox reactions such as water splitting for green hydrogen generation, carbon dioxide reduction to value added fuels and nitrogen reduction to ammonia. A successful architecture of these multi-metallic electrocatalysts relies on the overall electronic structure, optimization of the active centers, elemental ratio, heterogeneous localization of the elements, coordination environment, shape and size of the nanostructures, and the atomic scale defects. However, alloying the metals with dissimilar crystal structures and unmatched crystallographic facets is a non-trivial task. Therefore, an effective multi-metallic catalyst design needs a substantial all-round knowledge of chemistry, especially the branches of basic inorganic chemistry and solid state chemistry, besides electrochemistry. This lecture will highlight a part of our efforts in making the multi-metallic heterogeneous alloys having immiscible lattices of the metal components for water electrolysis.[1-5] Our electrocatalysts are typically composed of two metals that mutually tune the electronic structure to have a profound impact on the overall catalytic activity.[6-8]

Keywords: ELectrocatalyst, Bimetallic alloy, Electronic structure, Water electrolysis, Industrial scale

References

(1) Parvin, S.; Maji, M.; Majee, R. *ACS Catal*. **2025**, Accepted.

(2) Mondal, S.; Dutta, S.; Hazra, V.; Pati, S. K.; Bhattacharyya, S. *Nano Lett*. **2025**, *25*, 1296-1304.

(3) Maji, M.; Dutta, S.; Jena, R.; Dey, A.; Maji, T. K.; Pati, S. K.; Bhattacharyya, S. *Angew. Chem. Int. Ed*. **2024**, *63*, e202403697.

(4) Mondal, S.; Dutta, S.; Mal, S.; Pati, S. K.; Bhattacharyya, S. *Angew. Chem. Int. Ed*. **2023**, *62*, e202301269.

(5) Parvin, S.; Bothra, N.; Dutta, S.; Maji, M.; Mura, M.; Kumar, A.; Chaudhary, D. K.; Rajput, P.; Kumar, M.; Pati, S. K; Bhattacharyya, S. *Chem. Sci.* **2023**, 14, 3056-3069.

(6) Majee, R.; Kumar, A.; Das, T.; Chakraborty, S.; Bhattacharyya, S. *Angew. Chem. Int. Ed*. **2020**, *59*, 2881-2889.

(7) Parvin, S.; Kumar, A.; Ghosh, A.; Bhattacharyya, S. *Chem. Sci*. **2020**, *11*, 3893-3902.

(8) Sahasrabudhe, A.; Dixit, H.; Majee, R.; Bhattacharyya, S. *Nat. Commun*. **2018**, *9*, 2014.

Electrochemical Transformation of Pollutants to Value-Added Chemicals

Sangaraju Shanmugam,*

Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology (DGIST), Daegu, South Korea

* E-mail: sangarajus@dgist.ac.kr

Abstract

Single-atom catalysts have garnered significant attention in electrocatalysis due to their maximized atomic utilization, adjustable metal centers, and diverse coordination environments. Their key advantage stems from the fully exposed active sites, facilitating strong interactions with neighboring coordination atoms, thereby affording exceptional activity and stability to the single-atom catalysts. I will focus on our recent efforts to promote the single-atom catalyst's performance in electrochemical transformation of gas and water pollutants into value-added products (Fig.1). The synthesis and characterization of metal catalytic sites anchored on porous graphitic nanospheres [1] and Cu nanowires in multichannel carbon nanorods catalyst will be discussed [2,3]. Finally, their potential applications in single-cell electrolysis of NO to NH_3 and primary Zn-NO batteries will be presented.

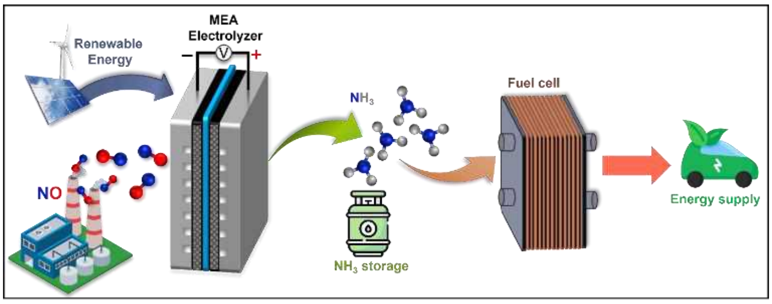


Fig. 1 Schematic of NH_3 economy that contains carbon-free fuel generation from the air pollutant NO utilized by the sustainable energy-driven electrolyzer and the produced NH_3 is used as energy supply.

Keywords: Electrocatalysis, Energy Storage, Ammonia, C-free fuels, Hydrogen

References

[1] Markandaraj, S.S,; Dhanabal, D.; Shanmugam, S, *J. Mater. Chem. A* 2023, 11, 23479.
[2] Dhanabal, D.; Markandaraj, S,S.; Shanmugam, S, *ACS Catal.*, 2023, 13, 9136.
[3] Dhanbal, D.; Song, Y,; Jang, J.S.; Shanmugam, S, *Appl. Catal.*, B 2025, 287, 119952.

Enhancing Hydrogen Evolution at Lower Potentials via Developing New Catalysts for Alternative Anodic Oxidation Reactions

Di-Yan Wang*

[1] *Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan*

* *diyanwang@ntnu.edu.tw*

Abstract

Traditional water electrolysis faces the challenge of high potential from the oxygen evolution reaction (OER). This research aims to reduce energy demand and increase hydrogen production efficiency by using the iodide oxidation reaction (IOR) and urea electrooxidation reaction (UOR) as alternative solutions. The first part of the study focuses on IOR, utilizing the delocalized π electron system of graphite materials to facilitate rapid charge transfer with iodide ions, thereby reducing the reaction onset potential. Experimental results show that carbon fiber paper (CFP), as a catalyst, exhibits excellent IOR catalytic activity, with an onset potential of only 0.54 V (vs. RHE). In a two-electrode system, only 0.59 V of voltage is required to achieve a current density of 10 mA cm^{-2}, significantly reducing energy consumption by 65% compared to traditional OER water electrolysis. The study emphasizes that the catalytic activity of the graphite structure is closely related to the electrode spacing, and optimizing the electrode spacing can further reduce voltage requirements. The second part of the study focuses on UOR, designing and synthesizing dynamically stable blended CoOOH–Ni(OH)$_2$ nanoclusters as highly efficient UOR electrocatalysts. These blended nanoclusters exhibit excellent electrocatalytic activity in an alkaline environment, with an onset potential of 1.24 V (vs. RHE) in 1 M KOH and 0.5 M urea solution, requiring only a low applied potential of 0.45 V to achieve a current density of 10 mA cm^{-2}. Density functional theory calculations show that, compared to CoNiOx, blended CoOOH–Ni(OH)$_2$ nanoclusters with more oxygen vacancies exhibit lower Gibbs free energy in the NCONH$_2$ / NCONH intermediate reaction pathway, which is beneficial for the UOR. The study also explores the application of asymmetric electrolyzers, utilizing a pH gradient to further reduce the operating potential while separating the anode and cathode products.

Our study successfully utilizes IOR and UOR as alternative oxidation reactions, significantly reducing the potential requirements for HER. The application of graphite materials and mixed metal oxide nanoclusters provides new solutions for high-performance electrochemical hydrogen production. The results emphasize the importance of catalyst design and optimization of reaction conditions in improving hydrogen production efficiency, paving the way for new industrial applications of electrochemical hydrogen production.

Keywords: Iodide oxidation reaction, Urea electrooxidation reaction, Blended CoOOH–Ni(OH)2 nanoclusters, Oxygen evolution reaction, Carbon fiber paper

References

1. Shih-Mao Peng,Shu-Ting Chang, Chia-Che Chang,Priyadarshini HN, Chun-Chih Chang,* Kuan-Chang Wu, Yung-Hung Huang, Yi-Chia Chen, Tsung-Rong Kuo,Chih-Wen Pao, Jeng-Lung Chen, Di-Yan Wang*, 2024: Boosted Urea Electrooxidation Activity by Dynamic Steady Blending CoOOH-Ni(OH)2 Nanoclusters for H2 Production in a pH-asymmetric Electrolyzer, *J. Mater. Chem. A*, **2024**, 12, 24126–24135.
2. Shih-Mao Peng, Shivaraj B. Patil, Chun-Chih Chang, Shu-Ting Chang, Yi-Chia Chen, Kuan-Chang Wu, Wei-Nien Su,* Bing Joe Hwang* and Di-Yan Wang* 2022: Fast charge transfer between iodide ions and a delocalized electron system on the graphite surface for boosting hydrogen production, *J. Mater. Chem. A,* **2022**, 10, 23982–23989. (Selected as front cover and *2022 HOT Journal of Materials Chemistry A article*).

Designing greener energy conversion system for a sustainable future

Tharamani C. Nagaiah

Department of Chemistry, IIT Ropar, Rupnagar, Punjab-140 001

tharamani@iitrpr.ac.in

Abstract

Global energy requirements are touching new meridians with the gradual advancement in the living standards and the day-by-day growing world population. This necessitates the exploration to seek for greener and sustainable energy reservoir systems which ought to be environmentally agreeable for such an intriguing purpose. Electrochemical energy conversion and storage devices offer some most alluring aptitudes for providing clean energy. To name a few of these include fuel cells, rechargeable metal-air/peroxide batteries and HCl/ H_2S electrolysis and likewise.[1,2] Oxygen being central to the processes in these devices, a lot of attention has been focused upon the study of oxygen chemistry in terms of oxygen reduction reaction (ORR) and also Hydrogen evolution reaction (HER) and thence to the melioration of the associated electrocatalysts. In the past decade research has depicted tremendous improvement towards the betterment of fuel cells/Zn based batteries/hydrogen production in its legions of shortcomings or corrigible features.[3,4] But still an infinite pursuit towards the exploration of effective, sturdy and energy efficient catalysts continues. The talk addresses,

- several strategies pursued to replace noble-metal free electrocatalysts for ORR/HER.
- Zn based battereis
- visualization of local electrocatalyic activity by SECM.

Keywords: ORR, HER, electrocatalyst, Zn based batteries, SECM

References

1. Zhang, M.; Guan, J.; Tu, Y.; Chen, S.; Wang, Y.; Wang, S.; Yu, L.; Ma, C.; Deng, D.; Bao, X., Energy Environ. Sci. 2020, 13 (1), 119-126.

2. Kumar, M.; Tharamani, C. Nagaiah, Journal of Materials Chemistry A, 2022, 10, 7048 - 7057

3. Mehta, S.; Kaur, S.; Singh, M.; Kumar, M.; Kumar, K.; Meena, S.K.; Tharamani, C. Nagaiah, Advanced Energy Materials 2024, 14, 2401515,

4. Kumar, M.; Tharamani, C. Nagaiah, Energy Storage Materials, 2022, 49, 390-400

Chemical Regeneration of Spent Battery Cathodes under Ambient Conditions

Minah Lee[1,*]

[1] *Department of Battery Engineering, Graduate Institute of Ferrous & Eco Materials Technology (GIFT), Pohang University of Science and Technology (POSTECH), 77 Cheongam-Ro, Nam-Gu, Pohang, Gyeongbuk, 37673, Republic of Korea*

* malee@postech.ac.kr

Abstract

Developing energy-efficient, economically viable, and environmentally safe technologies for lithium-ion battery (LIB) recycling is critical to sustaining their widespread adoption in electric vehicles and grid-scale energy storage. Conventional recycling methods primarily rely on destructive processes that recover elemental metals but require energy-intensive resynthesis steps to regenerate high-value cathode materials. Although non-destructive direct regeneration approaches have been explored, their industrial scalability remains limited due to the need for precise lithium quantification or the use of extreme processing conditions such as elevated pressure, temperature, or inert atmospheres.

Herein, we introduce a thermodynamically controlled chemical regeneration strategy that directly restores spent cathodes under ambient pressure and open-air conditions using recyclable electron donors (REDs). The redox potentials of REDs are precisely tuned between the operational and over-lithiation potentials, enabling topotactic lithiation via coupled electron and lithium-ion transfer while minimizing side reactions. Simple soaking of spent cathodes in a regeneration solution containing RED molecules and lithium salts fully restores both composition and electrochemical performance, without requiring prior lithium quantification or cathode separation. The regeneration solution can be refreshed by recharging the REDs, enabling closed-loop recycling with minimal waste and cost. This approach is demonstrated on spent cathodes from commercial 1-Ah pouch cells, highlighting its scalability and applicability across various cathode chemistries with heterogeneous lithium depletion. The RED-mediated regeneration provides an energy-efficient, cost-effective, and sustainable pathway for LIB recycling, potentially advancing circular battery manufacturing.

Keywords: Cathode regeneration, Recyclable electron donors, Closed-loop battery recycling

References

(1) Ko, S.; Choi, J.; Hong, J.*; Kim, C.; Hwang, U.; Kwon, M.; Lim, G.; Sohn, S. S.; Jang, J.; Lee, U.; Park, C. B.; Lee, M.* Thermodynamically Controlled Chemical Regeneration of Spent Battery Cathodes Using Recyclable Electron Donors under Ambient Conditions. *Energy Environ. Sci.* **2024**, *17*, 4064.

Analysis of Silicon-Anode Degradation Mechanisms in All-solid-state Batteries via X-ray Nano-CT

Mao Matsumoto[1], Arata Matsumoto[1], Nodoka Ishikawa[1], Kei Hirabayashi[1], Yuya Sakka[1], Yuki Orikasa[1,*]

[1] *Department of Applied Chemistry, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu, Japan*

* orikasa@fc.ritsumei.ac.jp

Abstract

Silicon is one of the attractive next-generation anode active materials due to its high theoretical capacity. However, its practical use is limited by poor cycle capabiity. In conventional liquid-electrolyte Li-ion batteries, silicon's large volume change of silicon leads to the formation of fresh surfaces on which the electrolyte continually decomposes, accelerating degradation. If solid electrolytes are employed, the newly created active surfaces are not easily covered by the electrolytes, which can suppress the electrolyte decomposition and improve cycle life. On the other hand, electrolytes' plastic deformation causes the active material to lose adhesion with the solid electrolyte, which reduces the effective interfacial area. We previously developed a pressure-controlled operando X-ray computed-tomography (CT) cell that enables in-situ observation of the contact interface between active material and solid electrolyte.[1,2] In this study, we utilize phase-contrast nano-X-ray CT to resolve the morphological evolution of silicon and its surrounding solid electrolyte during all-solid-state battery operation.

Tracking the same silicon particle during charge-discharge reveals cracks in the surrounding solid electrolyte during lithiation, induced by the stress of silicon's volumetric expansion. During delithiation the silicon particles contract and detach from the electrolyte, leaving a shell-like voild at the interface. If the expansion-induced stress is released, the plastic electrolytes can not follow the shape change. A large first-cycle irreversible capacity and the voltage drop at the initial discharge coincide with the onset of interfacial delamination. Importantly, the detachment progresses while small "bridges" of contact remaines between silicon and electrolyte, which stabilizes and the charge-discharge capacity from the second cycle.

Keywords: All-solid-state battery, Solid electrolyte, Silicon anode, Solid interface, X-ray CT

References

(1) Sakka, Y.; et al, *J. Mater. Chem. A* **2022**, *10*, 16602-16609.

(2) Sakka, Y.; et al, *J. Electrochem. Soc.* **2024**, *171*, 070536.

Acknowledgement: This work was supported by JST-Mirai Program Grant Number JPMJMI24G1, Japan.

Generation of Battery materials from end of life LIBs: Pros and Cons

Mamata Mohapatra [a,b] *
[a]CSIR-Institute of Minerals and Materials Technology, Department of Hydro, Bio & Electrometallurgy, Bhubaneswar, 751013, Odisha, India
[b] Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh, India
mamata@immt.res.in

Abstract

Despite substantial progress, advanced R&D in hydrometallurgical recycling remains crucial to address key challenges to enhance the design of LIBs for improved end-of-life recoverability, optimizing process parameters to maximize metal recovery while minimizing reagent use and waste generation, mitigating effluents to reduce secondary pollution, developing selective separation techniques for recovering battery-grade materials from complex leachates, and above all improving cost-effectiveness and scalability through efficient resource and energy management. Beyond metal recovery, the reintegration of purified metals into new energy storage materials is vital for closing the material loop and reducing dependence on virgin resources. Recovered lithium, cobalt, nickel, and manganese can be processed into electrocatalysts or cathode precursors, yet purification, controlled precipitation, calcination, and doping to meet electrochemical performance standards are the current ongoing research. CSIR-IMMT has been working for the above domain of research since a coupl of year for the Development of a leaching strategy for the recovery of valuable metals from spent LIBs to minimise overall processing cost and complexity of the recycling workflow. Recovering functional materails as promising candidate for next-generation energy storage and conversion systems from the processed leach liquor. Trials are made to develop functional cathode material. Overall, a holistic recycling approach was made for metal recovery efficiency through sustainable leaching strategies but also demonstrates the direct functional reuse of recovered materials in energy storage and conversion applications. By utilizing the recovered transition metal complexes as precursors for synthesizing LIB cathode materials, it reinforces the vision of a closed-loop, low-impact recycling system aligned with circular economy goals.

Keywords: End of life, LiB, recovery, Energy materials, leaching

References

1. M. Mohapatra, S. Basu, and S. Sahu, Zero waste process development for the recovery of energy grade critical materials from spent oxide-based li-ion batteries materials (filed, application no. 202411057123).

2. Kotkar, S. Dash, P. Bhanja, S Sahu, et al., “Microwave assisted recycling of spent li-ion battery electrode material into efficient oxygen evolution reaction catalyst,” Electrochimica Acta, p. 141 842, 2023.

Local Electrochemical Mapping of 2D Materials Using Scanning Electrochemical Cell Microscopy

He-Yun Du[1,2,3,4*], Kuei-Hsien Chen[5,6], Li-Chyong Chen[6,7,8]

[1] *Department of Chemical Engineering, Ming Chi University of Technology, New TaipeiCity, Taiwan*

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

[3] *R&D Centerof Biochemical Engineering Technology, Ming Chi University of Technology, New Taipei City, Taiwan*

[4] *Center for Sustainability and Energy Technologies, Chang Gung University, Taoyuan City, Taiwan*

[5] *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*

[6] *Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan*

[7] *Department of Physics, National Taiwan University, Taipei, Taiwan*

[8] *Center of Atomic Initiative for New Materials, National Taiwan University, Taipei, Taiwan*

* Heyundu@mail.mcut.edu.tw

Abstract

Layered two-dimensional (2D) materials, such as graphene and MoS_2, are widely recognized as promising photocatalysts for hydrogen evolution and water splitting. However, the interfacial electronic structure, particularly the influence of layer number and alloy composition, remains insufficiently understood. Accurate analysis of band offsets and charge transfer behavior is crucial for improving catalytic performance. In this study, we investigate the heterogeneous charge transfer properties of 2D materials with varying layer numbers and alloy compositions using scanning electrochemical cell microscopy (SECCM). Localized redox mapping reveals distinct area, layer, and composition-dependent reactivity, offering new insights into interfacial band alignment and the confinement of faradaic currents. Complementary structural characterizations, including Raman spectroscopy, photoluminescence mapping, and transmission electron microscopy, are used to correlate electrochemical activity with crystal structure, layer thickness, and alloy distribution. This study links local electrochemical activity to structure and composition, supporting catalyst design for hydrogen applications.

Keywords: 2D material, MoS_2, HER, SECCM

Electrochemical Dimerization of 1,3-Dicarbonyls through PCET Mechanisms: Many Routes, One Destination

Amit Paul*

[1] *Department of Chemistry, IISER Bhopal, Bhopal Bypass Road, Bhauri, Bhopal, MP 462066, INDIA*

*apaul@iiserb.ac.in

Abstract

Dimerized 1,3,-dicarbonyls are important building blocks for various natural products. Hence, green electrochemical synthesis of such molecules are of great interest. First, I will discuss the dimerization of 3-carboxylate-2-oxindole by direct electrode oxidation on the electrode surface.[1,2] A detailed mechanistic investigation involving proton-coupled electron transfer (PCET) will be discussed, wherein I will present three different PCET pathways for dimerization.[1] Thereafter, I will present electrocatalytic routes involving TEMPO as a redox mediator and TEMPO$^+$ as an active catalyst for the dimerization of 3-carboxylate-2-oxindoles following a hydride transfer mechanism.[3] Thereafter, I will discuss dimerization of β-ketoester following Multi-Site Concerted Electron Proton Transfer (MS-PCET), wherein I will demonstrate of polarization of nonpolar C-H bond through electrolyte for the operation of MS-PCET. Moreover, many aspects of green chemistry, such as minimizing waste generation, recovery of electrolytes etc., will also be discussed.[3]

Keywords: Proton-Coupled Electron Transfer (PCET), Hydride Transfer, Multi-Site Concerted Electron Proton Transfer (MS-PCET), Electro-organic Synthesis, Green Chemistry.

References

1) Sharma, S.; Roy, A.; Shaw, K.; Bisai, A.; Paul, A. *J. Org. Chem.* **2020**, *85*, 14926-14936.

2) Sharma, S.; Behera, H.; Ahlawat, S.; Paul, A. *Org. Biomol. Chem.* **2025**, *23*, 3288-3306.

3) Sharma, S.; Shaheeda, S.; Shaw, K.; Bisai, A.; Paul, A. *ACS Catal.* **2023**, *13*, 2118-2134.

Challenges of Electrochemical Ammonia Production: Pathways to Green Future

Ramendra Sundar Dey[1]*

[1] *Institute of Nano Science and Technology, Sector-81, Mohali-140306, Punjab, India*

* Corresponding author's email address: rsdey@inst.ac.in

Abstract

The rapid depletion of non-renewable energy sources made the researchers to incline towards the development of alternative approaches with a long-term vision of a sustainable society. With this advent, green hydrogen/green ammonia plays a dominating role towards a safe, reliable and electrified future. Although to meet the practical demands of ammonia, the Haber Bosch process is the sole option, but it deviates from the goal to a "net-zero" society. This calls for the electrochemical approach and we have thus keenly focused to develop suitable materials to achieve a significant ammonia production by nitrogen reduction reaction (NRR) in aqueous electrolytes. The structure-function relationship of the materials is extensively rendered emphasizing the impact of the synthesis strategy on the electronic properties of the materials that in turn modulate the elementary steps of NRR. The fundamental understanding between the electronic structure and adsorption energy of N_2 and apparent activity of the active site towards NRR are studied to gain a better understanding on the mechanisms of NRR ongoing on the material surface. On a broader perspective, with these improvisations we aim to develop a full NRR electrolyzer in laboratory scale having a potential of a better energy efficient ammonia synthesis.

Keywords: Green fuel; electrochemical ammonia synthesis; Nanomaterials; Net-zero.
Acknowledgement: R.S.D. acknowledges BRNS (Board of Research in Nuclear Sciences) (58/14/19/2023-BRNS) for financial support.

References

(1) Biswas, A.; Kapse, S.; Ghosh, B.; Thapa, R.; Dey, R. S.* PNAS, 2022, 119, 33, e2204638119.
(2) Biswas, A.; Kapse, S.; Thapa, R.; Dey, R. S.* Nano-Micro Letters, 2022, 14, 1-17.
(3) Biswas, A.; Nandi, S.; Kamboj, N.; Pan, J.; Bhowmik, A.; Dey, R. S.*, ACS Nano, 2021, 15, 20364–20376.
(4) Bhardwaj S., Das S. K., Biswas, A.; Kapse, S.; Thapa, R.; Dey, R. S.*, Chemical Science, 2023, 14, 8936.
(5) Biswas A., Barman N., Avinasj N., Thapa R., Dey, R. S.*, Mater. Horiz., 2024, 11, 2217.

Surface Active Ionic Liquids: The Electrocatalytic Electrolytes for Green ELectrochemistry

*Mohsin Ahmad Bhat**
Department of Chemistry, University of Kashmir, Srinagar,190006, India
e-mail; mohsin@kashmiruniversity.ac.in Tel: +91 9419033125

Abstract

Managing electron transfers across inteligently designed polarizable interfaces offers offers a promising route for developing green and efficient technologies for renewable energy storage and conversion, sustainable chemical synthesis, selective sensing of pollutants and disease biomarkers, and the electrochemical detoxification of environmental contaminants. However, electron transfer processes central to these applications are often intrinsically sluggish, warranting high overpotential requirements that compromises the overall efficiency and limits their practical implementation. These challenges have fueled extensive research into the design of electrocatalytic systems with potential to facilitate selective and efficient heterogeneous electron transfer, particularly in contexts such as fuel cells, electrosynthesis, and electrochemical sensing. Most studies reported so far in this regard have focused on the design and development of electrocatalytic electrode materials and additives (molecular electrocatalysts), with just few reports about the design and development of electrocatalytic electrolytes. Over the last few years, our and few other research groups, have demosntarted the potential use of aqueous solutions of Surface-Active Ionic Liquids (SAILs) as potential green electrocatalytic electrolytes for electrochemical sensing, electrochemical synthesis and electro-catalytic detoxification of environmental pollutants[1,2,3,4]. We have demonstrated that the special ability of SAILs to organize into interface-localized or bulk phase distributed organized structures with ability to stabilize, solubilize and activate a variety of electro-analytes or electrogenerated-analytes offer distinct electrochemical advantages to these systems. These fetures endow SAILs with electrochemical advantages not accessible with conventional solvent systems. Results from our detailed electrochemical investigations, showcasing the selective and highly efficient electrocatalytic dehalogenation and electrocarboxylation of halocarbons and pinacol coupling over inherently non-catalytic electrodes with aqueous micellar solutions of imidazolium based SAILs, will be presented[3,4,5,6,7]. The findings to be presented we belive highlight the underappreciated potential of electrocatalytic electrolytes as key components in next-generation green electrochemical technologies.

Keywords: Surface Active Ionic Liquid, Electrodehalogenation, Electrocarboxylation, pinacol coupling, CO_2 Electroreduction

References:

1. Buettner, C. S.; Cognigni; Schröder, A. C.; Bica-Schröder, K.; *J. Mol. Liq.* ***2022***, 347**,** *118160.*
2. Bailey, J. et al. M. *Green Chem.* **2024**, 26*, 1092-1131(2024)*
3. Bhat, P.A.; Pandit, S. A.; Rather, M. A.; Bhat, M. A. *J. Mol. Liq.* **2019**, 289, 111129.
4. Pandit, S. A.; Bhat, S. A.; Rather, M. A.; Ingole, P. P. ; Bhat, M. A. *Phys. Chem. Chem. Phys.* **2020**, 22, 16985-16997 (2020)
5. Pandit, S. A.; Bhat, S. A.; Rather, M. A.; Sofi, F. A.; Ingole, P. P.; Bhat, Z. M.; Thotiyl, M. O.; Bhat, K. A.; Rehman, S. U.; Bhat, M. A. *Green Chem.* **2021,** 23*, 9992-10005*.
6. Hassan, N.; Kuchey, M. Y.; Bhat, M. A. *Chem. Commun.*, **2024**,60, 9038-9041.
7. Sheikh, U.R.; et al. J. Electroanal. Chem.2025, 979, 118902.