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Toward Sustainable and Safe Battery

Atsuo Yamada*

Country Department of Engineering, The University of Tokyo, 7-3-1, Hongo, Bunkyo, Tokyo 113-8656, Japan

* yamada@chemsys.t.u-tokyo.ac.jp

Abstract

The current generation Li-ion batteries employ oxides such as $\text{Li}(\text{Ni}, \text{Mn}, \text{Co})\text{O}_2$ and olivine LiFePO_4 as cathodes. However, the growing concern on scarcity and large-scale applications of Li-resources have steered effort to realize sustainable sodium-ion batteries, Na and Fe being abundant and low cost charge-carrier and redox center. We have identified a hitherto-unknown $\text{Na}_2\text{Fe}_2(\text{SO}_4)_3$ with Alluaudite structure, registering the highest ever $\text{Fe}^{3+}/\text{Fe}^{2+}$ redox potential at 3.8 V (vs. Na) along with very fast rate kinetics, leading to ultra-cheap yet competitive energy density with lithium battery with LiFePO_4 cathodes. Our discovery is now on mass-production (> 50,000 ton per year) stage for yearly > 7 GWh sodium-ion battery to drive electric bike in China from 2024 to replace lead-acid batteries. At this juncture, details on electrode performances, reaction mechanisms, structure evolution, ionic/electron transport properties, moisture sensitivity, LCA impact, and their modification by forming solid solutions of Fe-Mn or $\text{SO}_4\text{-PO}_4$ system will be introduced as time permits.

Alongside, the increasing energy density and size requirements has necessitated establishing reliable safety technologies for rechargeable batteries. However, comprehensive safety evaluations at the full-cell level are limited by size requirements (greater than the ampere-hour scale) for performing accelerating rate calorimetry (ARC) tests that can provide critical information on heat generation during thermal runaway. We designed cylindrical-pouch-type miniature batteries (~21 mAh, ~0.1 g of cathode active materials) that are highly susceptible to heat generation, thus allowing to perform full-cell-level ARC tests on a laboratory scale. This enables rapid safety screening and early-stage feedback for battery design, which can help accelerate the development of high-safety batteries.

Keywords: Abundancy, Safety, ARC

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Nanocatalysts for Electrochemical Energy Conversion Reactions

Bing Joe Hwang^{1,2*}

¹*Sustainable Electrochemical Energy Development (SEED) Center, National Taiwan University of Science and Technology, Taipei, Taiwan*

²*Synchrotron Radiation Research Center, Hsinchu, Taiwan*

E-mail: bjh@mail.ntust.edu.tw

Abstract

Electrochemical green energy technologies—including energy conversion and storage—are critical to achieving net-zero carbon emissions. In this talk, I will present an integrated approach combining materials design, interfacial engineering, and operando characterization to enhance the catalytic activity, selectivity, and long-term durability of nanostructured electrocatalysts for applications in fuel cells, water splitting, value-added electrolysis, and CO₂ electroreduction. For the oxygen reduction and evolution reactions (ORR/OER), we have developed both precious and non-precious metal nanocatalysts with tailored morphologies and engineered supports to improve active site accessibility and mass transport. In the context of value-added hydrogen production and CO₂ electrolysis, our research highlights bifunctional and single-atom catalysts designed to modulate electronic structures and achieve precise control over reaction mechanisms. A central feature of this work is the use of in situ and operando techniques—complemented by density functional theory (DFT) calculations—to probe reaction pathways, active intermediates, and catalyst degradation mechanisms at the atomic level. These insights guide the rational design of highly efficient and robust catalysts under practical operating conditions. Finally, I will discuss how these nanocatalyst platforms have been successfully integrated into emerging electrochemical systems, including fuel cells and value-added electrolyzers, reinforcing their relevance to sustainable clean energy solutions.

Keywords: Nanocatalysts, Value-added Electrolysis, In-situ, Hydrogen, Carbon Dioxide

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Oxygen-redox chemistry in layered transition metal oxides for advanced lithium-ion battery cathode materials

Kisuk Kang^{1,2,*}

¹ Department of Materials Science and Engineering, Research Institute of Advanced Materials (RIAM), Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea

² Institute for Rechargeable Battery Innovation, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea

* matlgen1@snu.ac.kr

Abstract

The discovery of layered TiS_2 and LiCoO_2 compounds has led to the proliferation of modern lithium-ion batteries, exploiting the lithium-ion insertion/deinsertion chemistry toward the high-energy-density battery system. For the past decades, extensive efforts have been placed in improving the performance of these layered compounds for cathodes such as by compositional tuning and structural modifications. One of the notable approaches in recent years is to exploit the oxygen redox activity by adopting excess amounts of lithium-ions in the layered materials. This shift from the conventional cationic redox reaction relying on transition metals (Co, Ni and Mn) to the cumulative cationic and anionic (oxygen) redox reaction enables the boost of the specific capacity over state-of-the-art cathodes. In this journey to explore the 'lithium-excess layered cathodes', various new findings/challenges have been being disclosed. In this talk, I will present our recent understandings on these materials with respect to the lithium insertion mechanism that differs from what have been observed in conventional layered materials and the effect of the layered stacking sequences, and discuss on the outlook on the lithium-excess layered cathodes.

Keywords : Cathode material, Lithium-excess layered cathode, Anionic redox, Oxygen redox chemistry,

Layered stacking sequence

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Operando studies of intercalation processes

Clare P. Grey¹, Sian Dutton² and Akshay Rao²

¹ Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge UK

²Cavendish Laboratory, University of Cambridge, Cambridge UK

* cpg27@cam.ac.uk

Abstract

This talk will discuss the development and application of operando methods to study how ions are inserted into lithium- and sodium-ion electrode materials. Together with Prof. Akshay Rao, we have shown that optical methods that probe changes in light scattering can be used with sufficient time and spatial resolution to follow (de)intercalation processes in single, micron-sized particles. A variety of different mechanisms have been observed, which depend (i) on the ion diffusivities in the solids, and how they change as a function of e.g., Li⁺ content, (ii) the rate of ion insertion, (iii) particle size and (iv) in layered materials, coupling between the layers. In LiCoO₂, delithiation follows a shrinking core model, ions being removed from all surfaces of the particle, while the poor Li transport in the fully lithiated material results in an “intercalation wave” mechanism, involving a single nucleation site, the new phase propagating across the particle. A new mechanism is identified for intercalation in the dilute stages of graphite that is reminiscent of an “avalanche” phase transition, where layers within sub-domains of the particle are intercalated individually. In the dense stage, where there is stronger coupling between the layers, a more conventional intercalation wave mechanism is seen. Facet dependent processes can be followed, along with communication between particles.

The second part of my talk will compare lithium- and sodium-nickelates and the roles of Jahn-Teller distortions, antisite defects and charge and cation-ordering in phase transitions.

Keywords: Operando methods, phase transitions, Jahn-teller distortions

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Controlling Interface Phenomena in Batteries by Innovative Materials Engineering

Satishchandra Ogale^{*1,2}

¹ *Research Institute for Sustainable Energy, TCG-CREST, Sector V, Salt Lake, Kolkata, India*

² *Indian Institute of Science Education and Research, Pune, India*

* satishogale@gmail.com, satishogale@tcgcrest.org

Abstract

Batteries are perhaps the most sought after device systems at the present time in view of their implications for large scale implementation of clean and renewable energy technologies; but at the same time they are present a complex, non-trivial and intriguing electrochemical interplay of different materials and phases as well as their interfaces. Controlling the interface phenomena is the most challenging aspect of the emergent battery science if a robust high performance battery technology is to be realized for broader applicability. Amongst the multiple interface phenomena the solid electrolyte interphase (SEI) formation and dendrite formation most critically control the battery performance. In this talk, I will strive to address these with particular emphasis on innovative electrode and electrolyte engineering approaches, deriving from some of our recent research results. The battery systems in focus will be Li and Na ion batteries and anode-free Li/Na metal batteries.

Keywords (max 5): Battery, Electrode, electrolyte, Engineering, Anode-Free

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Practical solid batteries via in situ solidification technologies

Hong Li¹⁻⁴

¹*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

²*Beijing WeLion New Energy Technology Co., Ltd., Beijing 100176, China*

³*Tianmulake Excellent Anode Material Ltd., Liyang, 213399, China*

⁴*Tianmulake Institute of Energy Storage Co., Ltd., Liyang, 213399, China*

E-mail: hli@iphy.ac.cn

Abstract

Developing lithium ion batteries with high energy density, high power density, high safety, long cycle life, wide operation temperature, low cost and large production ability is an important target for various emerging applications. ASSB is regarded as the most promising solution to satisfy all these requirements simultaneously. The commercialization time of ASSB have been claimed from 2026-2030 by several famous manufacturers. We purposed to develop in-situ solidification technology for ASSB since 2016. Semi-solid batteries have been also developed based on this technology. The main advantage is to form continuous ion paths at atomic level in the cell during the whole operation life, aiming to solve the solid/solid contact problem in ASSB. In addition, the layered cathode coated by solid electrolyte, solid electrolyte coated and filled separator, low expansion nano-Si/C anode with high capacity, anode prelithiation, in situ solidification as well as the filling of the pores in the electrode and separator using nanosized oxide electrolytes have been developed and demonstrated. Consequently, LIB for 3C, drone , EV with high enegy density and energy storage cell with high safety have been developed. In this report, we will update related progresses on LIB using in situ solidification technology from semi-solid to ASSB.

Keywords: ASSB, LIB, oxide electolyte, in situ solidification, semi-solid