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

Scalable Electrode Engineering for High-Areal-Capacity Lithium Batteries

Sang-Young Lee*

Department of Chemical and Biomolecular Engineering, Department of Battery Engineering, Yonsei University, Seoul 03722, Korea
*syleek@yonsei.ac.kr

Abstract

Achieving high-energy-density batteries is pivotal for advancing the smart energy era. While extensive efforts have been devoted to developing new electrode active materials and electrolytes, comparatively less emphasis has been placed on the scalable engineering of electrode architectures that directly determine areal capacity and manufacturability. In this talk, we introduce a comprehensive materials-to-manufacturing framework that enables areal capacities exceeding 20 mAh cm^{-2}, while maintaining structural integrity, electrochemical stability, and compatibility with industrial-scale processes. Central to this platform is the development of PFAS-free binder systems and rheologically tuned slurries**,** designed to simultaneously address performance, processability, and environmental sustainability. We highlight strategies such as amphiphilic bottlebrush polymers, cationic semi-interpenetrating polymer networks (semi-IPNs), and surface-functionalized nanocellulose. These binder-driven approaches prevent drying-induced phase segregation, improve electrode uniformity and manufacturing yield, and are compatible with roll-to-roll processing. The proposed platform extends beyond lithium-ion batteries to systems such as lithium–sulfur batteries and other chemistries where engineered interfacial mechanics and chemical affinity are vital for stable cycling under constrained cell conditions. By seamlessly integrating molecular design with scalable processing, this approach offers a viable route toward environmentally responsible, high-energy-density batteries, bridging the gap between laboratory breakthroughs and industrial implementation.

Keywords: Lithium Batteries, High-Energy-Density, Electrode Engineering, High Loading, Binders

References

(1) S. Y. Lee et al., Regulating electrostatic phenomena by cationic polymer binder for scalable high-areal-capacity Li battery electrodes *Nature Comm.* 14 (2023) 5721.
(2) S. Y. Lee et al., Material challenges facing dry-processable battery electrodes *ACS Energy Lett.* 9 (2024) 5688.
(3) S. Y. Lee et al., Upscaling high-areal-capacity battery electrodes *Nature Energy* 10 (2025) 295.

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

A Robust Li-Ion Permeable Interphase to Address Interfacial Instability and Structural Degradation of Ni-Rich NCM Cathodes In Poly(ethylene oxide)-Based All-Solid-State Li-Ion Batteries

C. H. Liao, Yu-Ting Weng, Nae-Lih Wu

[1] *Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan*

* nlw001@ntu.edu.tw

Abstract

Poly(ethylene oxide) (PEO)-based solid polymer electrolytes (SPEs) are widely used for all-solid-state lithium-ion batteries (ASSLIBs) because they offer high processibility, good thermal stability and improved safety compared to traditional organic electrolytes. However, they encounter challenges of poor interfacial stability and significant degradation of the cathode structure when used with the high-voltage Ni-rich NCM cathodes. This presentation introduces lithium sulfonated poly(1,4-phenylene ether-ether-sulfone) (SPEESLi) as a robust artificial cathode-electrolyte interphase (A-CEI) for $LiNi_{0.83}Co_{0.12}Mn_{0.05}O_2$ (NCM83) cathodes to address those challenges. It is demonstrated that the SPEESLi A-CEI is capable of effectively enhancing the interfacial stability, reducing side reactions, and suppressing impedance growth, leading to substantially enhanced cycle stability. Meanwhile, as revealed by high-resolution microscopic analysis, its high mechanical strength minimizes cathode microcracks, limits volume changes, and reduces rock-salt layer thickness, preserving cathode integrity. Synchrotron X-ray absorption analysis confirms suppressed Ni reduction, further demonstrating the efficacy of SPEESLi in enhancing interfacial and structural stability, enabling improved performance of the Ni-rich NCM in the PEO-based ASSLIBs.

Keywords (max 5): Sulfonated polymer coating, Ni-rich cathodes, All-solid-state Li-ion batteries, PEO-based solid polymer electrolyte

References

(1) C. H. Liao, N. L. Wu, Chemical Engineering Journal 523, 168677 (2025).

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

Enhancing Lithium Metal Electrode Stability with Ceramic Layer Coatings

Nobuyuki Imanishi*, Riku Imanishi, Hiroya Sahashi, Soh Taminato, Daisuke Mori

School of Engineering, Mie University, Tsu, Mie, Japan

* imanishi@chem.mie-u.ac.jp

Abstract

Keywords: Lithium metal electrode, Solid Electrolyte Interphase, Deposition and dissolution, Dendrite, Coulombic efficiency

In recent years, the development of next-generation batteries with high energy density and enhanced safety has been accelerating, driven by the widespread adoption of renewable energy and the advancement of electric mobility. Many battery systems, such as lithium-ion batteries, are composed of a complex combination of materials with different functions. In these composite systems, while the performance of each individual material is certainly important, the interfacial properties between the materials significantly affect the overall performance and stability of the battery. Increased resistance at interfaces can reduce output characteristics and charge-discharge efficiency, while unstable interfaces can trigger side reactions and gas generation, leading to reduced safety and capacity degradation.

The importance of interfaces is particularly pronounced in next-generation batteries that use lithium metal as the anode. Lithium metal possesses a theoretical capacity (3860 mAh/g) far exceeding that of conventional graphite-based anodes, offering the potential for a dramatic increase in energy density. However, its high reactivity poses serious challenges. At the interface with the electrolyte, an inhomogeneous solid electrolyte interphase (SEI) is likely to form, leading to issues such as dendrite growth, electrolyte decomposition, low Coulombic efficiency, and cycle degradation. In all-solid-state batteries, chemical instability and poor contact at the electrode-solid electrolyte interface hinder efficient lithium-ion transport across the interface, presenting a major obstacle to practical application [1].

Many of these issues stem from the direct contact between the electrode and the electrolyte. Therefore, simply changing the combination of materials is not sufficient to fully resolve them. One promising strategy is to introduce an artificial interfacial layer between the electrode and the electrolyte. This study focuses primarily on systems where lithium metal is used as the electrode, and aims to control and suppress interfacial reactions by introducing electrochemically stable materials at the electrode-electrolyte interface, thereby promoting uniform lithium deposition and dissolution. In this work, we report on systems in which an inorganic interfacial layer is formed on the electrode.

References

(1) R. Zhang et al., Chemical Society Reviews, 49(14), 5101(2020).

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

Iron-based conversion electrode material -from lithium batteries to anion-shuttle system-

Hikari Sakaebe

Institute for Materials Chemistry and Engineering, KYUSHU UNIVERSITY, 6-1 Kasuga koen, Kasuga-shi, Fukuoka 816-8580, Japan

sakaebe@cm.kyushu-u.ac.jp

Abstract

Developing high-energy-density batteries without resource constraints is an important goal. The author has been working on the development of iron-based cathode materials. Among these, $LiFePO_4$ with an olivine structure is a representative example and has been adopted in commercial batteries. To further improve energy density, the author has aimed to expand the capacity by conversion reaction, using Iron(III) fluoride (FeF_3). FeF_3 can be operated in both lithium insertion/extraction and conversion reaction, with a high theoretical capacity of 712 mAh g^{-1}. The charge–discharge mechanism of FeF_3 as a conversion electrode has been investigated in detail, and methods to overcome its drawbacks have been explored. [1-3] In recent years, research on anion shuttle batteries has been gradually expanding. FeF_3 has been demonstrated to work as an electrode material for all-solid-state anion-shuttle batteries. [4] To further elucidate the potential of FeF_3, thin-film electrodes were prepared and a series of electrochemical measurements and analyses were conducted. These investigations revealed that FeF_3 enables intrinsically reversible electrode reactions. [5, 6] Furthermore, efforts are currently underway to explore its applicability under ambient temperature operating conditions. Some other progress would be presented.

Keywords: Iron trifluoride, conversion electrode, anion-shuttle system, High energy

Acknowledgement

This work was financially supported by the RISING2 (JPNP16001) and RISING3 (JPNP21006) of NEDO.

References

(1) K. Yoshii, H. Sakaebe, *et al*., *Chem. Commun.*, 2020, 56, 4878-4881.

(2) Y. Maeyoshi, H. Sakaebe, *et al*., *Chem. Commun.*, 2025, 61, 9222-9225.

(3) Y. Takabayashi, H. Sakaebe, *et al*., *Adv. Sustainable Syst.* 2024, 8, 2300571.

(4) A. Inoishi, H. Sakaebe, *et al*., *Adv. Energy Sustainability Res*. 2022, 3, 2200131.

(5) M. Yamamoto, . H. Sakaebe, *et al*., *J. Phys. Chem. C* 2025, 129, 26, 11831–11837.

(6) A. Yano, H. Sakaebe, *et al*., Submitted for publication

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

Unlocking the Power of Aqueous Batteries with Rationally Engineered Anode and Cathode

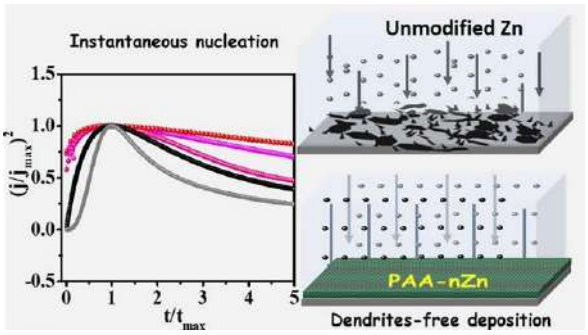
C. Retna Raj

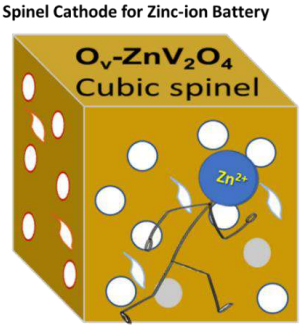
Functional Materials and Electrochemistry Lab, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India.

* crraj@chem.iitkgp.ac.in

Abstract

The recent advancement in renewable energy technologies towards carbon neutrality demands an efficient energy storage system. Non-aqueous lithium-based batteries (LiBs) dominate the landscape of rechargeable energy technologies. However, the safety and environmental sustainability issues and the cost of LiBs are matters of concern. Aqueous rechargeable batteries are promising in meeting the sustainability requirements and powering portable electronics and grid-scale storage. Among them, the aqueous zinc-ion batteries have emerged as strong contenders for sustainable energy storage due to the high theoretical specific capacity (820 mAh g^{-1}), low redox potential (−0.763 V vs. SHE), etc. However, their widespread adoption is limited by sluggish Zn^{2+} transport, suboptimal cathode performance, and dendritic growth at the anode due to inhomogeneous nucleation. We have developed electrochemical strategies to engineer (i) the anode with a zincophilic polymer interface and (ii) spinel and layer-structured cathode materials. The polymer interface decreases the nucleation overpotential and suppresses the undesired growth of zinc dendrites. Remarkable enhancement in the specific capacity and charge-discharge cyclability has been achieved with the engineered anode and cathode. The defect-engineered layer structured cathode delivers specific capacity as high as 692.8 mAh g^{-1} at 100 mA g^{-1} and has an ultra-long cycle-life of over 75,000 cycles at high current density and fast charging capability.





Keywords: Zinc batteries, Zincophilic interface, Vanadium cathode, Fast charging

References

(1) Mallick, S.; Choutipalli, V. S. K.; Subramanian, V.; Raj, C.R., *ACS Appl. Mater. Interfaces* 2022, 14, 33, 37577. (b) Bag, S.; Choutipalli, V. S. K.; Bhadra, A.; Shuford, L.L.; Kundu, K.; Raj, C.R., *J. Mater. Chem. A*, 2024, 12, 22998. (c) Mallick, S.; Raj, C.R., *ChemSusChem* 2021, 14, 1987.

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

Layered $NaMeO_2$ (Me = 3d metals): Synthesis, Polytypes, and Solid-State Redox

Shinichi Kumakura, Kodai Moriya, and Shinichi Komaba*

Department of Applied Chemistry, Tokyo University of Science, Tokyo 162-8601, Japan

* komaba@rs.tus.ac.jp

Abstract

Sodium-ion and potassium-ion batteries have been increasingly acknowledged as sustainable and cost-effective alternatives to lithium-ion batteries, due to the plentiful availability of their constituent elements. Layered oxide materials, particularly, hold great promise as positive electrodes for sodium-ion batteries (SIBs). In this presentation, we will provide an overview with the latest highlights about crystallographic and electrochemical properties of layered oxides, $NaMeO_2$ (Me = 3*d* metals). Enabling $Mn^{3+/4+}$ redox couple in the layered structure is one of the key factors to achieve high energy density without using expensive metals, such as cobalt and nickel. O'3-$NaMnO_2$ suffers a rapid capacity loss as well as multiple phase transitions during electrochemical cycling.[1] The impact of structural properties on electrode performance will be further discussed by comparing with the polytype, *β*-$NaMnO_2$ having corrugated MnO_2 layers instead of ordinary planar layers. Another layered polytype P2-type and P'2-type structures will also be addressed with respect to both phase formation, electrochemical activity, and doping.

We recently leveraged a specially constructed database for O3-type Na-ion batteries to predict the electrochemical properties of Ni-Mn-Fe-Ti-based layered oxides.[2] The database are consisted of compositions and electrochemical properties for O3-type layered oxides, which were previously published as well as unpublished results. Leveraging this data, we constructed a predictive model that determines electrochemical properties for virtual compositions. The predicted promising compositions are experimentally verified, showing an initial energy density of 549 Wh kg^{-1}.

Futher, we recently reported single-phase products of Sc-substituted P'2-$Na[Mn,Sc]O_2$ showing superior cycle stability and rate performance.[3] To utilize Na-deficient P2 materials, it is a necessary to compensate sodium on a positive electrode. We proposed an application of Na_2CO_3 as a sacrificial electrode additive to balance the sodium content (= state of charge) in sodium-free negative electrode and Na-deficient P2 based positive electrodes.[4] We will further discuss the perspective and future strategy of the layered oxide electrode materials in Na-ion battery.

References:

[1] K. Kubota, M. Miyazaki, E. J. Kim, H. Yoshida, P. Barpanda, S. Komaba, *J. Mater. Chem. A* **2021**, *9*, 26810.

[2] S. Sekine, T. Hosaka, H. Maejima, R. Tatara, M. Nakayama, S. Komaba, *J. Mater. Chem. A* **2024**, *12*, 31103.

[3] K. Moriya, S. Kumakura, E. J. Kim, R. Tatara, S. Komaba, *Electrochem. Commun.* **2025**, *174*, 107891.

[4] M. Matsuzaki, S. Komaba, et al., *Batteries & Supercaps* **2025**, *7*, e202400009.

Keywords: Na-ion battery, layered oxides, manganese oxide

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

Rational Interfacial-design of Sulfide-Based Solid Electrolytes for All-Solid-State Batteries

Sang-Min Lee[1,2*]

[1] *Department of Battery Engineering, Graduate Institute of Ferrous & Energy Materials Technology, POSTECH, Pohang, Korea*

[2] *Department of Material Science and Engineering, POSTECH, Pohang, Korea*

* sangma@postech.ac.kr

Abstract

Sulfide-based solid electrolytes (SEs), such as Li_6PS_5Cl and related argyrodite compounds, are among the most promising candidates for next-generation all-solid-state batteries (ASSBs) due to their high ionic conductivity and favorable mechanical properties (1). However, their practical application is significantly limited by interfacial instability when in contact with both lithium metal anodes and high-voltage cathodes. These interfacial reactions lead to the formation of resistive layers, capacity fading, and shortened cycle life.

In this presentation, we present a comprehensive interfacial engineering strategy to stabilize the interfaces between sulfide SEs, electrodes, and ambient environments. A range of approaches—including bulk-level material design, ionically conductive artificial interlayers, and in situ formed passivation layers—were systematically investigated to suppress interfacial side reactions and reduce interfacial resistance (2,3). Advanced characterization techniques were employed to elucidate structural and chemical transformations occurring at the interface during electrochemical cycling. The results demonstrate that targeted interfacial modification significantly enhances interfacial compatibility and long-term electrochemical performance. This work underscores the critical role of interfacial engineering in addressing the intrinsic limitations of sulfide-based SEs and provides practical insights into the design of stable, high-energy-density ASSBs incorporating both solid and liquid–solid hybrid electrolytes.

Keywords (max 5): All-solid-state batteries, Sulfide electrolyte, Argyrodite, Interfacial engineering

References

(1) Q. Zhao, and L.A. Archer, Nature Reviews Materials, 5(3) (2020) 229-252

(2) Taesoon Hwang, and Sang-Min Lee, J. Mater. Chem. A, 10, (2022) 16908

(3) Sumin Ko, and Sang-Min Lee, Chem. Eng. Journal, 496, 15, (2024) 154151

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

Solids-state Na-ion Batteries via Two Dimensional Filler based Composite Polymer Electrolyte

Sudharshan Vasudevan and Palani Balaya[1,*]

[1] *Department of Mechanical Engineering, School of Design and Engineering, National University of Singapore, 117575, Singapore*

* Email: mpepb@nus.edu.sg

Abstract

In the context of supply chain constraints and safer energy solution amid increasing energy safety and demand, solid-state Na-ion cells have gained importance at global ventures. [1] The flexible composite polymer electrolyte (CPE) are translatable for mass production due to lower energy requirement, interfacial mechanical and electrochemical properties with improved ionic conductivity and electrochemical voltage window for current cathode materials. Here, compositing with small fraction of functional two dimensional filler can take advantage of the size and morphology driven interface enhancenment between filler and polymer matrix for better ion conduction and mechanical properties. [2] Especially, this work aims at investigating a low cost graphitic carbon nitride (GCN) with high active surface area which lowers the polymer crystallinity, improves transport properties and mechanical strength to impede dendrite growth. A PEO-GCN based CPE using NaTFSI as salt, investigated in our previous study [3] was fabricated that offers several key improvements. The CPE exhibited ~2.5 times higher ionic conductivity, ~3 times higher tensile strength, better electrochemical voltage window of ~4.5 V and ion transference number of 0.51 when compared to pristine counterpart, PEO-NaTFSI. This stems from the reduction of crystallinity, introduction of high conductivity polymer-filler interface, improved oxidation stability of polymer matrix and N group influenced better salt/polymer interactions. Eventually, the Na metal plating/stripping behavior improved by offering more than twice the critical current density with stable cycling over 1000h at 0.1 mA/cm^2. Alongside, an all-solid-state Na-metal battery constructed with CPE using different cathodes in coin and pouch cell formats exhibited remarkable rate performance till 2C and a stable cycling performance by exploiting the multi-faceted improvements in CPE achived.

Keywords: Solid electrolytes, Sodium-ion batteries, Polymer electrolyte, 2D functional filler

References

(1) Zhou, W.; Li, Y.; Xin, S.; Goodenough, J. B. *ACS Cent. Sci.* **2017**, *3*(1), 52-57.

(2) Lan, X.; Luo, N.; Li, Z.,; Peng, J.; Cheng, H. M. *ACS nano* **2024**, *18*(13), 9285-9310.

(3) Vasudevan, S., Dwivedi, S., Morekonda Ganesh Babu, K. B., & Balaya, P. *ACS Appl. Mater. Interfaces* **2024**, *16*(38), 50736–50746.

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

Development of Next-Generation Fuel Cells in GteX Project in Japan

Minoru Inaba

Department of Molecular Chemistry and Biochemistry, Doshisha University, Kyotanabe, Kyoto 610-0321, Japan

* minaba@mail.doshisha.ac.jp

Abstract

Hydrogen is a key material for realizing carbon neutrality in 2050. It is important for us to accelerate production, transportation, storage, and utilization of hydrogen simultaneously for this purpose. Development of fuel cells started around 2000 by industry-academia-government collaboration in Japan, and big accomplishments have been made, especially on durability improvements. As a result, small household fuel cell co-generation systems (~1 kW) have been commercialized since 2009, and fuel cell vehicles (FCVs, e.g. MIRAI and Clarity Fuel Cells) have been on the market since 2014 in Japan. It is now believed that the application of fuel cells to heavy-duty vehicles (HDVs) such as long-range tracks and buses, construction machinery, ships, railway, etc. is needed for full-scale expansion of fuel cells. However, there remain many issues such as performance, durability, and cost for the state-of-the-art fuel cell systems on the application to HDVs. In our GteX (Green Technologies of Excellence) fuel cell project, which started in 2023, we are developing innovative materials for catalysts, electrolytes, ionomers, bipolar plates, etc. to realize the next-generation fuel cell systems for heavy duty vehicles. The fuel cell systems include (1) high-temperature proton-conductive membrane fuel cells (HT-PEMFCs), (2) anion-exchange membrane fuel cells (AEMFCs) and (3) (solid oxide) proton-conductive fuel cells (PCFCs). These fuel cell developments are supported by cross-sectoral (4) the system evaluation group and (5) the advanced analysis, calculation, DX-MI technology group as shown in Fig. 1. In this talk, the research and development in our GteX fuel cell project are overviewed.

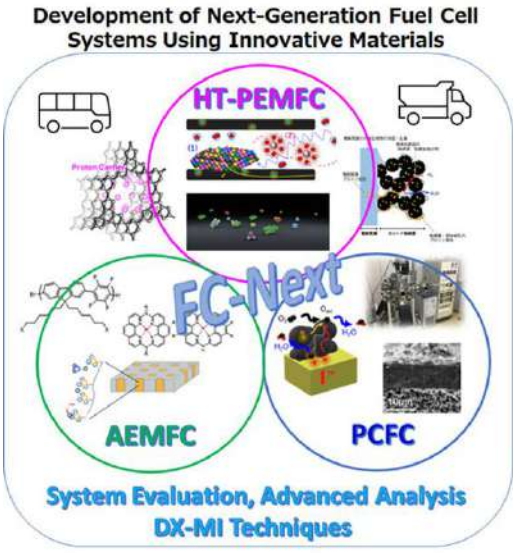


Figure 1 GteX fuel cell project.

Keywords: Fuel cell, HT-PEMFC, AEMFC, PCFC, Heavy Duty Vehicle

This study supported by JST GteX Program Japan Grant Number JPMJGX23H0.

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

Copper-Integrated Solid Polymer Electrolyte with Enhanced Li^+ Transport and Durability in Lithium Metal Batteries

Hsisheng Teng[1,*], Hanh T. T. Nguyen[1], Jyh-Chiang Jiang [2], Liang-Ting Wu[2]

[1] *Department of Chemical Engineering, National Cheng Kung University, Tainan 70101, Taiwan*

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

* hteng@mail.ncku.edu.tw

Abstract

The presence of permanant solvents in solid polymer electrolytes (SPEs) enhances ion transport by forming [Li^+-solvent] complexes, which create additional pathways for Li^+ movement and significantly boost the overall ionic conductivity. However, the low conduction band minimum of these complexes renders them continuously react with the Li metal anode, leading to an unstable solid electrolyte interphase (SEI) layer. This study synthesizes a SPE that enhances ionic conductivity while ensuring compatibility with lithium metal by using additives CuF_2 and $LiNO_3$. These additives resulted in a four-fold increase in the diffusion coefficient of Li^+ by altering the coordination environment of Li^+. The SPE achieves a high ionic conductivity of 1.3 mS cm^{-1} at 30 °C. Furthermore, CuF_2 and $LiNO_3$ synergistically facilitate the formation of a LiF-Li_3N-Cu containing SEI layer, promoting uniform Li deposition and suppressing reactions between the electrolyte and electrode. The Li||Li cell using SPE with additives achieves a critical current density of 6.3 mA cm^{-2}, enhancing electrolyte efficiency and permitting operation at elevated currents. A resulting Li||$LiFePO_4$ cell retains 87% of its initial capacity after 400 cycles at a high current density of 1.7 mA cm^{-2}, highlighting the durability and efficiency of this electrolyte system. A resulting Li||Cu cell exhibits a high deposition capacity of 6.0 mAh cm^{-2}, showing compatibility with high-loading cathodes. Overall, the incorporation of CuF_2 and $LiNO_3$ as additives significantly enhances the electrochemical performance of SPEs, providing a promising solution for developing high-performance, durable batteries suitable for various applications.

Keywords: Solid polymer electrolyte, Lithium metal battery, Solid-Electrolyte Interphase

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

Pseudocapacitive Properties of Birnessite Nanosheets

Wataru Sugimoto[1,2,*], Ryota Saito[2], Keisuke Muramatsu[1]

[1] *Institute of Aqua Regeneration (ARG), Shinshu University, 3-15-1 Tokida, Ueda, Nagano 386-8567, Japan*

[2] *Graduate School of Medicine, Science and Technology, Shinshu University, 3-15-1 Tokida, Ueda, Nagano 386-8567, Japan*

* wsugi@shinshu-u.ac.jp

Abstract

The interlayer space of layered birnessite-type manganese oxide (δ-MnO_2) can be utilized for charge storage[1] and can be converted into nanosheets via chemical exfoliation,[2] making it an attractive model material to understand the redox capacitance as a function of porosity and accessible surface area. We discuss here the enhancement in the redox kinetics by partially substituting Mn with Ir, δ-(Mn,Ir)O_2.[3] In addition, the incease in charge storage by the exfoliation of δ-(Mn,Ir)O_2 to nanosheets, δ-(Mn,Ir)O_2(ns), is discussed.

Exoliated δ-(Mn,Ir)O_2(ns) was obtained by the reaction of proton exchanged δ-(Mn,Ir)O_2 with quaternary ammonium hydroxides.[4] Acetylene black (AB) was added as the conductive additive to δ-(Mn,Ir)O_2(ns) colloid (mass ratio: (Mn,Ir)O_2 : AB = 1 : 4) and cast onto a glassy carbon electrode to prepare the working electrode (0.200 mg cm^{-2}). The amount of iridium subsitution was Ir/Mn = 0.05.

Cyclic voltammetry was conducted in 1.0 M Li_2SO_4 (25°C, 2-500 mV s^{-1}, 0.6-1.2 V vs. RHE). The specific capacitance of δ-(Mn,Ir)O_2(ns) was 226 F g^{-1}, considerably larger than δ-MnO_2(ns) of 140 F g^{-1}. The oxidation peak of Mn in the δ-(Mn,Ir)O_2(ns) shifted to a lower potential by about 40 mV, consistent with the features observed in the non-exfoliated layered δ-(Mn,Ir)O_2.[3] The increase in charge storage capability is be attributed to the improvement of the conductivity of the nanosheets due to iridium doping and the reduction of the contact resistance between the sheets.

Keywords: Birnessite, Manganese oxide, Iridum doping, Pseudocapacitance

References

(1) S. Boyd, K. Ganeshan, W.-Y. Tsai, T. Wu, S. Saeed, D. Jiang, N. Balke, A. C. T. Duin, and V. Augustyn, *Nat. Mater*., **20**, 1689 (2021).

(2) Y. Omomo, T. Sasaki, Wang, and M. Watanabe, *J. Am. Chem. Soc*., **125**, 3568 (2003).

(3) R. Saito, H. Tanaka, K. Teshima, D. Takimoto, S. Hideshima, and W. Sugimoto, *Inorg. Chem*., **61**, 4566 (2022).

(4) Z. Liu, R. Ma, Y. Ebina, K. Takada, and T. Sasaki, *Chem. Mater*., **19**, 6504 (2007).

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

Disorder-Engineered Oxide Cathodes and Solid-State Electrolytes: Mechanistic Insights into Structural and Ionic Modulation

Yong-Mook Kang[1,*] Jae-Bum Kim[1], Suwon Lee[1]

[1] *Department of Materials Science and Engineering, Korea University, Seoul 02841, Republic of Korea*

* dake1234@korea.ac.kr

Abstract

The functionalities of solid-state materials are governed by their atomic structures, and varying degree of inherent disorders which leads to unprecedented ion or electron conduction, phase transition, and electrochemical properties.[1,2] In this talk, I explore the role of structural disorders in two critical components of Li-ion batteries; oxide-based cathodes and solid-state electrolytes (SSE) to reach the fundamental disorder-property relationship.

The α-$NaFeO_2$-type layered structure in $LiCoO_2$ (LCO) underpins its high theoretical capacity and facile Li^+ transport. Deviations from this archetype, however, can yield enhanced cycling reversibility by modulating phase transition pathways. In Li-birnessite ($Na_{0.04}Li_{0.4}MnO_2{\cdot}0.14H_2O$), dehydration-induced structural disorder—manifested as interlayer contraction, turbostratic distortion, and Mn vacancies—diminishes cooperative distortions and stabilizes the host framework, thereby suppressing Mn migration/dissolution and irreversible spinel conversion. In high-Ni NCM ($Li_{0.999}Ni_{0.903}Co_{0.046}Mn_{0.48}Nb_{0.004}O_2$), trace Nb doping induces local off-centering of NbO_6 units, mitigating lattice strain associated with the H2–H3 transition and promoting structural reversibility. In the solid-state electrolyte domain, disorder also governs ionic transport. Ta substitution in LLZTO disrupts Zr–O bonding networks, activates low-frequency anharmonic phonons, and enhances Li^+ migration entropy via delocalized configurations. Phonon-based machine learning and thermodynamic analyses confirm that such disorder enables temporally desynchronized Li^+ dynamics. Collectively, these findings underscore the utility of disorder as a design parameter: in cathodes, it reconfigures phase evolution pathways to avert degradation; in electrolytes, it redefines ion transport through entropy-driven lattice fluctuations—recasting disorder not as a defect but as a functional enabler of performance..

Keywords (max 5): Phase transition, Layered oxide cathodes, Phonon mode, Solid-state electrolytes, Machine learning

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

Compressible Lightweight Solid Electrolytes for Durable Batteries

Stefan Adams[1,*]

[1] *Dep. of Materials Science & Engineering, National University of Singapore, 5 Engineering Drive 2, Singapore 117579 Singapore*

* mseasn@nus.edu.sg

Abstract

Low-density solid electrolytes that are both electrochemically and mechanically compatible with high energy density cathode materials are necessary for energy-dense, long-lasting solid- state batteries. Here, we design and implement two types of compressible electrolytes that retain close interfacial contact with breathing cathodes, extending cycle life. One strategy to enhance compressibility and reduce mass density of solid electrolytes is to boost the ionic conductivity of Li-salt doped polymers by surface-active nanoceramics that create a percolating network of fast-conductive interphases. The resulting Ceramic-in-polymer Composite Electrolytes consisting of Li-salt doped polymers, plasticizers, and surface-active nanoceramics achieve Li^+ conductivities up to 1 mS/cm at densities <2 g/cm^3 and maintain broad electrochemical windows.[1] Symmetric cells cycle steadily at up to 5 mA/cm^2. Oriented nanoceramics [2] and electrolyte:electrode interface engineering [3] lead to further advancements.

An alternative all-inorganic approach is based on glass-ceramic oxyhalides $A_xMO_xCl_{5-x}$ (A=Li, Na; M=Nb, Ta; x≈1 [3,4]), which reach Li+ conductivities of about 10 mS/cm, we instead take use of the relationship between conductivity and glass forming ability. Large-angle rotations of NbCl4 groups around the axis of the one-dimensional NbCl4O2/2 chains facilitate the alkali ion transport perpendicular to the chains both in tetragonal LiNbOCl4 as well as in orthorhombic NaNbOCl4. Slightly above room temperature both phases transform into a viscoelastic “plastic-crystalline” state, which explains their good catholyte performance, according to our X-ray and neutron structure determinations, MD simulations, as well as thermo- and electrochemical characterisations. As catholytes in combination with sulphide anolytes both oxychlorides enable stable solid-state battery performance.

Keywords: Ceramic-in-Polymer Composites Solid Electrolytes, Oxychlorides, Solid State Batteries

References

(1) He, L. et al. *Energy Stor. Mater.* 2023, 60 102838.

(2) Wang, K. et al. *Adv. Science* 2024, 34, 2403797.

(3) Wang, K. et al. 2025 DOI: 10.22541/au.174492565.58592171/v1

(4) Tanaka, Y. et al. *Angew. Chem. Int. Ed.* 2023, 62, e202217581.

(5) Adams, S. *Energy Stor. Mater.* 2024, 68, 103359.

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

Beyond intercalation – Solvent co-intercalation and spillover in layered sulfides and sulfur/carbon composites

Philipp Adelhelm[1,2*]

[1] *Humboldt-University Berlin, Institute of Chemistry, Berlin, Germany*

[2] *Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Joint research group on operando battery analysis (CE-GOBA), Berlin, Germany*

* philipp.adelhelm@hu-berlin.de

Abstract

The use of sulfur and layered sulfides in batteries provides alternatives for the classical intercalation chemistry.

Layered sulfides enable reversible charge storage through solvent co-intercalation, a process that allows not only to minimize the charge transfer resistance but also to design new electrode materials. Solvents such as diglyme or propylene carbonate have been recently demonstrated to enable such a mechanism in Na_xTiS_2 and other layered sulfides.[1] When combined with co-intercalation anodes, the concept may enable the development of high-rate "co-intercalation batteries"[2,3] This talk will present recent findings on solvent co-intercalation and address key challenges and bottlenecks in the field.

Sulfur, on the other hand, offers a low-cost, high-capacity alternative to conventional intercalation materials. In metal-sulfur batteries, the cathode typically consists of a sulfur/carbon composite that is prepared by melt-infiltration. Surprisingly, sulfur/carbon composites exhibit a "sulfur spillover" process at room temperature, where sulfur wets the carbon surface and fills the carbon pores without requiring melt infiltration. This leads to a loss of carbon porosity and erases characteristic properties of sulfur—such as its melting point and x-ray diffraction signals—even at sulfur loadings of 50 wt%.[3] The presentation will discuss details of the spillover process and the impact on the cycling behavior of solid-state sulfur batteries.[4,5]

References

(1) Sun, Y.; Åvall, G.; Wu, S.-H.; Ferrero, G. A.; Freytag, A.; Groszewicz, P. B.; Wang, H.; Mazzio, K.; Bianchini, M.; Baran, V.; Risse, S., Adelhelm, P.; *Nature Materials*, 2025, DOI: 10.1038/s41563-025-02287-7

(2) Ferrero, G. A.; Åvall, G.; Janßen, K.; Son, Y.; Kravets, Y.; Sun, Y.; Adelhelm, P.; *Chem. Reviews* 2025, 125 (6), 3401-3439. DOI: 10.1021/acs.chemrev.4c00805.

(3) Medenbach, L.; Escher, I.; Köwitsch, N.; Armbrüster, M.; Zedler, L.; Dietzek, B.; Adelhelm, P. *Angew. Chem. Int Ed.* 2018, 57 (41), 13666-13670, Article. DOI: 10.1002/anie.201807295.

(4) Piccolo, F. et al., Healy et al. (unpublished data)

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

Expanding the Frontiers of Dye-Sensitized Photoelectrochemical Cells: Solar Valorization of Biomass and Beyond

Hyeong Cheol Kang[1] and Jae-Joon Lee[1]

[1] *Department Energy & Materials, Research Center for Photoenergy Harvesting & Conversion Technology (phct), Dongguk University, Seoul, 100-715, Republic of Korea*

* *jjlee@dongguk.edu*

Abstract

We actively explored dye-sensitized photoelectrochemical cells (DSPECs) as a sustainable platform for solar-driven chemical conversions, particularly targeting the selective transformation of lignocellulosic biomass. By integrating molecular dye systems with hydrogen atom transfer (HAT) mediators, we have demonstrated highly efficient photoelectrocatalytic pathways for the oxidative cleavage of C–O and C–C bonds in lignin-derived model compounds. Building upon these foundations, our current efforts focus on (1) tuning TiO_2 photoanode architectures through surface passivation strategies such as screen-printable blocking layers and $TiCl_4$ treatment, (2) engineering donor–π–acceptor (D–π–A) organic dyes to enhance charge transfer and stability, and (3) optimizing HAT co-catalysts for bond-selective oxidation.

Recent results include photocurrent densities exceeding 2.0 mA cm^{-2} and conversion efficiencies above 80% using ACT-based mediators. Notably, we achieved ambient-condition C(aryl)–C(alkyl) bond cleavage with turnover numbers >3000, and demonstrated that rational dye–surface interface design is crucial for minimizing recombination losses. In parallel, we have expanded DSPEC applicability toward reductive reactions and alcohol oxidation using Ru-based dyes, non-aqueous solvents, and real lignin substrates. These advances offer insight into the development of modular DSPEC systems applicable to solar biorefineries, artificial photosynthesis, and value-added chemical production.

Keywords (max 5): lignin valorization, dye-sensitized photoelectrochemical cell, hydrogen atom transfer, selective oxidation, solar biorefinery

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

Electrode materials synthesized by soft chemistry

Hajime Arai[1,*], Atsunori Ikezawa[1], Takeyoshi Okajima[1]

[1] *Institute of Science Tokyo, 4259 Nagatsuta, Midori-ku, Yokohama 226-8501 Japan*

* arai.h.9d0c@m.isct.ac.jp

Abstract

Soft chemistry is one of synthetic methods to prepare metastable materials, involving high-temperature calcination to form highly crystalline templetes with uniform chemical compositions, followed by chemical treatment at low temperatures such as acid leaching [1] and alkaline titration [2] to maintain the templete host structures. For example, $LiNiO_2$ obtained at 700°C can be modified to form Li_xNiO_2 (x~0) by acid leaching and spinel $Li_xNi_2O_4$ by low-temperature heating [3,4]. This presentation describes how soft chemistry can be applied to form various electrode materials.

Delithiated Li_xNiO_2 (x~0) was used to produce hydrated nickel hydroxides with potassium [5] or magnesium [6] located in the interlayer, which were examined for alkaline rechargeable cells. $NaMnO_2$ was converted to hydrated manganese dioxides that works high-capacity electrodes in alkaline rechargeable cells [7]. These highly crystalline materials are suitable for observing their structural changes during battery operation. Delithiated spinel manganese dioxides can be cycled in rechargeable proton cells that can replace conventional lead-acid batteries with insertion-extraction electrodes [8]. $NaNi_{1-x}Fe_xO_2$ was treated by hydration and ion-exchange to form (Ni,Fe)-based layered double hydroxides (LDHs) that works as a good electrocatalytic material for oxygen evolution reaction (OER) [9].

Keywords: Soft chemistry, Nickel hydroxide, Layered double hydroxide (LDH), Nickel metal-hydride, Oxygen evolution reaction (OER)

References

[1] Hunter, J.C. , *J. Solid State Chem*. **1981**, *39*, 142-147.

[2] Li, W.; McKinnon, W.R.; Dahn, J.R., *J. Electrochem. Soc*. **1994**, *141*, 2310-2316.

[3] Arai, H., Tsuda, M.; Saito, K.; Hayashi, M. et al., *J. Solid State Chem*. **2002**, *163*, 340-349.

[4] Arai, H., Tsuda, M.; Hayashi, M.; Ohtsuka, H. et al., *Electrochim. Acta* **2005**, *50*, 1821-1828.

[5] Imai, K.; Ikezawa, A.; Sato, S.; Arai, H., *Chem. Commun.* **2024**, *60*, 10192-10195.

[6] Xiao, M.; Ikezawa, A.; Arai, H., *Electrochem. Soc. Japan Fall. Meet. 2021* **2021**, 1F02, Sapporo, Japan.

[7] Kosasa, R.; Ikezawa, A.; Okajima, T.; Arai, H. et al., *Batt. Symp. Japan* **2024**, 2H06, Kyoto, Japan.

[8] Kida, Y.; Ikezawa, A.; Okajima, T.; Arai, H., *PRiME2024* **2024**, A09-1406, Hawaii, USA.

[9] Ikezawa, A.; Koito, S.; Arai, H., *J. Mater. Chem. A* **2024**, *12*, 31603-31611.

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

Degradation mechanism and ADT protocole for alkaline water electrolyzers

Shigenori Mitsushima[1,2,*], Ashraf Abdlhaleem[1], Yoshiyuki Kuroda[1, 2]

[1] *Institite of Advanced Sciences, Yokohama Naitonal University, 79-5 Tokiwadai, Hodogayaku, Yokohama 240-8501, Japan*

[2] *Graduate School of Engineering Science, okohama Naitonal University, 79-5 Tokiwadai, Hodogayaku, Yokohama 240-8501, Japan*

* mitsushima-shigenori-hp@ynu.ac.jp

Abstract

Hydrogen is expected to serve as both an energy carrier and a fuel for hard-to-decarbonize sectors. Therefore, cost-effective hydrogen production with low carbon emissions is essential. Hydrogen produced via water electrolysis powered by renewable electricity is considered CO_2-free "green hydrogen." To reduce production costs, durability under fluctuating renewable power conditions is required.

Alkaline water electrolysis (AWE) is considered a promising approach for low-cost, large-scale hydrogen production because it does not require precious metals; however, degradation under fluctuating renewable electricity remains a significant issue. In particular, start-stop operations are severe, as electrodes are exposed to wide potential ranges. Understanding the degradation mechanisms and developing accelerated durability testing (ADT) protocols are crucial for designing durable materials.

In AWE stacks, due to shunt currents, the anode and cathode potentials can become nearly identical. We proposed an ADT protocol involving alternating chronopotentiometry at 0.6 A cm^{-2} and chronoamperometry at 0.5 V vs. RHE every 60 seconds. Under this ADT, a standard NiCo oxide-coated Ni anode exhibited degradation involving Co dissolution and subsequent catalyst layer detachment. This detachment was found to be suppressed by optimizing the coating temperature of the NiCo oxide layer.

Keywords: Water electrolysis, Hydrogen production, Degradation, Accelerated durability testing

Acknowledgments

This research was supported by JPNP 20003 project that was commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

References

(1) Mitsushima, S.; et. Al., *Electrochemistry* **2025**, 93 (4), 046001.

(2) Abdel Haleem, A.; et. Al., *J. Power Sources* **2022**, *535*, 231454.

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

Fabrication of Lithium Metal Powder with Surface Protection Shells for High-Performance Lithium Batteries

Jagabandhu Patra, Ming-Kuen Huang, Jeng-Kuei Chang*

Department of Materials Science and Engineering, National Yang Ming Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan

* Email: jkchang@nycu.edu.tw

Abstract

Surface-engineered stabilized lithium metal powder (SLMP) is synthesized using a simple, safe, and energy-efficient method that eliminates the need for high temperatures and hazardous molten lithium handling. By optimizing the processing parameters, we successfully engineers a tailored surface protection shell, enabling the dual functionality of SLMP as both an anode material and a prelithiation reagent. The synthesized SLMP is employed to fabricate a thin Li electrode (Li_{SLMP}) via a binder-free slurry casting method. The resulting electrode exhibits excellent stability in dry air and strong mechanical durability, as confirmed by bending, coiling, and adhesion tests. Compared to conventional lithium foil, a Li_{SLMP}-based symmetric cell exhibits significantly improved interfacial stability and uniform lithium stripping/plating, maintaining stable voltage hysteresis for approximately 700 hours of cycling and achieving a high critical current density of 25 mA cm^{-2}. A full cell paired with a $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ cathode demonstrates superior electrochemical performance, including excellent high-rate capability (130 mAh g^{-1} at 1500 mA g^{-1}) and outstanding cycling stability (95% retention after 100 cycles). A three-electrode study reveals reduced anode polarization, which reaults in imoproved cell charge-discharge capacities, especially at high rates. Moreover, precise control over Li_{SLMP} thickness enables a tunable areal capacity and predictable cycle life. This advancements also contribute to enhanced battery energy density and safety. Additionally, using SLMP as a prelithiation agent for Si/C anodes significantly improves the initial coulombic efficiency from 72% to 92%. Collectively, these attributes position the developed Li_{SLMP} as a key enabler for high-energy-density and high-perforamce lithium batteries.

Keywords: Stabilized Lithium Metal Powder, Thin Lithium Electrode, Critical Current Density, Prelithiation Agent

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

Computation-Aided Design of Materials Related to Lithium-Ion/Metal Batteries

Jyh-Chiang Jiang

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 106, Taiwan

Abstract

Various battery configurations related to Li metal anodes have been proposed in recent decades. These include anode-free rechargeable Li-metal batteries (AFLMBs), Li–S batteries, and Li batteries with high-voltage cathode materials, which differ significantly from those of commercial Li-ion batteries. Furthermore, the liquid range of electrolytes is crucial for maintaining optimal electrochemical performance under various battery operation scenarios, such as extreme weather conditions that can reduce the effective range of electric vehicles and uncrewed underwater or aerial vehicles that rely on batteries to operate at low or high temperatures. In addition, high-energy-density lithium-ion batteries have been widely studied and have received considerable attention for their application as a primary power source. Since the cathode often experiences issues with oxygen evolution and transition metal dissolution during charging and discharging, it is crucial to design and develop innovative cathode materials with high specific capacity and high redox potential.

Here, I will introduce how we systematically studied the surface instability of Li-rich and Ni-rich cathodes, including the formation of superoxides and the dissolution of transition metals (TMs), using density functional theory and ab initio molecular dynamics calculations. We also explored the effects of S and Cl anion substitution on structural stability and electrochemical performance.[1] Furthermore, I will demonstrate how the investigation combines density functional theory and the conductor-like screening model for realistic solvents to identify electrolytes with a wide liquid temperature range and high LiTFSI solubility.[2,3]

Keywords (max 5): Lithium ion bartteries, Density functional theory, Ab initio molecular Dynamics, Conductor-like screening model

References

1. (1) Kuan-Yu Lin, Santhanamoorthi Nachimuthu, Han-Wen Huang, and Jyh-Chiang Jiang*, npj Comput. Mater. (2022) 8:210.

2. Wu, LT; Zhan, YT; Li, ZL; Chen, PT; Hwang, BJ; Jiang, JC*, Journal of Materials Chemistry A 2024, 12, 15792-15802.
3. Liang-Ting Wu, Bing Joe Hwang, and Jyh-Chiang Jiang*, Chem. Eng. J. 515 (2025) 163801.

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

Work Function Centric Theory for Heterogeneous Electron Transfer Kinetics : ORR on Single Crystal Pt (h k l)

Rama Kant
Department of Chemistry, University of Delhi
Delhi 110007, India
Email: rkant@chemistry.du.ac.in

Abstract

A novel electrode work function centric theoretical approach for heterogeneous electron transfer (HET) is developed. Theory is based on the activation barrier, dependent on electron affinity ratio for the electrode and, the energy gap between electrode and the frontier molecular orbital. Theory postulate that the electrode quasi-Fermi energy level (in presence of surface dipoles and adsorbates) alignment with the fluctuating frontier molecular orbital of electroactive species results in the formation of transition state. This stochastic processes-based approach for HET is applied to many complex electrochemical systems: (i) the outer sphere heterogeneous electron transfer (OS-HET) rate constant[1-4] at atomically stepped nanocorrugated metal surface[1], and application to oxygen reduction reaction (ORR) on single crystal Pt of varying Miller indices, (ii) anion bridge assisted electron transfer kinetics on stepped metal, (iii) graphene covered metal electrode. Our theory circumvents limitations of Marcus-Hush theory for HET and show quantitative agreement with various experimental observations. Predictions for HET kinetics for oxygen reduction reaction and surface kinetics heterogeneity is used to generate EIS response on Pt (h k l) with and without adsorbing halide ions.

Keywords (max 5): EIS for electric double layer coupled electron transfer, Electrochemical Work Function, FMO of Electroactive Species, Bridging Ligand, Anion Adsorption

References

[1.] *Neha and R. Kant, J. Phys. Chem. C, 2024, 128, 12399-12413.*
[2.] *R. Kant and G. K. Mishra, J. Phys. Chem. C, 2023, 127, 14, 6884–6899.*
[3.] *G. K. Mishra and R. Kant J. Phys. Chem. A, 2023, 127, 13, 3048-3062.*
[3.] *R. Kant, G. K. Mishra and Neha, 2022, Nanoscale, 14. 5600.*
[4.] *G. K. Mishra and R. Kant, 2021, J. Phys. Chem. C, 125, 25774−25783.*
[5.] *J. Kaur and G. K. Mishra, J. Phys. Chem. C, 2020,124, 2273-2288.*

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

Modulating the Electronic Structure of Ni Single-Atom via Phosphorous for Efficient CO_2 Electroreduction

Kuei-Hsien Chen[1,2,*], Mengstu Etay Ashebir[1], Omran Moradlou[1], Li-Chyong Chen[2,3]

[1] *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*

[2] *Center for Condensed Matter Sciences, National Taiwan University, Taipei City 10617, Taiwan*

[3] *Department of Physics, National Taiwan University, Taipei 10617, Taiwan*

* chenkh@pub.iams.sinica.edu.tw

Abstract

The electrocatalytic carbon dioxide reduction reaction (eCO2RR) in an acidic environment is crucial for mitigating carbonate and bicarbonate formation while enhancing CO2 conversion efficiency. However, the hydrogen evolution reaction (HER) often outcompetes eCO2RR in a proton-rich microenvironment, posing a significant challenge. This study introduces an in-situ phosphatizing method to alter the electronic structure of a Ni–N4 single-atom catalyst (Ni–N3PC), thereby suppressing HER and promoting eCO2RR performance in acidic environments. The Ni–N3PC catalyst achieves a CO Faradaic efficiency (FE) exceeding 90% over a wide potential range, high carbon conversion efficiency, a CO partial current density of –357.7 mA cm–2, and long-term stability for 100 hours at –100 mA cm–2 with a FE of 85%. Electrochemical impedance spectroscopy and turnover frequency analysis reveal that Ni–N3PC exhibits lower charge-transfer resistance and higher intrinsic activity, respectively. The structural characterization using X-ray absorption spectroscopy confirms the formation of Ni–P and Ni–N bonds while scanning transmission electron microscopy shows atomically dispersed Ni atoms on carbon networks. Density functional theory calculations further support the experimental results, showing that Ni–N3PC significantly lowers the energy barrier for the key *COOH intermediate, resulting in outstanding eCO2RR performance. This research provides valuable insights into the design of highly efficient Ni single-atom catalysts for industrial eCO2RR applications.

Keywords: single atom; electronic structure; electroreduction; proton microenvironment

References

(1) Mengstu Etay Ashebir, Palani Sabhapathy, Osama Nasr, Varad Modak, Omran Moradlou, Amr Sabbah, Chih-Yang Huang, Santhanamoorthi Nachimuthu, Jyh-Chiang Jiang, Ying-Li Hu, Chen-Hsiung Hung, Li-Chyong Chen, Kuei-Hsien Chen, Chem. Engineering J. 509, 161319 (2025)

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

In situ visualization of local electrochemical activity of 2D catalysts

Li-Chyong Chen[1,2,3*], Septia Kholimatussadiah[1,2,3], Yu-Ling Liu[2], Mohammad Qorbani[2,3], Kuei-Hsien Chen[2,4]

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

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

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

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

*E-mail: chenlc@ntu.edu.tw

Abstract

Scanning electrochemical microscopy (SECM) is a versatile technique that can locally capture electrochemical current generated by any specified chemical reaction. Meanwhile, two-dimensional (2D) transition metal dichalcogenides (TMDs), such as MoS_2 and WSe_2, have recently emerged as promising materials for energy applications. Understanding and optimizing these materials is crucial for the development of systems that efficiently interconvert electrical and chemical energies. Here we use atomic force microscopy coupled with SECM to spatially resolve and quantify the local electrochemical activity of various 2D TMDs, *i.e.*, WSe_2, V-alloyed MoS_2, and NbS_2–WSe_2 heterostructures, which are amongst some emerging materials for next-generation energy storage and conversion. Firstly, we found the number of layers play a significant role in the basal plane electrochemical activation of WSe_2. Local variations in electrochemical activity was also observed in V-alloyed MoS_2, indicating that alloying MoS_2 strongly alternates its electrochemical properties. Lastly, we investigate electrochemical activity of NbS_2–WSe_2 vertical heterostructures. High work function metallic NbS_2 forms an ohmic contact with p-type WSe_2, improving charge injection by reducing its contact resistance. Our SECM results show NbS_2 enhances the basal plane activity of WSe_2, whereas WSe_2 electrochemically screens the activity of NbS_2, indicating its potential as a protective layer for NbS_2 from rapid surface oxidation. We suggest that this type of metal–semiconductor heterostructures to be suitable for photoelectrochemical energy devices. In conclusion, in situ visualization of nanoscale electron transfer and electrocatalytic hydrogen evolution reaction was achieved using SECM. The methodology and results reported in this study can be applied for other nanomaterials, particularly in finding and designing future energy devices.

Keywords: electron transfer, hydrogen evolution reaction, scanning electrochemical microscopy, transition metal dichalcogenides, two-dimensional materials