ICNaB 2025

The 10th International Conference on

Sodium Batteries

6-10 October 2025 Sydney

Conference Abstracts

Ionic Electrolytes for Sodium Batteries: The Impact of Ion Structure on Properties and Performance

Jenny Pringle,*[1] Lukasz Kufel,[1] Faezeh Makhlooghiazad,[1] Rachel Mah[1] and Maria Forsyth[1]

[1]Deakin University Burwood Campus, 221 Burwood Highway, Burwood,
VIC 2125, Australia.
E-mail: jenny.pringle@deakin.edu.au

Keywords: ionic liquids • plastic crystals • zwitterions • polymer electrolytes

Abstract: Electrolytes composed entirely of ions offer important safety and performance advantages over traditional molecular solvent-based systems, particularly for devices utilising reactive metals such as sodium. The benefits of ionic liquid (IL) based electrolytes are increasingly being recognised, while Organic Ionic Plastic Crystals (OIPCs) offer many of the same advantageous features and they are solid at room temperature. [1,2] An important approach to developing these safer electrolytes is increasing the range of known and well-characterised families. The nature of the cations and anions used to make IL and OIPC electrolytes for sodium batteries can have a significant impact on the chemical, physical and electrochemical properties and device performance, but the structure-property relationships are not well understood. Furthermore, the different sodium salts that can be used in combination with the IL or OIPC introduces further complexities in terms of understanding and optimising the thermal, electrochemical and transport properties. The field of ionic electrolytes can be further expanded by tethering the cation and anion together to form zwitterions. The development of zwitterions with molecular disorder allows their use as the main electrolyte matrix or as additives to polymers.[3]

Here we discuss our development of new, non-volatile ionic electrolytes for sodium batteries. Insights into the relationships between the different ionic structures of ILs, OIPCs and zwitterions and the physical, thermal and electrochemical properties of the resultant electrolytes will be presented.

References:

[1]. J. Sun, C.S.M. Kang, G. Huang, F.M.F. Vallana, A. Kumar, L.A. O'Dell, M. Galceran, O. Hutt, P.C. Howlett, M. Forsyth, J.M. Pringle, *J. Mater. Chem. A*, 2023 11, 22329-22339.

[2]. M. Salado, T. H. Smith, N. Sirigiri, F. Chen, L. A. O'Dell, J. M. Pringle, M. Forsyth, *JACS Au* 2025, *5* (4), 1663-1676.

[3]. F. Makhlooghiazad, L. A. O'Dell, L. Porcarelli, C. Forsyth, N. Quazi, M. Asadi, O. Hutt, D. Mecerreyes, M. Forsyth, J. M. Pringle, *Nat. Mater.*, 2022, 21, 228.

Biography: Jenny Pringle works in the Institute for Frontier Materials at Deakin University, Melbourne. She received her degree and PhD at The University of Edinburgh in Scotland, working on ionic liquids, before moving to Monash University in 2002 and then Deakin University in 2013. She leads research into the development and use of ILs and OIPCs for applications including sustainable cooling, thermal energy storage, CO_2 separation membranes, sodium and lithium batteries.

Fading Mechanism of Na-ion Batteries: Particle Cracking vs. Interfacial Reactivity

Xiaolin Li

Pacific Northwest National Laboratory, United States

Email: xiaolin.li@pnnl.gov

Abstract: Sodium-ion batteries continue to gain traction as promising alternatives to Li-ion batteries across various applications. In this presentation, the progress of Sodium-ion Alliance for Grid Energy Storage (SAGES) is briefly summarized. Using layered oxide cathodes and alloy anodes as model materials, the fading mechanisms of sodium-ion batteries including particle cracking and interfacial reactivity are discussed. The electrode-electrolyte interaction is believed to be more dominant than particle cracking in determining the performance fade.

Biography: Xiaolin Li currently is a scientist in the group of Electrochemical Materials and Systems in Energy Processes and Materials Division. He joined Pacific Northwest National Laboratory (PNNL) in December 2009. Before that, he conducted his postdoctoral research on carbon nanotubes and graphene with Prof. Hongjie Dai, NAS fellow, at Stanford University. Dr. Li has extensive experience with carbon nanotubes, graphene, and is an expert in designing nanostructured functional materials for various applications. He has authored/co-authored more than 80 papers including Science, Nature Nanotechnology, Journal of the American Chemical Society, Angewandte Chemie International Edition, Energy Environmental Science, Nature Communications, and Advanced Materials, to name a few. According to Google Scholar, he has a total citation of more than 20,000 times.

Tailoring Transport of Charge Carriers in Electrochemical Energy Storage Systems

Yuping Wu*

Confucius Energy Storage Lab, School of Energy and Environment & Z Energy Storage Center, Southeast University, Nanjing 211189, China
E-mail: wuyp@seu.edu.cn

Keywords: energy storage • electrolyte • anode • cathode • separator

Abstract: In the case of lithium or sodium batteries, the charge/discharge processes are related to the movement of charge carriers (electrons and cations). As a result, this movement is very crucial to electrochemical performance and safety for batteries. In this report, our main works on tailoring the transport of electrons/cations in anodes, cathodes, separators and solid electrolytes will be expounded.

Biography: Yuping Wu, chair professor of Southeast University, FRSC, executive dean of Z Energy Storage Center. He got his PhD in 1997 from Chinse Academy of Sciences. So far he has published over 560 papers in SCI-indexed journals with H-index of 110, editored over 10 books, and got over 30 licensed patents from China, US, EP and Japan. He was awarded as one of the Most Influential Minds over the World in 2015 (less than 20 every year) by Thomson Reuters from the Highly Cited Researchers. His main research work is on electrochemical energy storage systems and their key materials. His researches led to some edge-cutting technologies such as pore-free separators for lithium batteries, hybrid supercapacitors, and aqueous rechargeable lithium batteries. He is the founding as editor-in-chief of Energy Materials (IF=11.8) since 2021, and associate editor of Energy & Environment Materials (IF=13).

Functional Electrolytes for Sodium Secondary Batteries

Kazuhiko Matsumoto,* [1] Shaoning Zhang,[1] Duanfei Han,[1] Kohei Nishimoto,[1] Kentaro Kamada,[1] Fumiyasu Nozaki,[1] Jinkwang Hwang[1]

[1]Graduate School of Energy Science, Kyoto University, Yoshida, Sakyo-ku, Kyoto 606-8501, Japan

E-mail: matsumoto.kazuhiko.4c@kyoto-u.ac.jp

Keywords: additive • Na metal • ionic liquid • chemical oxidation

Abstract: Although some additives are known to improve initial coulombic efficiency, their effects have not been studied in detail. In this study, we systematically evaluated a series of fluoro(oxo)-borate and -phosphate addtives in sodium ion batteries. The use of NVP ($Na_3V_2(PO_4)_3$) counter electrode is a key strategy to avoid the physical and electrochemical contamination from Na metal counter electrode.[1] The resulting data exhibits the different role of additives at the cathode and anode sides.

Direct synthesis of triphylite $NaFePO_4$ is not achieved because of its thermodynamic metastability, which leads to the formation of maricite $NaFePO_4$. It is typically prepared through heterosite $FePO_4$ by electrochemically delithiating $LiFePO_4$. Our previous study revealed $LiFePO_4$ can be chemically oxidized to $FePO_4$ by Cl_2 gas in the presence of $AlCl_3$, which enables a large-scale preparation of $FePO_4$.[2] We recently confirmed that O_2 gas can also delithiiate $LiFePO_4$ in the presence of acetic acid, which allows the repeated synthesis of $LiFePO_4$ from the recovered lithium acetate. The resulting $FePO_4$ serves as a positive electrode for charged-state sodium metal batteries,[3] especially in ionic liquid electrolytes at elevated temperatures by making use of high thermal stability of ionic liquids.[4,5]

References:

[1]. J. Hwang, K. Takeuchi, K. Matsumoto, R. Hagiwara, J. Mater. Chem. A 7 (2019) 27057.

[2]. F. Nozaki, S. Shomura, J. Hwang, K. Matsumoto, R. Hagiwara, ACS Sustain. Chem. Eng. 11 (2023) 1037.

[3]. F. Nozaki, S. Zhang, M. H. Petersen, J. Hwang, J. H. Chang, J. M. García-Lastra, K. Matsumoto, Energy Environ. Sci. 18 (2025) 1408.

[4]. A. Basile, M. Hilder, F. Makhlooghiazad, C. Pozo-Gonzalo, D. R. MacFarlane, P. C. Howlett, M. Forsyth, Adv. Energy Mater. 8 (2018) 1703491.

[5]. K. Matsumoto, J. Hwang, S. Kaushik, C.Y. Chen, R. Hagiwara, Energy Environ. Sci. 12 (2019) 3247

Biography: Kazuhiko MATSUMOTO received his PhD degree at Kyoto University in 2004. He extended his research areas as a postdoc at Aichi Institute of Technology, McMaster University, and Kyoto University. He was appointed Assistant Professor in 2010 at Kyoto University and was promoted Associate Professor and Professor in 2015 and 2024, respectively. His research interests are in evaluation of electrolyte and electrode materials for electrochemical devices and applications of ionic liquids and fluoride materials. He received the Sano Award for Young Researchers (the Electrochemical Society of Japan) in 2013 and Commendation for Science and Technology by the MEXT (Young Scientist Award) in 2017. He is currently a director of the Electrochemical Society of Japan and Society of Fluorine Chemistry, Japan.

Design of High-Performance Sodium-Ion Polyanion Systems for Electrode and Solid Electrolyte Materials from Theory and Computation

Pieremanuele Canepa,[1,2,*] Wang Ziliang,[2,3] Sunkyu Park,[4,5] Eunike Mahayoni,[4,5] Zeyu Deng,[3] Jean-Noël Chotard,[4] Vincent Seznec,[4] Laurence Croguennec,[5] and Christian Masquelier[4]

[1]Department of Electrical and Computer Engineering and Texas Center of Superconductivity, University of Houston, Houston, TX, USA

[2]Department of Materials Science and Engineering, National University of Singapore, Singapore

[3]Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA

[4]Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie Jules Verne, CNRS, Amiens, France

[5]Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB), Université de Bordeaux, Bordeaux INP, CNRS, Pessac, France

E-mail: pcanepa@uh.edu

Abstract: Identifying substitutes for lithium (Li)-ion batteries is crucial for enhancing and diversifying energy storage technologies. When the life-cycle analysis is examined in the design of batteries, sodium (Na) is attractive because it can be "harvested" directly from seawater, making Na ~50 times lower in cost than Li. An important class of phosphate electrodes and electrolytes discovered by Hong and Goodenough is the Natrium Super Ionic Conductors (NASICONs) with the chemical formula $Na_xM_2(XO_4)_3$, where M is a transition metal, and X = Si and/or P. NASICON electrode and electrolyte materials display significant Na-ion mobility. In this talk, we will demonstrate that first-principles methods can guide the design of better NASICON electrodes and electrolytes, with superior energy densities and improved ion transport. For example, our *ab initio* predictions indicate that suitably doped NASICON compositions, especially with high silicon content, can achieve high Na^+ mobilities. We will showcase "smart" synthesis procedures to drastically reduce or even eliminate the impurities of these NASICON compositions.

We will show how these NASICON solid electrolytes can be integrated with novel high-energy density $Na_xV_2(PO_4)_3$ positive and negative electrode materials to incorporate into All-NASICON monolithic batteries that do not require any stacking pressure for operations. These findings push the optimization of mixed polyanion solid electrolyte and electrode compositions, including sulfide-based polyanion frameworks, which are known for their superior ionic conductivities.

Biography: Pieremanuele Canepa is the Assistant Professor in the Department of Electrical and Computer Engineering at the University of Houston and a member of the Texas Center for Superconductivity. His research focuses on computational materials science, using first-principles and high-throughput methods to design and understand materials for energy storage and conversion. He works extensively on electrodes, solid electrolytes, and multivalent ion batteries, applying advanced thermodynamics, electrochemistry, and spectroscopy tools to accelerate the development of next-generation energy technologies.

Agricultural Biomass-Derived Materials for Sodium-Ion and Lithium-Ion Battery Anode Applications

Zhanying Zhang

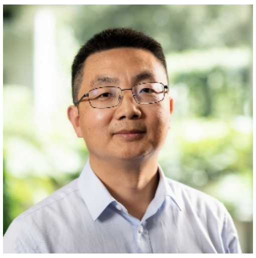
School of Mechanical, Medical and Process Engineering, Centre for Agriculture and the Bioeconomy, Queensland University of Technology, 2 George Street, Brisbane, Queensland 4000, Australia

E-mail: jan.zhang@qut.edu.au

Keywords: biomass • lignin • hard carbon • SiO_x/C • battery • anode

Abstract: Lignocellulosic biomass, such as sugarcane bagasse, is an abundant, low-cost, and renewable bioresource. It is primarily composed of three major components: cellulose, hemicellulose, and lignin. Lignin, a phenolic biopolymer, possesses a high carbon content (60%–65%), making it an attractive precursor for the production of hard carbon materials for sodium-ion battery (SIB) anode applications. Additionally, certain types of lignocellulosic biomass, such as rice husk, contain up to 20% silica, offering the potential for the synthesis of SiO_x/C composite anodes suitable for high-energy-density lithium-ion battery (LIB) applications.

Professor Zhang's research group is actively developing methodologies for the synthesis of lignin-derived hard carbon for SIB anode applications. Through various strategies involving biomass pretreatment, lignin processing and modification, and precise control of the carbonization process, the group has successfully produced lignin-derived hard carbon materials exhibiting high reversible sodium storage capacities exceeding 330 mAh/g and initial coulombic efficiencies above 80%. Furthermore, Professor Zhang has proposed sustainable and cost-effective strategies for the synthesis of high-performance SiO_x/C materials from lignocellulosic biomass, with the aim of replacing conventional SiO_x/C materials produced via costly chemical vapor deposition techniques for LIB applications. In this presentation, Professor Zhang will provide an overview of the group's recent progress in the synthesis of lignin-derived hard carbon for SIB applications and outline their ongoing efforts to develop biomass-derived SiO_x/C materials for LIB anodes.



Biography: Zhanying Zhang is an ARC Mid-Career Industry Fellow at QUT. His group focuses on converting agricultural biomass into nanocellulose, silica nanoparticles, lignin nanoparticles, hybrid nanoparticles, porous carbon, hard carbon and SiO_x/C for energy storage, thermal energy management, enhanced (bio)polymer composites, packaging, and other applications. Prof Zhang's group also works on the production of functional ingredients from food processing waste for food and beverage applications. Additionally, he previously developed biomass pretreatment technologies for producing fermentable sugars and biofuels, as well as waste processing technologies for resource recovery from municipal sludge, waste textile and used carpet.

Precursor Tuning Towards High Performance Hard Carbon for Sodium-Ion Batteries

Yuki Fujii,[1] Aoto Koizumi,[1] Naoki Rokuhira,[1] Zachary. T. Gossage, Changhee Lee, Tomooki Hosaka, Daisuke Igarashi, and Shinichi Komaba* [1]

[1]Department of Applied Chemistry, Tokyo University of Science, Shinjuku, Tokyo 162-8601, Japan
E-mail: komaba@rs.tus.ac.jp

Keywords: negative electrode • hard carbon • high capacity • carbonization yield • rate capability

Abstract: Now after much development, researchers are highly focused on hard carbon (HC) as the most promising negative electrode for Na-ion batteries with long cycle lifetimes, high power, and low-temperature operation to surpass the $LiFePO_4$//graphite cell.[1] Issues with cycling can be caused by unevenes of sodium insertion into the HC anode which has a low redox potential plateau close to Na deposition potential. Herein, we discuss about our latest design of HCs not only oringinal templated HC achieving high capacity[2] but also synthesis with H_3PO_4 addition or lignin carbonization as a renewed insight of HC research.

Figure 1 (a) shows galvanostatic charge-discharge curves of our latest HCs; H_3PO_4 added ZnO-templated HC and lignin-derived HC. An inrease in capacity via addition of H_3PO_4 addition has been recently reported,[3,4] which was also effective for improving our templated HC by impacting the pore structure mediated ZnO crystallite in precorsor. Lignin-derived HCs have relatively less capacity, as shown in **Fig.1 (b)**, but they remain promising as a low cost precursor and more than twice the carbonization yield than templated HC.[5] Furthemore, optimization of synthesis conditions of lignin-derived HC allowed us to control the pore and surface, delivering a superior rate-capability during sodiation (**Fig.1 (c)**). The impact of precursor tuning on performance will be discussed in this talk.

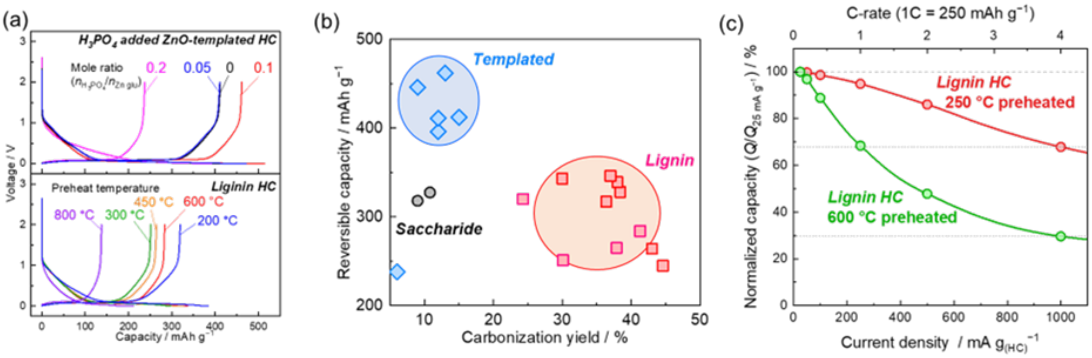
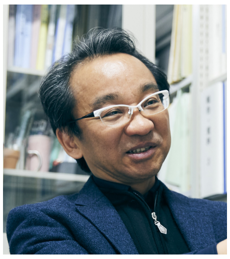


Figure 1. (a) Galvanostatic charge-discharge curves of H_3PO_4 added ZnO-templated HCs and lignin HCs. (b) Diagram of carbonization yield and reversible capacity of synthesized HCs. (c) Rate capabilities of diluted electrode of lignin HC synthesized through different pre-heat temperartures.

Acknowledgement:
This study was partially funded by ASPIRE (JPMJAP2313), and GteX(JPMJGX23S4), and JSPS-Grant-in-Aid for JSPS Fellows(24KJ2024).

References:

[1]. H. Hijazi, M. Metzger et al., *J. Electrochem. Soc.*, **171**, 050521 (2024).
[2]. D. Igarashi, S. Komaba et al., *Adv. Energy Mater.*, **13**, 2302647 (2023).
[3]. X. Zhao, Y. S. Hu et al., *Energy Storage Mater.*, **70**, 103543 (2024).
[4]. H. Ando, K. Gotoh et al., *Carbon Trends*, **16**, 100387 (2024).
[5]. Y. Fujii, S. Komaba et al., *ACS Appl. Energy Mater.*, **8**, 6577 (2025).



Biography: Shinichi Komaba is a Professor in the Department of Applied Chemistry at the Tokyo University of Science, Japan. He joined the Tokyo University of Science as a faculty member in 2005. He was awarded the 2014 Resonate Award from Caltech, USA, and JSPS Prize in 2014. He also received a Prize for Science and Technology, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science, and Technology, Japan, in 2019. He was selected as Highly Cited Researcher 2019 – 2023. His current research focuses on material science and electrochemistry in rechargeable Li-, Na-, K-, and Rb-ion batteries, capacitors, and electrochemical sensors.

Stretching the Limits of Na-Ion Cathodes

Robert House* [1]

[1]Department of Materials, University of Oxford, Oxford, OX1 3PH, UK

E-mail: Robert.house@materials.ox.ac.uk

Keywords: cathodes • oxygen redox • layered oxides • disordered rocksalt • Na-rich

Abstract: One of the biggest challenges that Na-ion batteries face is how to increase their energy density. The cathode material represents a major fundamental limitation. Layered oxides, such as $NaNi_{1/3}Mn_{1/3}Fe_{1/3}O_2$, remain the best class of materials for the highest energy density Na-ion cells. However, to increase further the amount of energy they can store requires moving to alkali-rich cathodes and contending with the challenges arising from high voltage instability and oxygen redox.

In this talk, I will discuss recent advances we have made in understanding the mechanisms of charge storage using oxide ions in next generation cathode materials.[1-3] I will illustrate how we have applied this understanding to overcome some of the critical issues they face and to develop improved O-redox cathode materials.[4-5] I will also look beyond layered oxides to discuss advances and opportunities in disordered rocksalt cathodes Na-ion batteries.[6]

Reference:

[1]. House, R. A. et al. Nature 577, 502–508 (2020).

[2]. House, R. A. et al. Nature Energy 6, 781-789 (2021).

[3]. Marie, J. J. et al. Nature Materials 23, 818–825 (2024).

[4]. House, R. A. et al. Nature Energy, 8, 351–360 (2023).

[5]. Marie, J. J. et al. Advanced Energy Materials, 14, 41, 2401935 (2024).

[6]. Mitchell, N. et al. Advanced Materials, 2419878 (2025).

Biography: Robert House is an Associate Professor in the Department of Materials, Fellow of ZERO Institute at Oxford and Non-Tutorial Fellow of Keble College. He holds a Research Fellowship with the Royal Academy of Engineering and affiliations with the Faraday Institution and Henry Royce Institute for advanced materials.

Professor House's research interests are in novel sustainable energy materials, particularly for electrochemical energy storage, and in developing and applying advanced X-ray, neutron and muon scattering techniques to study ion diffusion, charge storage mechanisms and structure-function relationships in energy storage materials.

His research group are actively engaged in materials discovery and development for next generation batteries, and work closely with a range of industry partners. Their activities cover future lithium-ion technology, and more sustainable alternative chemistries such as sodium-ion and magnesium-ion.

Sodium Ion Solid State Batteries for Fast and Long Cycling

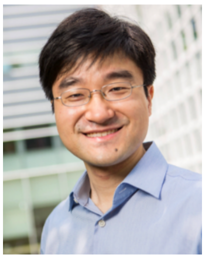
Xin Li [1]

[1]Harvard University, 29 Oxford Street, Cambridge, MA, 02138, USA

E-mail: lixin@seas.harvard.edu

Keywords: sodium • solid state battery• solid electrolyte • interface reaction • ionic conductivity

Abstract: Sodium ion solid state battery is a complementary cost-effective technology to Li ion solid state battery. The sodium version, however, for a long time cannot demonstrate sufficiently fast and stable cycling capability in comparison to the Li one. This talk will demonstrate our development of such a battery technology with fast Na ion conductors for high cathode loading and stable battery configurations that can prevent Na dendrite penetration for batteries cycled at high areal capacity and C-rate.



Biography: Xin Li is an associate professor of materials science at Harvard John A. Paulson School of Engineering and Applied Sciences. Xin Li's research group designs new energy-related materials and systems through advanced synthesis, characterization, and simulation, with the current focus on Li and Na ion batteries, solid-state batteries, and unconventional superconductors. Xin Li received his B.S. degree in physics from Nanjing University, China, his Ph.D. degree in materials science and engineering at Pennsylvania State University and performed postdoctoral research at CalTech and MIT before joining Harvard in 2015. Prof. Li is also a cofounder of Adden Energy, Inc, which is a solid-state battery start-up company aiming at combating climate-change with next-generation battery technologies.

Atomic Engineering and Structural Confinement for High-Performance Sodium Storage

Bin Luo*

Australia Institute for Bioengineering and Nanotechnology (AIBN) & School of Chemical Engineering, The University of Queensland, 4072 Brisbane, QLD, Australia

Email: b.luo1@uq.edu.au

Keywords: anode free • atomic engineering • sodium battery • confinement

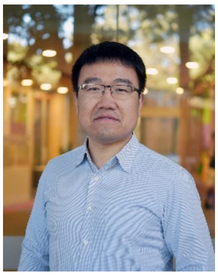
Abstract: Sodium-ion batteries (SIBs) hold great promise as a sustainable and cost-effective alternative to lithium-based systems, but their widespread deployment is hindered by challenges in anode stability, ion transport kinetics, and full cell reversibility. In this talk, I will present two recent advances that address these limitations through materials design at the atomic and nanoscale. The first part focuses on the confinement of ultrafine tin monophosphide (SnP) nanocrystals within $Ti_3C_2T_X$ MXene interlayers. SnP, with its robust three-dimensional crystallographic framework, offers high theoretical capacity, yet suffers from structural disintegration during cycling. By in situ growing ultrafine SnP within a conductive and flexible MXene matrix, we effectively mitigate phase separation and accommodate volume changes. The strong confinement and nanosizing synergistically enhance Na^+ transport and preserve structural integrity. The second part highlights a novel single-atom strategy for promoting uniform sodium deposition in anode-free configurations. We engineered carbon hosts doped with atomically dispersed Sn under a dynamic coordination environment. The coordination-governed modulation of Sn activity is critical in enabling uniform plating/stripping and minimising dead sodium formation. Symmetric cells demonstrate a stable operation for 1200 hours at 100 mA cm^{-2} and 100 mAh cm^{-2}, while full anode-free cells retain 94% capacity over 700 cycles at 10C. Together, these works underscore the importance of atomic-level control and hierarchical design in pushing the boundaries of sodium-ion battery performance.

References:

[1]. S. Gao, Y. Zhu, K. Shi, P. Liu, Y. Zhang, W. Tan, Z. Wen, L. Wang,* J. Hu,* L. Wang, B. Luo,* J. Zhou*. Nature Communication, 2025, accepted.

[2]. J. Tang, X. Peng, T. Lin, X. Huang, B. Luo*, L. Wang*. eScience, 202, 2, 203-211.

[3]. J. Tang, X. Huang, T. Qiu, X. Peng, T. Wu, L. Wang, B. Luo, L. Wang, *Chem. Eur. J.* **2021**, *27*, 1921.



Biography: Bin Luo is an Associate Professor & Group Leader in Australian Institute for Bioengineering and Nanotechnology (AIBN) at the University of Queensland (UQ). He received his doctoral degree in Physical Chemistry from National Centre for Nanoscience and Technology of China, University of Chinese Academy of Sciences in July 2013. Since joining UQ in 2014, he has worked as UQ Postdoctoral Research Fellow (2014-2018), ARC DECRA Fellow (2018-2021), and ARC Future Fellow & Group Leader (2021-2025) at AIBN. Dr Luo's research focuses on the design of new functional nanomaterials for energy storage applications.

Opportunities and Challenges in the Computational Design of Poly(ionic liquids) for Solid-State Sodium Batteries

Fangfang Chen

Fangfang Chen[1,]*, Jhonatan Soto Puelles[1], Kewei Cai[1], Shinji Kondou[1,2], Luis Miguel Guerrero Mejía[1], Maria Forsyth[1]

Email: fangfang.chen@deakin.edu.au

[1]Institute for Frontier Materials, Deakin University, 221 Burwood Highway, Burwood, Victoria 3125, Australia

[2]Department of Materials Engineering Science, Osaka University, 1-3, Machikaneyama, Toyonaka, Osaka 560-8531, Japan

Polymeric ionic liquids (polyILs) distinguish themselves from conventional polymer electrolytes through their positively charged cationic backbones, which lead to distinctive ion coordination structures and metal ion transport mechanisms.[1] These features promote decoupled metal cation transport within certain high salt concentration range,[2-3] offering advantages for solid-state electrolyte design. Molecular modelling plays a crucial role in revealing these underlying mechanisms and serves as a powerful tool for designing new polyIL-based electrolytes and predicting their physical properties. In this presentation, we demonstrate the strong potential of polyILs for the development of solid-state solidum batteries. We discuss our recent modelling design and exploration of new polyIL systems,[4] and we identify key challenges in both computational modelling and experimental translation.

References:

[1]. X Wang, F Chen, et al Joule, 2019, 3, 2687-2702.

[2]. F Chen, et al Nature Materials, 2022, 21, 1175-1182.

[3]. S Kondou, et al Journal of the American Chemical Society, 2024, 146, 33169-33178.

[4]. K Cai, et al, Batteries & Supercaps, 2025, https://doi.org/10.1002/batt.202500484

Biography: Fangfang Chen research interests focus on molecular modelling and simulation of material structures and properties using modern computational chemistry methods, such as molecular dynamics and Density Functional Theory. After graduating with a B.Sci from the Northeastern University (China), Dr Chen earned her Master degree in Material Engineering from Chinese Academy of Sciences (China) and PhD degree in Computational Chemistry from Swinburne University of Technology (Australia). Then she joined IFM, Deakin University as a research fellow, working on solid and liquid electrolyte materials.

Enhancing Sodium Battery Design through Nanoscale Characterisation

A/Prof. Ruth Knibbe[1], Dr. Ming Li[2], Dr. Qingbing Xia[1], Ms Emily Cooper[1], A/Prof. Jeffrey Harmer[2], Prof. Ian Gentle[3].

[1]School of Mechanical & Mining Engineering, University of Queensland, Brisbane, Australia,

[2]Queensland University of Technology, Brisbane, Australia,

[3]Centre for Advanced Imaging, Brisbane, Australia,

[4]School of Chemistry and Molecular Biosciences, Brisbane, Australia.

Keywords: sodium metal batteries • anode free batteries • cryo-TEM • in-situ TEM

Abstract: While lithium-ion batteries remain the dominant choice for commercial electric vehicles, they present limitations in cost and safety for applications such as grid-connected and flexible energy storage.

This presentation will highlight recent advances made by my group on visualising metal formation in zinc and sodium-metal batteries. The presented work will include operando liquid electrochemical transmission electron microscopy (TEM), cryo-TEM, and high-resolution TEM (HRTEM) for epitaxial characterisation.

Our cryo-TEM results reveal that dendrite size decreases with increasing current density, while nucleation density increases. Sodium was deposited onto copper TEM grids within coin cells using a $NaPF_6$-based electrolyte. Cryo-TEM imaging enables atomic-scale visualisation of sodium dendrites and the solid electrolyte interphase (SEI) layer. This identifies the key SEI components, including NaF, Na_2CO_3, and RCH_2ONa, formed in the ethylene carbonate/propylene carbonate electrolyte system.

To further enhance nucleation uniformity, we explored epitaxial growth of sodium on various current collectors. Crystallographic screening identified zinc and α-brass as promising CC materials due to their low lattice misfit with sodium and practical applicability. Zinc CCs demonstrated stable cycling performance and a low sodium overpotential of -16.5 mV (vs Na/Na^+). To confirm the role of epitaxial matching we developed a novel TEM workflow to enable high-resolution TEM imaging of sodium metal without cryogenic conditions, confirming epitaxial relationships and facilitating broader accessibility for researchers.

References:

[1]. Yang, T., et al., iScience, 2023. 26(3): p. 105982.

[2]. Cooper, E.R., Knibbe, R. et al., Angewandte Chemie International Edition, 2023. 62(51): p. e202309247.

[3]. Li, M., Knibbe, R., et al. The Journal of Physical Chemistry Letters, 2021. 12 (2): p. 913-918.

[4]. Li, M., Cooper, E.R., Knibbe, R. et al.. ACS Appl. Mater. Interfaces 2023. 15: p. 53333−53341.

[5]. Cooper, E.R., Li, M., Gentle, I., Xia, Q., Knibbe, R. 2023. 6(22): p. 11550-11559.

Biography: Ruth Knibbe is a leading researcher in electrochemical energy systems at the School of Mechanical & Mining Engineering, University of Queensland, Brisbane. She earned her PhD in Chemical Engineering from UQ in 2007, then worked at DTU Energy (Denmark) and the Robinson Research Institute in Wellington, New Zealand before returning to UQ in 2016. Her research combines electrochemistry, advanced electron microscopy (including operando / in-situ techniques), and machine learning to study battery and electrolyser materials, especially sodium-based and solid-state batteries, and to understand degradation mechanisms, interfaces, and large-scale safety for energy systems.

Multifaceted Reconsideration of Alluaudite Cathodes

Atsuo Yamada*

The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8654, Japan
E-mail: yamada@chemsys.t.u-tokyo.ac.jp

Keywords: alluaudite variety • transport properties • moisture sensitivity • LCA

Abstract: Rechargeable batteries have ushered the wireless revolution over last two decades and are now matured to enable green automobiles. The current generation Li-ion batteries employ oxides such as $Li(Ni,Mn,Co)O_2$ 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. In this pursuit, numerous Fe-based cathode compounds capable of efficient Na (de)insertion have been reported. However, their performance is limited owing to low operating voltage and sluggish kinetics. We have identified a hitherto-unknown $Na_2Fe_2(SO_4)_3$ with Alluaudite structure as a sodium-ion battery cathode, registering the highest ever Fe^{3+}/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 bateries. 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 SO_4-PO_4 system will be introduced as time permits.

Biography: Atsuo Yamada is professor at the university of Tokyo since 2009, known as one of the earliest adaptor of olivine cathode research, having published the first report on room-temperature theoretical capacity operation of $LiFePO_4$ in 2001. He has published over 280 refereed journal papers exceeding 40,000 citation, ranked as a Highly Cited Researcher. Among his many honors, Atsuo has been awarded the Spriggs Award and the Purdy Award from ACerS, the Scientific Achievement Award from ECS Japan, and IBA Research Award from International Battery Association, Battery Division Research Award from the Electrochemical Society, and Science &Technology award from MEXT Minister.

Na-Ion States and Dynamics in NIB Electrodes Revealed by DFT and MD Simulations

Yoshitaka Tateyama[1] *

[1]Laboratory for Chemistry and Life Science (CLS), Institute of Integrated Research (IIR), Institute of Science Tokyo, R1-25, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8501, JAPAN

E-mail: tateyama@cls.iir.isct.ac.jp

Keywords: density functional theory • molecular dynamics • hard carbon • prussian blue analogue • layered oxide

Abstract: Many efforts have been made so far toward realization of Na-ion batteries, and the commercialization is being realized in practice nowadays. Yet, the atomic-scale behaviors of Na-ions, such as diffusion/migration, adsorption/desorption in the NIBs are still open questions. Elucidation of those states and dynamics surely contribute to the improvement of NIB performance and NIB fabrication. To this end, we have addressed computational studies based on density-functional-theory (DFT) and molecular dynamics (MD) about the Na-ion behaviors in the NIB electrodes such as hard carbon (HC) anode [2] and cathodes of layered oxides and Prussian Blue analogue (PBA) [3].

For the HC anode, we already reported stable formation of 3-4 layers and pseudometallic Na-ion cluster in the HC nano pore by DFT geometry optimizations with rather small supercells [1]. However, recent finite-temperature DFT-MD indicated that 2-3 layers for 1.5 nm pore are more suitable at room temperature [2]. Caculated self-diffusivity of Na-ion was much higher than the reported experimental values, implying that the bottleneck of Na-ion diffusion does not seem the pore region. Concerning the supercell size effect, we also performed neural network potential based MD simulations with larger supercells, and demonstrated that HC models with more inhomogeneous structures and sizes may provide more reasonable self-diffusivity. The dependence of the structure and cell size will be discussed in the talk. For the cathode materials, we also demonstrated that Na-Mn-O systems can undergo the phase transitions, with the change of SOC, which may facilitate more reversible Na-insertion/elimination. On the PB materials, we carried out a comparative study of stable site occupations and diffusion manners among Li, Na and K-ions, and found that both are quite dissimilar. Besides, we evaluated lower barries of Na-ion diffusion than Li-ion, indicating that NIBs have an advantage under low tempearture condition.

These works were done in collaboration with Dr. Yong Youn, Prof. Huu Duc Luong, Dr. Che-an Lin, Dr. An Niza El Aisnada, Mr. Dan Ito, and Prof. Shinichi Komaba The works were supported by JST GteX project (NIB team) and ASPIRE project as well as MEXT DxMT project.

References:

[1]. Y. Youn, K. Kubota, S. Komaba, Y. Tateyama *et al.*, npj Comput. Mater. 7, 48 (2021).

[2]. C.-A. Lin, H.-D. Luong, Y. Tateyama, in preparation.

[3]. D. Ito, Y. Tateyama *et al.,* under review.

Biography: Yoshitaka Tateyama earned his MSc and PhD in physics from Graduate School of Science, The University of Tokyo. He has then worked as a permanent researcher in National Research Institute of Metals and National Institute for Materials Science (NIMS) since 1998. He finally got promoted to Director of Research Center for Energy and Environmental Materials (GREEN) in NIMS. During his NIMS term, he has worked in the Department of Chemistry at the University of Cambridge as a visiting researcher for 2003-2004, and got awarded JST PRESTO researchers twice for 2007-2015. He also received Gottfried Wagener Prize in 2015. In 2023, he partially moved to Tokyo Institute of Technolgy as a full professor, and is now Professor of Laboratory for Chemistry and Life Science (CLS), at the Institute of Science Tokyo (Science Tokyo). His research interest is computational materials science, mostly at the DFT level, on electrochemical and ionics phenomena, and those devices such as battery. In particular, he has played a project leader role of Fugaku materials science projects, under “Program for Promoting Research on the Supercomputer Fugaku” by MEXT since 2020.

High-Capacity and Long-Life Microsized Sn-Based Anodes for Sodium-Ion Batteries

Yansong Zhu,[1] Cheng Zheng,[1] Qian Yao,[1] Zhongchao Bai,*[,2] Nana Wang,*[,3] and Jian Yang*[,1]
[1]Key Laboratory of Colloid and Interface Chemistry, Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100 P. R. China
E-mail: yangjian@sdu.edu.cn
[2]Institute of Energy Materials Science (IEMS), University of Shanghai for Science and Technology, Shanghai 200093, P. R. China
E-mail: baizhongchao@tyut.edu.cn
[3]Centre for Clean Energy Technology, School of Mathematical and Physical Sciences, Faculty of Science, University of Technology Sydney, Sydney, NSW, 2007 Australia
E-mail: Nana.Wang@uts.edu.au

Keywords: sodium ion batteries • anode materials • alloy-type anode • microsize particles • tin

Abstract: Sn-based composites are considered as one of the promising anode materials for sodium-ion batteries (SIBs) due to their high theoretical capacities and suitable operation voltages. However, they suffer the huge volume change and unstable electrolyte/electrode interface during sodiation/desodiation, which causes structure collapse and serious capacity loss.[1,2] In recent years, our group has focused on investigating the electrochemical performance of alloy-type anodes, using microsized tin (u-Sn) as a model system. The electrochemical performance is greatly enhanced through structure design and electrolyte optimization (Figure 1). The fundamental mechanisms underlying these results are elucidated by examining the Sn/electrolyte interface. These findings are being validated and extended to other sodium-ion battery anode materials.[3-6]

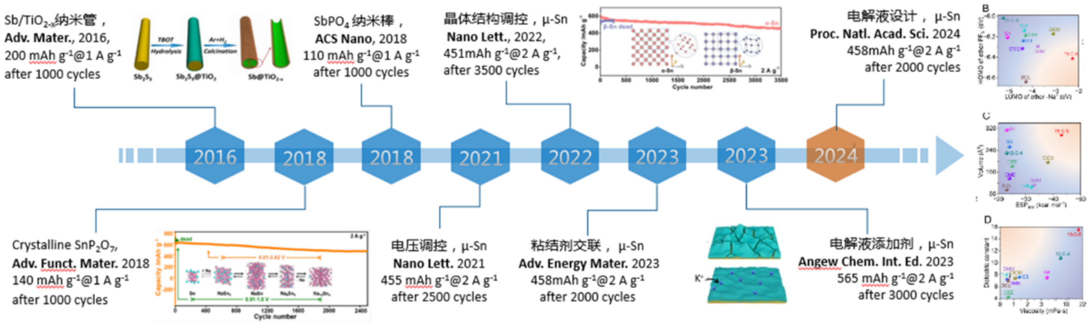


Figure 1. Advances of the electrochemical performance of μ-Sn in sodium-ion batteries.

References:

[1]. Li, Y.; Wu, F.; Li, Y.; Liu, M.; Feng, X.; Bai, Y.; Wu, C. *Chem. Soc. Rev.* **2022**, *51*, 4484.

[2]. Usiskin, R.; Lu, Y.; Popovic, J.; Law, M.; Balaya, P.; Hu, Y.; Maier, J. *Nat. Rev. Mater.* **2021**, *6*, 1020.

[3]. Sun, Y.; Zheng, C.; Yao, Q.; Lv, H.; Ma, X.; Yang, J. *Angew. Chem. Int. Ed.*, **2025**, 64, e202420573.

[4]. Yao, Q.; Wang, N.; Yang, J.; Dou, S.; Qian, Y., et al., *Proc. Natl. Acad. Sci.,* **2024**, 121, e2312337121.

[5]. Zheng, C.; Ji, D.; Liu, D.; Wang, N.; Yang, J.; Dou, S., et al., Angew. *Chem. Int. Ed.*, **2023**, 62, e202214258.

[6]. Zhu, Y.; Yao, Q.; Shao, R.; Wang, C.; Yan, W.; Ma, J.; Liu, D.; Yang, J.; Qian, Y. *Nano Lett.*, **2022**, 22, 7976.

Biography: Jian Yang is a professor at the School of Chemistry and Chemical Engineering, Shandong University. His research interests focus on the interface chemistry of electrochemical energy storage. To date, the results have been published on high-impact journals, such as Proc. Natl. Acad. Sci., Angew. Chem. Int. Ed., Energy Environ. Sci., Adv. Mater., ACS Nano, and so on. He has been awarded with National Natural Science Award of China, New Century Talent Program of the Ministry of Education (China), Special Government Allowances of the State (China), Most Cited Chinese Researcher (SCOPUS), etc.

Transport, Kinetics & the Path to New Materials Discovery

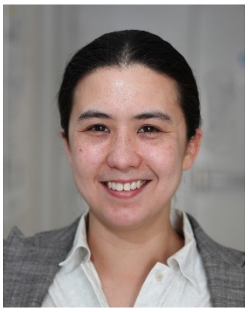
Karena Chapman

Stony Brook University, United States

Email: karena.chapman@stonybrook.edu

Abstract: Advances in safer, higher-energy batteries, durable catalysts, and efficient solar conversion depend on the discovery of new inorganic materials. The main challenge is not identifying promising targets—computational methods generate many—but the ability to synthesize these often metastable materials, which remain out of reach because the outcome of synthesis reactions cannot yet be designed or predicted. The critical gap is a lack of mechanistic understanding of the dynamic transformations that drive synthesis.

Solid-state reactions, the most common route to crystalline oxides, are typically slow, limited by atomic and ionic transport through solids. We use time-resolved in situ X-ray scattering with custom operando reactors to track reaction kinetics from the atomic to the particle and system scales. By pinpointing what causes reactions to slow, our goal is to extend the fast kinetic regimes observed at early stages, enabling solid-state synthesis at lower temperatures and shorter times. This will expand access to metastable materials that would otherwise decompose or transform at higher temperatures.



Biography: Karena joined the faculty of Stony Brook University in Fall 2018 as the inaugural Endowed Chair in Materials Chemistry. She completed her B.Sc. in 2001 at the University of Sydney, Australia and earned her Ph.D. at the same institution in 2006 before moving to Argonne National Laboratory as the Arthur Holly Compton Fellow. Prof Chapman's honors include the 2015 Materials Research Society Outstanding Young Investigator Award, for contributions to understanding the coupled structure and reactivity of energy-relevant systems and for developing incisive experimental tools to interrogate these complex materials, and as a 2016 C&E News Talented Twelve honoree. Dr Chapman's work impacts broad materials and applications including energy storage in batteries, porous materials for gas capture, storage and catalysis, and nanomaterials to remediate nuclear waste. She both designs high fidelity tools to explore materials' function and applies these to solve important questions for key systems. More broadly, her efforts have transformed niche X-ray analyses attempted by a handful of experts into robust, broadly useful tools capable of addressing complex problems in chemistry and material science. While probing material function under real operating conditions in real time is widely valued, doing so without changing the function—a "Schrödinger's cat" problem—is a challenge that Dr Chapman has recognized and addressed, thereby resolving misleading, inconsistent results in the literature. As co-director of a new energy research center at Stony Brook, Dr Chapman's ongoing innovations aim to revolutionize how we interrogate, understand and control reactions leading to the discovery of new materials and materials' states.

Flexible and High-Performance Sodium Ion Micro-Batteries

Zhong-Shuai Wu* [1]

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, China

E-mail: wuzs@dicp.ac.cn

Keywords: sodium ion micro-batteries • 3D printing • photolithgrapy • integrated microsystems • microelectronics

Abstract: The conventional batteries with fixed design/form factors have difficulties in fulfilling the requirements of flexible/wearable electronics. Therefore, we need to shift our focus towards innovative energy storage devices design. Micro-batteries (MBs) with in-plane geometry are emerging micro-electrochemical energy storage devices for flexible, miniaturized, integrated microelectronics. This talk highlights our recent advances in planar sodium ion MBs. First, we developed several microelectrode fabrication methods, such as photolithography, screen printing, inkjet printing, laser scribing, and 3D printing. Using these techniques, we developed a series of high-energy sodium ion MBs, especially, based on the design of high-capacity electrodes and high-voltage ionic liquid and ionogels. Second, our planar MBs achieve high current/voltage through series/parallel connections. Third, integrated microsystems for diverse applications—such as gas sensors, wearable pressure sensors, and biodegradable medical devices—are developed. These self-powered systems combine energy harvesting, storage, and consumption, enabling broad microelectronic applications.

Biography: Zhong-Shuai Wu is a leading scientist at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, specializing in 2D materials, micro-electrochemical energy storage systems, advanced batteries, and energy catalysis. His distinguished research portfolio includes over 370 publications in high-impact journals such as *Nature*, *Nature Communications*, with more than 47,000 citations. He has been recognized as a Highly Cited Researcher from 2018 to 2024 and elected as a Fellow of the Royal Society of Chemistry. He is serving as Associate Editor of *Energy Storage Materials* and Associate Editor of *Applied Surface Science*, Section Editor of *Journal of Energy Chemistry*, Editorial Group Member for *National Science Review,* and editorial board members of *Science Bulletin, Nanomaterials, Carbon Futures, Mater. Res. Express, Interdisciplinary Materials, Chin. Chem. Lett., eScience, Materials Futures,* and *Engineering.*

Prediction of Stability and Voltage of Layed Oxide Materials for Sodium-ion Batteries

Payam Kaghazchi

Institute of Energy Materials and Devices (IMD-2): Werkstoffsynthese und Herstellungsverfahren, Forschungszentrum Juelich, Germany; MESA+ Institute for Nanotechnology, University of Twente, Enschede, 7500 AE The Netherlands

Email: p.kaghazchi@fz-juelich.de

Keywords: classical potential • DFT • continuum • cathode • sodium-ion batteries

Abstract: Layered oxides (LOs) are among the most promising cathode materials for Na-ion batteries (SIBs) because of their potentially high energy densities. There are, however, still some challenges in applying LO cathodes for SIBs, in particular because of their low cyclability, which is mainly related to their structural evolution (i.e. phase transition). We have recently developed an efficient Coulomb energy optimizer using advanced sampling methods. Our optimization package, GOAC (Global Optimization of Atomistic Configurations by Coulomb), can achieve a speed up of several orders of magnitude compared to existing softwares and more importantly can be used to sample gigantic configurational spaces of up to ten to the power of several thousands configurations. By applying our software package GOAC we optimized Coulomb energies in complex multi-element LOs ($Na_x[M_yM'_{1-y-\ldots}\ldots]O_2$) to simulate their phase stability and transition during charge/discharge. The predictive capability of this approach will be discussed. Besides the cationic potential, which has been reported before by other groups, we found other parameters that determine the phase stability of LOs. Afterwards, our recently developed classical potential to predict the voltage profile $V(x)$ of LOs will be presented. It is shown that $V(x)$ can be computed with a high accuracy. Parameters controlling the voltage range and plateaus, which influence the stability of LOs, will be discussed. Finally, our multiscale modelling and simulation studying the mechanism of cracking in LOs by desodiation/sodiation will be presented. In particular, the influence of composition on the mechanical stability will be discussed.

Biography: Payam Kaghazchi is a theoretical physicist (Ph.D.: Fritz-Haber-Institute/FU Berlin, 2009). He is currently head of the modeling team at the Institute of IMD-2 in the Forschungszentrum Jülich in Germany, and associate professor in the Department of Inorganic Materials Science at University of Twente in the Netherlands. His research has focused on developing and applying multiscale modeling approaches to simulate and design materials for energy storage and conversion systems.

Molten Na Battery Chemistries for Energy Storage System Applications

Guosheng Li, Ph.D.

Battery Materials and Systems Group, Pacific Northwest National Laboratory, Richland, WA 99354

Email: guosheng.li@pnnl.gov

Abstract: As the demand for electricity rises, effective energy storage systems (ESS) are increasingly crucial to balance supply and demand across various time scales. While lithium-ion batteries (LIBs) dominate the grid storage and electric vehicle markets, their application in ESS is challenged by high costs, limited material availability, and inherent safety issues. Moreover, LIBs are well-suited for short-term storage (< 4 hours) but inadequate for long-duration energy storage (LDES) exceeding 10 hours.

These constraints have renewed interest in molten sodium (Na) battery technologies, including sodium-sulfur (Na-S) and sodium metal-halide (Na-MH) batteries. Molten sodium batteries offer benefits such as abundant material availability and reduced costs, effectively addressing sustainability and supply chain challenges. Notably, Na-MH batteries, despite utilizing a molten sodium anode, are known to be free from thermal runaway due to their use of a robust β”-alumina solid-state electrolyte and inorganic molten salts. Additionally, their high-temperature operation renders the battery's performance independent of ambient temperature, removing the necessity for HVAC systems during operation.

Current research focuses on lowering their operating temperatures from 250–350°C to around sodium's melting point (~100°C). Achieving this would simplify thermal management, reduce costs, and enhance cell performance, including longer cycle life and improved capacity utilization. Additionally, using more affordable metals such as iron (Fe), zinc (Zn), or aluminum (Al) in place of traditional nickel (Ni) cathodes—whose price has recently been quite volatile—offers potential for further cost savings and improved supply chain security.

This presentation will highlight recent advancements in molten sodium battery technology, emphasizing their promise for low material costs and extended durability. These breakthroughs represent significant strides towards resolving storage challenges tied to grid integration, paving the way for a more sustainable and resilient energy future.

Biography: Guosheng Li is a Senior Scientist in the Battery Materials & Systems Group at Pacific Northwest National Laboratory (PNNL), Richland, Washington, USA. His expertise spans advanced electrolytes (both liquid and solid-state), cathode materials synthesis, cathode reaction mechanisms, and interfacial challenges in rechargeable battery technologies. He is particularly noted for pioneering work on high-temperature batteries, including molten sodium and sodium-aluminum battery chemistries, and efforts to lower their operating temperature while improving performance. He has published widely (h-index >40), working on grid-scale energy storage systems, flow batteries, Na-based and multivalent battery systems, and in-situ spectroscopic/structural characterization. His work contributes toward making energy storage more cost-effective, durable, and capable for long-duration/seasonal and grid flexibility applications.

Design of New Material Used as Cathode for Na-Ion Batteries

T. Soudant[1,3], V. M. Kovrugin[1,3], A. Sagot[1,3], L. Stievano*[2,3]*, E. Bigard[1,3], M. Sougrati[2,3], and V. Pralong[1,3,*]

[1]Laboratoire de Cristallographie et Sciences des Matériaux CRISMAT, ENSICAEN, Université de Caen, CNRS, 6 Bd Maréchal Juin, F-14050 Caen, France.

[2]Institut Charles Gerhardt Montpellier, UMR 5253, CNRS, Université Montpellier, ENSCM, Montpellier 34095, France

[3]Réseau sur le Stockage Electrochimique de l'Énergie (RS2E), FR CNRS 3459, 80039 Amiens, France

Email: valerie.pralong@cnrs.fr

Keywords: manganese • iron • oxide • cathode

Abstract: Energy storage technologies are highly dependent on the used materials, necessitating the search for advanced, cost-effective and environmentally friendly alternatives – a surprisingly challenging task. However, only a limited number of elements satisfy these constraints, including abundant alkali ions (mostly Na and K)[1,2], non-hazardous transitions elements (Ti, Nb, Mn, Fe, Zr, Cu or Al), or anions such as oxides or sulfides[3]. Despite the high performance of materials based on lithium, their cost is driving the development of alternative systems based on sodium and potassium, more abundant on Earth's crust by several orders of magnitude. Moreover, Mn-based oxide materials emerge as promising cathodes for alkaline-ion batteries due to their high energy density, low-cost and low-toxicity. Focusing on layered-type structures, the A_xMnO_2 families show interesting insertion properties in systems based on lithium, sodium and more recently potassium[4]. For instance, the system A-Mn/Fe-O with A=Cu, Li, Na, K are extremely rich in term of original structural types. While the exploration of these ternary diagrams has already allowed us to synthesize and study numerous phases, new compositions still remain to be discovered with the goal of finding an economical and non-toxic cathode material for metal-ion batteries. For example, our research has led to the discovery of $Li_4Mn_2O_5$, a lithium-rich disordered rocksalt material showing an exceptional capacity of about 300 mAh/g[5]. In sodium based systems, the honeycomb layered $Na_2Mn_3O_7$ shows highly reversible cationic and anionic redox activity achieving a reversible capacity of 240 mAh/g[6,7]. Recently, we also reported the electrochemical activity of A_3MnO_4 with A=K, Na demonstrating reversible potassium and sodium extraction/insertion[8,9]. This presentation will discuss the relationship between structural and insertion properties in the A-Mn-O system, emphasizing our strategy for the generation of green materials for energy storage playing with the chemist's toolkit.

References:

[1]. W. M. Haynes, Handbook of Chemistry and Physics, 93rd Edition.; CRC Press, 2012.

[2]. I. A. Shiklomanov, J.Rodda, Press Syndicate of the University of Cambridge 2003, 41 (07), 41-4063-41–4063.

[3]. B. C. Melot, J.-M. Tarascon, Acc. Chem. Res. 2013, 46 (5), 1226–1238.

[4]. K. Kubota, M. Dahbi, T. Hosaka, S. Kumakura, and S. Komaba, Chem. Rec. 2018, 18, 459 – 479

[5]. M. Freire, N. Kosova, C. Jordy, et al., Nature Mater, 2016, 15, 173.

[6]. E. Admaczyk, V. Pralong, Chem. Mater. 2017, 29, 11, 4645–4648.

[7]. A. Tsuchimoto, XM. Shi, K. Kawai, et al., Nat Commun, 2021, 12, 631.

[8]. A. Sagot, L. Stievano, and V. Pralong, ACS Applied Energy Materials, 2023, 6(15), 7785-7789.

[9]. A. Sagot, L. Stievano, V. M. Kovrugin, et al., under preparation, 2025.

Biography: Valérie Pralong is a CNRS research director at Normandy University in the Crystallography and Materials Science laboratory (CRISMAT) in Caen, France. She obtained her doctorate in materials science from the University Picardie Jules Verne in 2000 on alkaline batteries. After three years of postdoctoral training on the research of new materials for Li-ion batteries, she joined the CNRS in 2003 as a research fellow. Her research focuses on the synthesis by soft chemistry and the electrochemical characterization of new ionic conductive materials, new structures, likely to be used for energy storage in the field of batteries and fuel cells. She focusses on the exploration of ternary diagram based on non-toxic and abundant element (Mn, Fe), trying to propose new composition that could be used as electrode or solid state electrolyte for metal ion batteries. She is the co-author of more than 180 publications, 3 book chapters and 10 patents in this field; she delivered more than 40 invited talks.

Interface Regulation Strategies of Na Metal Anodes

Yan Yu* [1]

[1]University of Science and Technology of China, Hefei 230026, China

E-mail: yanyumse@ustc.edu.cn

Keywords: Na metal batteries • Na metal anodes • interface regulation • artificial interface protective layer

Abstract: Sodium (Na) metal batteries have been considered as the most promising energy storage systems because of their high theoretical capacity and low cost of Na resource. However, the practical application of Na metal anodes faces several challenges in terms of unstable SEI structure, dendrite growth and huge volume expansion during the plating and stripping process, which may cause the structure damage of electrode and poor electrochemical performance of Na metal batteries. To address the above key problems, we have developed some effective strategies to regulate the interface of Na metal anodes: 1) designing three-dimensional conductive skeleton can reduce local current density and induce uniform interface deposition of alkali metal ions. 2) constructing the artificial interface protective layer on the surface of alkali metal anode could not only improve the mechanical toughness and ion diffusion ability, but effectively reduce the nucleation overpotential of metal ions. 3) modifying the electrolyte and separator can induce uniform metal ions deposition process and suppress the dendrite growth. Our research may provide scientific guidance to promote the commercial development and application of Na metal batteries.

Biography: Yan Yu is a faculty member in the Department of Materials Science and Engineering at the University of Science and Technology of China (USTC), where she leads the Clean Energy and Nanomaterials Research Group. She received her PhD from USTC in 2006 and subsequently worked as a postdoctoral researcher at Florida International University (USA) and as a Humboldt Research Fellow at the Max Planck Institute for Solid State Research (Germany). Her research focuses on the design, synthesis, and mechanistic study of advanced energy storage materials and devices, including lithium-, sodium-, and potassium-ion batteries as well as lithium-sulfur systems. Prof. Yu has been recognized as a highly cited researcher in materials science, has received multiple national and international awards, and serves on editorial and advisory boards of leading scientific journals.

Improving Energy Density of Sodium-Ion Cells: From Hard Carbon to Tin Anodes

Carla Albenga, [1] Faduma M. Maddar [1] and Ivana Hasa* [1]

[1]WMG, University of Warwick, Coventry CV4 7AL, United Kingdom

E-mail: ivana.hasa@warwick.ac.uk

Keywords: hard carbon • Sn anode • energy density • full-cells

Abstract: Sodium-ion batteries (SIBs) are increasingly recognized as the next generation sustainable energy storage technology, offering advantages such as greater sustainability and lower projected material costs when compared to lithium-ion batteries (LIBs), compatibility with existing LIB manufacturing facilities, and enhanced safety features like 0V storage capability[1]. The recent industrial investments reflect the accelerated progress toward commercial viability.

While various cathode materials have been proposed, hard carbon (HC) has emerged as the anode of choice for SIBs. This presentation shows research conducted on the development of industrially relevant 1Ah sodium-ion pouch cells using Prussian White (PW) cathodes[2] and bio-mass derived hard carbon anodes. The use of aqueous processing for both materials, matches the requirements for low toxicity, low cost, and sustainability in large-scale applications. Despite the promising results, the intrinsically low density of both PW and HC anode, limits substantially the volumetric energy density of these Na-ion cells. A comprehensive understanding of the intrinsic limitations of HC anodes further tested in combination with layered oxide cathode, also confirms HC to be the limiting electrode for high energy density cells[3].

To address this limitation, alloying-type anodes such as tin (Sn) are being explored due to their high theoretical capacity, superior conductivity and notably higher density compared to HC. However, large volume changes experienced by these materials during (de-)sodiation often cause mechanical degradation and unstable solid-electrolyte interphase (SEI). We investigated the influence of both Sn content and particle size on the structural and electrochemical stability of Sn/HC-based anodes. While nanosized Sn suffers from severe instability, micrometric Sn (μ-Sn) demonstrates enhanced stability, particularly in glyme-based electrolytes. Contrary to expectations, increasing the Sn content does not compromise the cycling stability. The structural resilience is attributed to the formation of a robust porous "coral-like" Sn network, which mitigates volume expansion and structural degradation. The successful formation of this morphology relies on both Sn content and the degree of sodiation[4].

These findings demonstrate that μ-Sn anodes can overcome key limitations of HC, offering a viable pathway to substantially improve the volumetric energy density of sodium-ion batteries and accelerate their commercial potential.

References:

[1]. I. Hasa et al, Journal of Power Sources, 2021, 482, 228872.

[2]. F. M. Maddar et al, J. Mater. Chem. A, 2023, 11, 15778-15791.

[3]. C. Constable, et al, J. Electrochem. Soc., 2024, 171, 023506.

[4]. C. Albenga, et al , J. Mater. Chem. A, 2025, Advance Article.

Biography: Ivana Hasa is Associate Professor of Electrochemical Materials in WMG at the University of Warwick. Her research activities are directed toward the understanding of the processes governing the chemistry of the next generation's sustainable battery technologies. Design of technically relevant materials and the understanding of their structure-property correlation and electrochemical behaviour are the core of her research interest. Her work is inherently interdisciplinary, tackling challenges at the interface of chemistry, materials science, and electrochemistry. At the Energy Innovation Centre in WMG, she is also working toward the development and scale up of new battery chemistries from concept to full proven cell prototypes.

Manganese-based Cathode Design and Interface Modulation in Sodium-Ion Batteries

Hui Xia*

[1]School of Materials Science and Engineering, Nanjing University of Science and Technology, 200 Xiaolingwei, Nanjing, 210094, China

E-mail: xiahui@njust.edu.cn

Abstract: Manganese-based cathode materials are promising low-cost candidates for sodium-ion batteries (SIBs), yet their practical application is hindered by suboptimal Na storage performance. In this report, we present the development of a Na-rich birnessite cathode material with enhanced electrochemical properties. The structural design incorporates Mn-O hexahedral coordination within the birnessite framework, and we systematically investigate the impact of interlayer chemistry and Mn defects on Na storage behavior. Furthermore, we highlight the critical role of electrode/electrolyte interface engineering in improving battery performance. Strategies such as electrolyte additive incorporation are explored to expand the electrochemical stability window and enhance cycling durability. This work provides valuable insights into optimizing both bulk material design and interfacial properties for high-performance SIBs.

Biography: Hui Xia received his B.E. and M.E. from University of Science and Technology Beijing in 2000 and 2003, and Ph.D. from National University of Singapore in 2007. From 2007 to 2011, he was a postdoc research fellow at National University of Singapore. Prof. Xia joined Nanjing University of Science and Technology (NUST) in 2011 and is currently the principal investigator of the research group - Nano Energy Materials (NEM, http://nem.smse-njust.com). The NEM research focuses on developing new materials and architectures for electrochemical energy storage systems, including all-solid-state microbatteries, supercapacitors, and new energy storage systems.

Electron Paramagnetic Resonance as a Tool to Determine the Sodium Charge Storage Mechanism of Hard Carbon in Na-Ion Batteries

Nuria Tapia-Ruiz

Imperial College London, United Kingdom

Email: n.tapia-ruiz@imperial.ac.uk

Abstract: Emerging rechargeable battery technologies such as sodium-ion batteries have attracted much attention in recent years due to the low cost and large natural abundance of sodium sources. Non-graphitic hard carbons (HC), formed by randomly orientated and curved graphene sheets with expanded interlayer distance (3.6–4 Å) and with the possibility of being derived from biosources, are promising anode candidates for Na-ion batteries, showing typical reversible capacities of ca. 300 mAh g^{-1}. The reaction mechanisms that drive the sodiation/desodiation properties in hard carbons are complex and relate to (1) Na^+ ion adsorption at edge sites and defects, (2) Na^+ intercalation into graphene–graphene interlayer spacing, and (3) Na^+ ion insertion into nanopores. These storage mechanisms and their subsequent electrochemical response are strictly linked to the characteristic slope and plateau regions observed in the voltage profile of these materials.

In this work we show that electron paramagnetic resonance (EPR) spectroscopy is a powerful and fast diagnostic tool to predict the extent of the charge stored in the slope and plateau regions during galvanostatic tests in pristine hard carbon materials. EPR lineshape simulation and temperature-dependent measurements help to separate the nature of the spins in mechanochemically modified hard carbon materials synthesised at different temperatures. This proves relationships between structure modification and electrochemical signatures in the galvanostatic curves to obtain information on their sodium storage mechanism. Furthermore, we show through the use of ex-situ EPR the evolution of these EPR signals at different states of charge to further elucidate the storage mechanisms in these hard carbons, to answer questions related to the nature of the Na clusters.

Biography: **Nuria** was born in Barcelona and graduated in Chemistry from the University of Barcelona in 2009. After this, she travelled to Scotland (Glasgow) to pursue her PhD studies with Prof. Gregory in the Chemistry Department at the University of Glasgow. In 2013, she moved to the east coast of Scotland (School of Chemistry, University of St. Andrews) to work as a Postdoctoral Fellow with Prof. Peter Bruce in energy storage materials. In 2014, she moved with Prof. Bruce and his research group to Oxford (Materials Department, University of Oxford) to work as a Research Fellow where she took up the role of Team Leader of the Sodium-ion battery team. She started her independent career as a Lecturer in Chemistry at Lancaster University in 2017 and was promoted to Senior Lecturer in 2020. In November 2022 Nuria, her research group and lab moved to Imperial College London where she is Senior Lecturer. She currently holds a CAMS-UK fellowship.

From Resources to Reuse – Optimisation of a Sustainable Sodium-Ion Battery

Emma Kendrick* [1]

[1]School of Metallurgy and Materials, University of Birmingham, Edbaston, B15 2TT, UK

E-mail: e.kendrick@bham.ac.uk

Keywords: critical materials • BOM • recycling • sodium-ion • ice-stripping

Abstract: Sodium-ion batteries (SIBs) offer a sustainable alternative to lithium-ion systems by reducing reliance on critical raw materials while enabling competitive performance for stationery and transport applications. Recent research has advanced hard carbon anodes paired with sodium layered oxide cathodes, demonstrating full-cell energy densities approaching ~150 $\mathrm{Wh\,kg^{-1}}$ and cycle life exceeding 500 cycles with ~80% capacity retention. Optimized formation protocols, such as controlled low-current conditioning within a restricted voltage window, have been shown to improve solid electrolyte interphase (SEI) uniformity, suppress irreversible sodium loss, and significantly enhance long-term stability.[1–3] At the materials level, engineered hard carbons with tailored porosity and surface chemistry deliver high reversible capacities (~300 $\mathrm{mAh\,g^{-1}}$) and stable Na^+ diffusion kinetics. Layered oxides, including $NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$, benefit from dopant incorporation and morphology control to mitigate phase transitions and electrolyte degradation. Together, these advances yield full cells with balanced N/P ratios and robust high-voltage operation.[4,5] To address end-of-life sustainability, direct recycling strategies such as ice-assisted electrode delamination and low-temperature reconditioning enable recovery and reuse of hard carbon and layered oxide materials without intensive chemical processing. Reclaimed electrodes retain near-pristine electrochemical performance, demonstrating ~86–89% capacity retention after 200 cycles post-reassembly. Complementary re-sodiation treatments restore sodium inventory losses, supporting closed-loop circularity.[6–8]

This integrated approach which combines materials optimization, controlled formation, and direct recycling, promotes a circular approach towards new battery technology development, for low cost, low supply chain risks, long-life and recyclability.

Reference:

[1]. Kishore B, Chen L, Dancer C E J and Kendrick E 2020 Electrochemical formation protocols for maximising the life-time of a sodium ion battery *Chemical Communications* **56** 12925–8.

[2]. Chen Y, Lakhdar Y, Chen L, Kishore B, Choi J, Williams E, Spathara D, Jackowska R and Kendrick E 2024 Accurate voltage prediction for lithium and sodium-ion full-cell development *Next Energy* **5** 100166.

[3]. Song T, Chen Y, Chen L and Kendrick E 2024 Areal capacity balance to maximize the lifetime of layered oxide/hard carbon sodium-ion batteries *J Power Sources* **624** 235599.

[4]. Song T, Zhang Q, Chen Y, Zhu P and Kendrick E 2023 Synthesis and design of NaNi1/3Fe1/3Mn1/3O2 cathode materials for long-life sodium-ion batteries *Chemical Engineering Journal Advances* **16** 100572.

[5]. Song T, Chen L, Gastol D, Dong B, Marco J F, Berry F, Slater P, Reed D and Kendrick E 2022 High-Voltage Stabilization of O3-Type Layered Oxide for Sodium-Ion Batteries by Simultaneous Tin Dual Modification Chemistry of Materials 34 4153–65.

[6]. Stephens I D R, Slater P and Kendrick E 2025 A Perspective on Cell Bill of Materials Using BatPaC J Power Sources 631 236170.

[7]. Liu B, Song T, Chen L, Shekhar A T, Mirolo M, Vinci V, Drnec J, Cornelio J, Xie D, Driscoll E H, Slater P R and Kendrick E 2025 Sustainable Recovery and Reuse of Hard Carbon From Scrap and End-of-Life Sodium-Ion Batteries Adv Energy Mater 2405894.

[8]. Chen L, Kishore B, Liu B, Song T, Lakhdar Y, Omoregbe O, Britton M M, Slater P R and Kendrick E 2025 A “Cool” Route to Battery Electrode Material Recovery Adv Energy Mater 2405924.

Biography: Emma Kendrick, CChem FRSC FIMMM - Professor of Energy Materials, School of Metallurgy and Materials, University of Birmingham and co-lead of the Energy Materials Group (EMG). Her research focuses on the design and development of sustainable battery technologies and chemistries. Materials, manufacturing and recycling. Prior to academia, she worked in the battery industry, as Chief Technologist in Energy Storage at SHARP Laboratories of Europe Ltd (SLE) and as Lead Scientist of two lithium-ion battery SMEs, Fife Batteries Ltd and Surion Energy Ltd. Her work on battery parameterisation was spun out into a company, About:Energy, in 2021, and is currently chair of their scientific advisory board. Prof Kendrick holds a PhD from Keele University, obtained as part of a postgraduate transfer partnership (PTP) scheme with CERAM Research, an MSc in new materials from the University of Aberdeen and a BSc in chemistry from the University of Manchester. She has been recognised for her research in sustainable batteries, including, as part of RELIB, the 2024 RSC Horizon Prize for work in battery recycling. 2021 Faraday Institution (FI) Researcher Development Champion, Royal Society of Chemistry (RSC) 2021 Environment, Sustainability and Energy Division Mid-Career Award, and the 2019 Hothersall Memorial Award for outstanding services to Metal Finishing.

NASICON-based Materials: A Wonderful “Crystal Chemistry” Playground

Nikhil Subash [1,2], Pierre-Etienne Cabelguen [3], Christian Masquelier [1,2] and J.N. Chotard [1,2]*

[1]Laboratoire de Réactivité et de Chimie des Solides (LRCS), CNRS UMR 7314, Université de Picardie Jules Verne, 80039 Amiens Cedex, France.

[2]RS2E, Réseau Français sur le Stockage Electrochimique de l’Energie, FR CNRS 3459, F-80039 Amiens Cedex 1, France.

[3]Umicore, Brussels BE-100, 512 Belgium

Keywords: NASICON • battery • operando • all-solid-state battery

Abstract: NASICON -based materials have a regain interest in the last decade. Originally known for their high ionic conductivity, their chemical versatility allows them to be used as electrode materials as well as as coating materials for different battery technologies (Li-ion, Na-ion, multivalent-ions and all-solid-state batteries) by tuning its composition. Indeed, the NASICON crystal structure of general formula $A_xMM'(XO_4)_3$, allows a wide range of chemical substitutions. Among them, the vanadium phosphate $Na_3V_2(PO_4)_3$ (NVP) is of particular interest because of its fantastic rate capacity and thermal stability, with a theoretical capacity of 117.6 mAh/g at 3.4 V and an energy density of 396 Wh/kg. Because of the wide oxidation range of Vanadium, NVP can be used either as an anode or a cathode. NASICON materials have also proven to be among the best solid electrolyte material for sodium All-Solid-State-Batteries (ASSBs). As an example, $Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$ attains ionic conductivity as high as 10 mS/cm with 3D diffusion path. Because of those electrochemical properties, their chemical stability and compatibility, NASICON-type are perfectly matching for building All-Solid-State-Batteries. Finally, on the anode side, Ti and Nb based NaSICon materials, allow to play with several redox couples from Nb+V to Nb+III as well as Ti+IV to Ti+III and display really interesting charge and discharge mechanisms investigated via XRD Operando measurements.

In this presentation, I will discuss the astonishing diversity of the crystal chemistry of the NASICON materials (both as electrodes or electrolyte) mostly studied through operando X-Ray Diffraction as well as its use in ASSBs.

Biography: Jean-Noël Chotard is Associate Professor of the University of Picardie Jules Verne, France with research activities conducted at the Laboratoire de Réactivité et Chimie des Solides (LRCS).

He graduated a PhD in Crystallography in 2008 from University of Geneva (Switzerland) on Hydrogen storage materials and spent one year as a Post Doc at the LRCS Amiens, France. His research activities, mainly based on solid state chemistry and crystal-chemistry, focus on the design, shaping and understanding of mechanism occurring upon cycling of material for energy storage and conversion (active material for Li / Na-ion batteries, Solid electrolyte and Hydrogen storage materials). He is also developing operando electrochemical cells for X-Ray and Neutron diffraction measurements. He is actively involved in the French Network on the Electrochemical Energy Storage (RS2E) and in the MESC + Master Program. He mentored 15 PhD students and publish about 95 papers.

Emerging Electrolyte for Sodium Batteries

Xiang Chen and Qiang Zhang*

Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

E-mail: zhang-qiang@mails.tsinghua.edu.cn

Keywords: organic electrolyte • sodium batteries • solid electrolyte interfaces • solium metal anode • gas evolution

Abstract: The development of advanced energy storage devices, the efficient use of renewable energy, and the construction of a sustainable energy system are urgent needs to achieve the goal of "carbon neutrality". Due to the limitations of energy density and other aspects, it is increasingly difficult for traditional lithium-ion battery technology to meet the energy needs of future social development. The development of sodium-ion battery technology has become the focus of current research, but at the same time, higher requirements are put forward for electrolyte design. It is an important prerequisite for the development of a new electrolyte system to deeply understand the solvation structure and structure-activity relationship of electrolyte and explore its microscopic chemical principle. In order to solve the problem that the instability mechanism of the interface between the conventional organic electrolyte and the anode is unknown, an ionic-solvent chemical model was established to reveal the chemical nature of the reductive decomposition of solvent molecules on the surface of the metal anode at the molecular and electronic levels. The cation in the electrolyte interacts with the solvent to form an ion-solvent composite structure, which significantly reduces the minimum unoccupied molecular orbital (LUMO) energy level of the solvent, making it easier for the solvent molecule to obtain electrons at the negative electrode, reduce decomposition, and even produce flammable gases. Based on the ion-chemical model, electrolyte design strategies such as cationic additives, weakly solvated electrolytes, lithium-ion solvated shell anions, and anion acceptors were proposed, and a stable electrolyte-anode interface was constructed, which provided important theoretical support for the development of the next generation of high-safety new battery systems.

Biography: Qiang Zhang is a professor at Tsinghua University. He held the Newton Advanced Fellowship from Royal Society, UK and the National Science Fund for Distinguished Young Scholars. He is the dean of Department of Chemical Engineering, Tsinghua University. He is selected as highly cited researchers at 2017-2024 by Clarivate Analytics. His current research interests are advanced energy materials and energy chemistry, including dendrite-free lithium metal anode, lithium sulfur batteries, and electrolyte, especially the structure design and full demonstration of advanced energy materials in working devices. His h-index is 172 now. He is the Editor-in-Chief of EES Batteries, Advisor Editor of Angew. Chem.. He is sitting on the advisory board of Joule, Chem Soc Rev, Matter, Adv Funct Mater, ChemSusChem, J Mater Chem A, Chem Commun, Energy & Fuels, and so on. He is the deputy head of the expert group on energy storage and smart grid of the national key research and development plan. He has won the first prize of Natural Science of the Ministry of Education, the first prize of Fundamental Science of the Chemical Engineering Society.

Hard Carbon anodes and ionic liquid electrolytes

N.Byrne

ARC Industry Transformation Training Centre for Future Energy Technologies, Institute for Frontier Materials (IFM), Deakin University, Burwood, Victoria 3125, Australia

Emai: nolene.byrne@deakin.edu.au

Abstract: Energy storage devices are a critical component in the transition to net zero. Currently lithium ion batteries dominate the market, however lithium ion batteries have many drawbacks, including the high use of critical minerals, resulting in potential supply volatility and the inherent safety issues . Many of the limitations associated with Lithium-ion batteries can be overcome by Na-ion batteries, with target application in stationary energy storage. However, Na-ion battery performance needs to improve, a key to this improvement is better performing anodes. Unlike current LIBs which require highly structure graphite as the anode, Na-ion batteries perform best with carbon anodes which are non-graphitizable known as hard carbons. In recent times, hard carbons from waste streams have gained significant interest however despite the precursors choice some inherent limitations remain for hard carbons such as low initial columbic efficiency and rate capability. In this talk we explore these limitations by examining the impact of precursor choice and carbonization protocol, and the impact this has on the material properties of the hard carbon and subsequently the electrochemical performance is discussed including porosity. Additionally, as the electrolyte choice, ionic liquids are used and we discuss the impact of ionic liquid choice on performance and SEI formation.

Deconstructing The Role of Water on Phase Transitions in Prussian Blue Analogue Cathodes

William R. Brant

[1]Department of Chemistry – Ångström Laboratory, Uppsala University, Sweden

Abstract: The fundamental appeal of Sodium-ion batteries is that they can achieve performance on par with some Lithium-ion technologies but at a substantially reduced cost and with vastly more abundant raw materials. The one class of materials which meets these requirements are iron based Prussian blue analogues (PBAs) $A_xM[Fe(CN)_6]_{1-y}\cdot zH_2O$, which are comprised of corner linked FeC_6 and MN_6 (where M is commonly Mn or Fe) octahedra forming a porous framework structure. A common feature for all PBAs is a phase transition which occurs for high cation content (when $x > 1\text{-}1.2$). This phase transition is particularly damaging when water is removed from the structure, leading to an 18% reduction in the unit cell volume. Subsequently, during electrochemical cycling, sodium extraction and insertion, a second phase transition occurs leading to a 16% volume change. This potentially carries consequences for the cycle life of PBA electrode materials. Thus, this contribution will undertake a deep dive into the consequences of the phase transition during electrochemical cycling and unravel the role that water plays in stabilising the structure.

Intriguingly, via a series of *operando* diffraction studies it was revealed that the phase transition is only responsible for a loss of capacity during the initial formation cycles. However, the losses are still substantial enough to warrant a deeper understanding of the phase transition to design solutions to stabilise the structure, minimise particle cracking, electrode delamination and subsequently capacity loss. To this end we applied a combination of neutron scattering techniques including QENS, neutron pair distribution function analysis and inelastic neutron scatting to build a deep understanding of the interaction between water and the host PBA structure. The investigation revealed the complex dynamics of water positioning and orientation as a function of temperature and sodium content. By understanding the relative affinity of water towards the mobile sodium ion or the host framework, alternative small guest molecules can be rationally selected which fulfill the role of structure stabilisation without the risk of damaging side reactions with the electrolyte.

Biography: **William R. Brant** is a Senior Lecturer / Associate Professor in the Structural Chemistry group at the Department of Chemistry – Ångström Laboratory, Uppsala University. His research investigates dynamic non-equilibrium processes in crystalline materials—how atoms move, relax, and rearrange both on sub-nanometer to macroscopic scales—and how those changes affect performance in battery and energy storage materials. He uses advanced diffraction techniques (operando X-ray, neutron, etc.) to follow structural evolution during cycling and non-equilibrium transitions, with the goal of informing design of better energy storage materials.

Insight on bio-based hard carbon anodes for Na-ion Batteries

L. Simonin*[1,4], C. Saavedra Rios[1,2] J. Michell[2], A. Qaterneh[2], A. Beda[3,4], A. Escamilla[3,4], C. Dupont[2], C. Matei-Ghimbeu[3,4]

[1]Université Grenoble Alpes, CEA, LITEN DEHT LM, 17 rue des Martyrs, Cedex 9, Grenoble 38054, France.
E-mail: loic.simonin@cea.fr

[2]Department of Water Supply, Sanitation and Environmental Engineering, IHE Delft, Westvest 7, 2611 AX Delft, The Netherlands

[3]Institut de Science des Matériaux de Mulhouse (IS2M), CNRS UMR 7361, F-68100 Mulhouse F-68100

[4]Reseau sur le Stockage Electrochimique de l'Energie (RS2E), CNRS FR3459, 33 Rue Saint Leu, 80039 Amiens Cedex, France

Keywords: bio-based hard Carbon • raw biomass • hydrothermal carbonization • biopolymers • Na-ion negative electrode

Abstract: Hard Carbon (HC) is considered as the most promising anode material for Sodium-Ion Batteries (SIBs). State-of-the-art reversible capacities exceed 300 mAh.g^{-1}, Initial Colombic Efficiencies (ICE) are above 90% and average operating voltages are around 0.2 V[1]. HC is typically produced by pyrolyzing oxygen- rich precursors under inert atmosphere, at temperature above 1000°C. The three main types of precursors sources are biomass, biopolymers, or fossil-based synthetic polymers. Their physicochemical properties, such as porosity, structure, and surface chemistry, and thus electrochemical performances can be tailored through precursor selection and synthesis conditions. The search for bio- sourced precursors is widely promoted as a sustainable and cost effective alternative to fossil-based synthetic polymers. In this study, we present a comprehensive investigation into the influence of the precursor type, precursor purity, synthesis methods, synthesis parameters on the properties and performances of HC. First of all, 25 dry biomasses precursors were prepared by pyrolysis, showing a great influence of the elemental composition, inorganic elements type and precursors morphology on HC characteristics[2]. Subsequently, Hydrothermal Carbonization (HTC) was employed to prepare HC out of uvularized low cost wet biomasses. We evaluated the impact of this pretreatment compared to direct pyrolysis, on the leaching of inorganic elements and their impact on carbon properties[3]. Furthermore, we identified river driftwood as a highly promising low cost wet biomass for high- performance HC[4]. Finally, bio-polymers[5], and bio-molecules[6] were used to produce HC with notable high specific capacities and initial coulombic efficiencies. We also examined the influence of impurities, porosities and surface chemistries on the electrochemical performances were reported of HC. The best performance was observed for materials with low impurity levels, more disordered structures, and low specific surface areas.

References:

[1]. C. Matei Ghimbeu et al., Advanced Energy Materials (2024), https://doi.org/10.1002/aenm.202303833
[2]. C Saavedra et al., Fuel Processing Technology, https://doi.org/10.1016/j.fuproc.2022.107223
[3]. J. Michel et al., Biomass Conversion and Biorefinery, https://doi.org/10.1007/s13399-023-05105-94
[4]. Qaterneh et al., Journal of Environmental Chemical Engineering, https://doi.org/10.1016/j.jece.2021.106604
[5]. Escamilla et al., ACs Appl. Energy Mater., https://doi.org/10.1021/acsaem.3c00640
[6]. Beda et al., Acs Appl. Energy Mater., https://doi.org/10.1021/acsaem.2c00215

Biography: Loïc Simonin is a senior scientist at the Laboratory for Innovation in New Energy Technologies and Nanomaterials (LITEN) at the French Alternative Energies and Atomic Energy Commission (CEA) in Grenoble, France. He leads the Na-ion battery innovation program at LITEN. He is a member of the French Network for Electrochemical Energy Storage (RS2E). He has coordinated several EU-funded projects and is involved in the Battery 2030+ initiative. He earned his PhD from Delft University of Technology in 2009 (The Netherlands). His research focuses mainly on cathode and anode materials as well as prototyping of Na-ion battery. For the past decade, he has made significant contributions to this field. For example, he played a key role in the RS2E Na-ion task force and coordinated the EU project NAIADES, which led to the creation of the TIAMAT battery manufacturer.

Tuning The Microporosity and Surface Chemistry of Hard Carbons for High Electrochemical Performance

Da Huo,[1-2] Marion Bermont,[1-2] Raphaël Janot* [1-2]

[1]Laboratoire de Réactivité et Chimie des Solides, LRCS, UMR 7314 CNRS, Université de Picardie Jules Verne, 15 rue Baudelocque, 80039 Amiens, France

[2]Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR 3459 CNRS, 33 Rue Saint Leu, 80039 Amiens, France

Email: raphael.janot@u-picardie.fr

Keywords: hard carbon • microporosity • surface chemistry • biomass • Na-ion battery

Abstract: Non-graphitizing carbons, such as hard carbons (HCs), are the most investigated materials to date as negative electrode for Na-ion batteries due to their good electrochemical performances, although the exact mechanism of sodium storage remains under debate. HCs can be prepared from a large variety of precursors ranging from preoxidized pitch to biosourced polyphenolic molecules. The pyrolysis temperature has a huge impact on the heteroatom contents and structural defects and thus on the electrochemical performances (reversible capacity, Initial Coulombic Efficiency (ICE), rate capability).

This presentation will present an in-depth characterization of the HCs meso/microporosity, e.g. open and closed pores were characterized by gases adsorption/desorption (N_2, CO_2, H_2) and SAXS (Small Angle X-ray Scattering), respectively. An original experiment by in-situ environmental TEM (i.e. pyrolyis performed in the TEM chamber under various atmospheres) will reveal the mechanism of nanopore formation during the pyrolysis of different carbonaceous materials. We will show that the development of the closed microporous volume (i.e. pores size below 2 nm) allows to promote the plateau capacity (< 0.1 V vs. Na^+/Na) on the galvanostatic sodiation profiles of the HCs. This reveals that the plateau capacity is related to the pores filling mechanism.

The presentation will also discuss the coating of the HC particles by a soft carbon (prepared by CVD using ethylene, or by an impregnation method using petroleum pitch dissolved in THF). This coating method is known for reducing the BET surface area for many materials and thus limiting the SEI formation and promoting the ICE. Actually, we will show that the BET surface area is not the major parameter controlling the ICE value, but that the nature of the surface groups is also very important. Thanks to XPS experiments, we will clarify the effects of surface chemistry on the SEI formation and the ICE value of the HCs.

As a conclusion, we will present some facile synthesis routes for bio-based hard carbons exhibiting high electrochemical performance: namely, a reversible capacity above 320 mAh/g at C/20 and a high coulombic efficiency at the first cycle (above 85 %).

Biography: Raphaël Janot studied solid-state chemistry at University de Lorraine, France where he received a PhD degree in 2001 on the synthesis of negative electrode materials for Li-ion batteries by mechanochemical methods. He extended his research to hydrogen storage materials during two successive post-doctoral fellowships. Since 2005, Raphaël JANOT is CNRS Researcher at Laboratoire de Réactivité et Chimie des Solides (LRCS) in Amiens, France. His current research activities are focused on complex hydrides for solid state hydrogen storage and carbonaceous materials for metal-ion batteries. This latter aspect includes the development of hard carbon negative electrodes for Na-ion batteries.

Diverse Connected and Air-Free Analysis Workflows for Battery Research

Bernd Schulz*[1], Kashmira Raghu[1], Yulia Trenikhina[2], Steve Kelly[2]

[1]Carl Zeiss Pty Ltd, 65 Epping Road, Macquarie Park NSW 2113, Australia

Email: bernd.schulz@zeiss.com

[2]Zeiss Research Microscopy Solutions, 5300 Central Pkwy, Dublin, CA 94568, USA

Keywords: air-free handling • scanning electron microscopy • x-ray microscopy • microstructure

Abstract: The increasing demand for grid storage is propelling significant advancements in battery technology. However, several critical materials challenges must be addressed before next-generation batteries can become standard in these applications. Modern battery research is confronted with complex challenges that span across various length scales, from component engineering at the cell level to intricate material characterisation challenges at the nanometre scale. As materials used in batteries react strongly with air, careful sample handling and preparation considerations must be addressed to successfully investigate these systems.

This presentation will explore correlative multi-scale microscopy workflows that integrate 3D X-ray microscopy (XRM) imaging connected Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM) techniques. XRM can reveal sub-surface details non-destructively and with high spatial resolution, guiding further investigations with detailed 3D maps of internal material microstructures. FIB-SEM can target specific regions within these volumes for nanoscale imaging and chemical analysis of specific features. Additionally, we will discuss the introduction of air-free sample transfer shuttles, which are crucial for preserving the integrity of reactive materials during analysis.

These advanced workflows provide profound insights into the material properties of complex battery systems, paving the way for enhanced understanding and development of next-generation energy storage solutions.

Biography: Bernd Schulz oversees the Materials Research portfolio at ZEISS Australia and New Zealand. He holds a PhD from UNSW Sydney and has over 10 years' experience as Materials Scientist within academic research and the manufacturing industry. This extensive experience has cultivated a deep understanding of microscopy techniques and their applications, equipping him to offer tailored solutions to a wide range of challenges.

Temperature-Dependent Degradation of Fast-Charging Commercial Sodium-Ion Batteries

Jiaxing (Gaaseng) Liang, [1] Sherman Wong,[1] Adam Best,[1] and Tony Hollenkamp* [1]

[1]CSIRO Manufacturing, Clayton, VIC 3168, Australia

E-mail: Tony.Hollenkamp@csiro.au

Keywords: sodium-ion batteries • fast-charging • temperature-dependent • cyclic aging • sodium transition metal oxides

Abstract: Sodium-ion batteries (SIBs) have garnered significant attention as a promising electrochemical energy system, offering high power density and cost-effective scalability. However, their commercial viability remains constrained by temperature-dependent degradation during cycling, especially under fast-charging conditions. In this study, we examined the aging behaviour of a typical commercial SIB featuring a $Na_{0.94}Ni_{0.33}Mn_{0.34}Fe_{0.33}O_2$ cathode and a hard carbon anode under varying temperature conditions (0–50°C) with rapid charge and discharge cycling. While these batteries demonstrate a prolonged lifespan at elevated temperatures (50°C), their significant degradation at lower temperatures presents a critical barrier to practical applications, particularly in cold environments. This performance decline is commonly attributed to sluggish sodium ion desolvation from the electrolyte, yet the underlying mechanisms remain insufficiently understood. To address this gap, we systematically investigated the mechanical integrity of the cells, along with structural transformations of the active materials and changes in electrode/electrolyte interfacial chemistry. By correlating temperature effects with cell structure changes, ion diffusion kinetics, redox activity variations, and overall electrochemical performance, this study provides valuable insights into the fundamental processes governing temperature-dependent cyclic aging behaviour of SIBs. These findings contribute to the optimization of battery design, particularly SIBs, aiming to enhance resilience and operational stability across wide temperature ranges, expanding their feasibility for energy storage applications in diverse environmental conditions.

Biography: Jiaxing (Gaaseng) Liang is currently a CSIRO Early Career Research (CERC) Fellow and Project Leader in the Battery Material and Design (BMD) team at CSIRO Manufacturing (2024-present). Before this, he served as a postdoctoral research assistant at University of New South Wales (UNSW Sydney) and Shenzhen University of Advanced Technology in the development of extremely fast charging batteries (2024). He received his B.E. degree from South China Normal University in 2017, followed by a M.Phil. degree in 2019 and a Ph.D. degree in 2024, both in Chemical Engineering from UNSW Sydney. His research specializes in sustainable electrochemical energy systems, with a particular focus on lithium/sodium/dual-ion batteries and supercapacitors. His expertise spans functional materials design and electrode-electrolyte interface engineering.

From 1 mAh to 1 Ah: Bridging Fundamental Research and Practical Na-Ion Cells through Innovation

Jon Ajuria[1]

[1]Alava Technology Park, Albert Einstein 48, 01510 Vitoria-Gasteiz, Spain

Keywords: advance materials • prototype • electrode fabrication • cell design • performance evaluation

Abstract: Sodium-ion batteries (SIBs) are gaining momentum as a sustainable and cost-effective alternative to lithium-based systems, particularly for grid-level and stationary storage. Yet, the gap between fundamental discoveries and practical device implementation remains significant. Advanced active materials—such as high-performance hard carbon anodes and layered oxide cathodes—often demonstrate potential breakthroughs beyond the state of the art. However, without a proper evaluation platform, their practical impact remains limited. In this work, we present an innovation-driven approach that scales sodium-ion technology from lab-scale 1 mAh cells to 1 Ah-class pouch cells, a platform that can be used for demonstrating the feasibility of transitioning from fundamental insights to real-world prototypes.

The process includes slurry formulation, roll-to-roll processing, electrode calendering, and cell assembly. By iteratively optimizing key parameters—including the negative-to-positive (N/P) ratio, electrolyte composition, and formation protocols—promising materials, processes, and components can be evaluated in a more relevant TRL 4–5 environment, advancing them toward practical innovation.

Biography: Jon Ajuria is Research Line Manager for Sodium-Ion Batteries at CIC energiGUNE. With over 20 years of experience in process engineering and energy generation and storage technologies, his work focuses on electrode manufacturing optimization, hybrid batteries, and the upscaling of supercapacitors and sodium-ion batteries. He has authored over 40 scientific publications (h-index: 24), holds 2 patents, and has led multiple technology transfer projects in collaboration with private industry. Jon also coordinates European research initiatives, contributing to the advancement of sustainable and scalable battery technologies across various TRL levels.

Sodium-Ion Batteries for High-Power Applications

Chloé Pablos[1,2,3], Matilda Fransson[4], Sandrine Lyonnard[4], Laurence Croguennec[2] and Mathieu Morcrette[1,3]

[1]Tiamat Energy, HUB de l'Energie, 80000 Amiens, France * chloe.pablos@tiamat-energy.com

[2]Univ. Bordeaux, Bordeaux INP, ICMCB, UMR 5026, 33600 Pessac, France

[3]LRCS, UMR 7314, HUB de l'Energie, 80000 Amiens, France

[4]CEA IRIG, F-38054 Grenoble, France

Keywords: Na-ion batteries • NVPF • high-power batteries

Abstract: Alternatives to lithium-ion batteries for energy storage have been intensively studied, with sodium-ion emerging as a strong candidate due to sodium's abundance and wide distribution [1]. Carbon-coated $Na_3V_2(PO_4)_2F_3$ (NVPF) // hard carbon (HC) chemistry has been successfully implemented in Tiamat Energy's high-power cells [2], including commercial 18650-format device, such as Leroy Merlin screwdrivers [3] and lately in 52148-prismatic cells for peak shaving in datacentres. These prismatic cells demonstrate excellent performance, retaining 93% of its capacity after more than 750 cycles at 20C charge and discharge rates.

To better understand the origin of this exceptional cyclability, structural analyses were performed on 18650-format cells that retained 85% of their capacity after more than 1800 cycles at 20C, with no evidence of sodium plating. These investigations relied on ex situ and in situ Small- and Wide-Angle X-ray Scattering Computed Tomography (SWAXS-CT), conducted at beamline ID31 of the European Synchrotron Radiation Facility (ESRF). This technique enables high-resolution mapping of structural heterogeneities and spatially resolved detection of sodium deposition within full cells. WAXS-CT revealed no crystalline metallic sodium satisfying Bragg diffraction conditions, confirming the absence of plating. In parallel, WAXS also provided insight into phase transitions in the positive electrode material during the desodiation process, offering a detailed understanding of the internal structural evolution throughout cycling.

Backed by strong market interest, Tiamat is currently preparing the construction of a 5 GWh sodium-ion gigafactory in France, aiming to scale up production and support the industrial rollout of its high-power battery technology.

References:

[1]. Mariyappan, S.; Wang, Q.; Tarascon, J. M. Will Sodium Layered Oxides Ever Be Competitive for Sodium Ion Battery Applications? *J. Electrochem. Soc.* **2018**, 165 (16), A3714-A3722

[2]. Broux, T.; Fauth, F.; Hall, N.; Chatillon, Y.; Bianchini, M.; Bamine, T.; Leriche, J.-B.; Suard, E.; Carlier, D.; Reynier, Y.; et al. High Rate Performance for Carbon-Coated Na3V2(PO4)2F3 in Na-Ion Batteries *Small Methods* **2019**, 3 (4), 1800215-1800226

[3]. https://www.leroymerlin.fr/conseils/conseils-pratiques/tout-savoir-sur-batterie-sodium-nouvelle-alternative-au-lithium.html

Biography: Currently a PhD student at Tiamat Energy, I have been working on NVPF electrode positive material for the past five years.

Promising Phosphate and Sulfate-Based Electrode Materials for Na-Ion Batteries

L. Croguennec[1,]*, S. Park[1,2,3], G. Minart[1], A. Grebenshchikova[1,2,4], F. Fauth[5], F. Weill[1],
P. Canepa[6], L. Simonin[4], D. Carlier[1], J.N. Chotard[1], J. Olchowka[1], C. Masquelier[2]
[1]ICMCB, Université de Bordeaux, UMR CNRS 5026, Pessac, France
[2]LRCS, Université de Picardie Jules Verne, UMR CNRS 7314, Amiens, France
[3]TIAMAT Energy, Amiens, France
[4]CEA Liten, Grenoble, France
[5]ALBA synchrotron, Spain
[6]University of Houston, USA
Email: laurence.croguennec@icmcb.cnrs.fr

Abstract: During this talk, I will discuss about new attractive phases and mechanisms identified in the vanadium-rich (fluoride) phosphates $Na_3V_2(PO_4)_3$ and $Na_zMn_xV_{2-x}(PO_4)_2F_{3-y}O_y$, as well as in iron-rich mixed phosphates and sulfates, all being interesting candidates as positive electrode materials in Na-ion batteries.

A new class of NASICON-related materials has been obtained. A whole series of new single-phase $Na_xV_2(PO_4)_3$ compositions (x = 1.5, 1.75, 2, 2.25, and 2.5) was discovered using an innovative and straightforward synthesis route.[1] Typically, $Na_2V_2(PO_4)_3$ is obtained by annealing an equimolar mixture of $Na_3V_2(PO_4)_3$ and $NaV_2(PO_4)_3$ and exhibits a structure and an electrochemical signature different from the "conventional" NaSICON structure. Disorder is observed in the Na^+ distribution within the channels of the 3D framework. Furthermore, a significant increase (0.6 V) of the average operating voltage due to changes in the extraction/insertion mechanism - a solid solution reaction all along the composition domain - leads to an increase in energy density of ~10%.

The feasibility of synthesizing stable Na-deficient polyanionic phases within the Mn and O substituted $Na_zV_{2-x}Mn_x(PO_4)_2F_{3-y}O_y$ ($0 \leq x, y \leq 2$ and $z \leq 3.6$) material family has been demonstrated.[2] They are obtained via topochemical reaction in an ionic liquid medium, starting from a tailored precursor $Mn_{x/2}(VO)_{1-x/2}PO_4 \cdot 2H_2O$. The resulting active materials exhibit promising electrochemical performance, delivering a specific capacity of 90 mAh/g at 1C and an average potential of 3.75 V vs. Na^+/Na. An excellent capacity retention of 94% was demonstrated after 200 cycles at C/5. Besides, X-ray absorption spectroscopy analysis reveals the redox activity of both manganese and vanadium transition metals.

Development of new sulfate and/or phosphate sodium iron positive electrode materials for Na-ion batteries has been achieved recently in our groups. Among them, sodium iron sulfate $Na_2Fe_3(SO_4)_4$, a new compound made only of non-critical elements was obtained by ball milling synthesis method, interestingly from Na_2SO_4 and $FeSO_4$, and preliminary electrochemical tests showed promising results.[3]

I will demonstrate that only the in-depth control of the relationship synthesis/composition/atomic and electronic structure allows to tune the properties in the battery.

References:

[1]. S. Park, Z. Wang, K. Choudhary, J.-N. Chotard, D. Carlier, F. Fauth, P. Canepa, L. Croguennec, C. Masquelier, *Nature Materials*, **2024**, 1-9.

[2]. G. Minart, M. Duttine, A. Iadecola, J.-P. Salvetat, F. Weill, S. Buffière, R. Wernert, J. Olchowka, L. Croguennec, *Chemistry of Materials*, **2024**, *36* (20), 10186-10197.

[3]. A. Grebenshchikova, J. Olchowka, L. Simonin, S. Yaroslavtsev, M. Duttine, F. Fauth, L. Stievano, C. Masquelier, L. Croguennec, *submitted*.

Biography: Laurence Croguennec is CNRS Research Director at the Institut de Chimie de la Matière Condensée (ICMCB-CNRS, France) at the Bordeaux University. She graduated (PhD) in 1996 from Nantes University at the Institut des Matériaux Jean Rouxel (France) and spent one year as a Post-Doc at the Bonn University (Germany). She became CNRS researcher at ICMCB in 1997, led the research group "Energy: Materials and Batteries" between 2004 and 2021 and is Deputy Director of ICMCB since 2022. She is also actively involved in the French Network on the Electrochemical Energy Storage (RS2E), in the ALISTORE European Research Institute devoted to battery research and in the France 2030 acceleration program with the PEPR batteries.

Laurence Croguennec has been working for more than 25 years now on the crystal chemistry of electrode materials developed for Metal-ion batteries, and more recently all-solid-state batteries, and on the characterization of mechanisms involved upon their cycling, especially for layered and spinel oxides and polyanionic-type positive electrode materials. She develops also research in collaboration with European neutrons and synchrotron large scale facilities for *in situ* and *operando* characterization of materials during the operation of the batteries. She is the co-author of 180 publications, 5 book chapters and 8 patents in this field; she delivered 90 invited talks, and organized 19 international and 7 national meetings or symposiums.

Revisiting Fe-based Layered Cathode Material: Stable Cycling Stability Achieved by Integrated Surface Engineering

Seung-Taek Myung* [1]

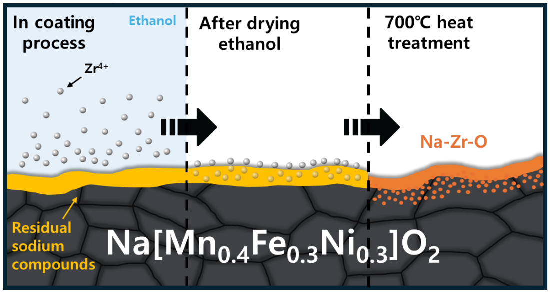
[1]Hybrid Materials Research Center, Department of Nanotechnology and Advanced Materials Engineering & Sejong Battery Institute, Sejong University, 98 Gunja-dong, Gwangjin-gu, Seoul 05006, South Korea

E-mail: smyung@sejong.ac.kr

Keywords: zirconium• coating • doping• sodium• battery

Abstract: Achieving high performance in O3-type layered cathodes for sodium-ion batteries is hindered by various chemical and mechanical issues such as phase transitions, voltage decay, and particle cracking. In this study, we explore the impacts of simultaneous surface doping with Zr^{4+} and surface coating with Zr-based oxides on the performance of the O3-type $Na[Mn_{0.4}Fe_{0.3}Ni_{0.3}]O_2$. The integration of a robust Zr-O bond and the chemically inert characteristics of the surface coating significantly enhances both the structural and interfacial stability of the $Na[Mn_{0.4}Fe_{0.3}Ni_{0.3}]O_2$ in Na cells. The associated charge compensation reaction was assisted by not only the redox pairs of Ni^{2+}/Ni^{4+}, Fe^{3+}/Fe^{4+}, and Mn^{3+}/Mn^{4+} but also the $O^{2-}/(O_2)^{n-}$ pair that is triggered by releasing the lattice oxygen from the OP2 phase, as verified by comprehensive analyses and density functional theory calculation. The bare and Zr-modified $Na[Mn_{0.4}Fe_{0.3}Ni_{0.3}]O_2$ paired with hard carbon anodes demonstrate capacity retention of 5% and 43% after 500 cycles at 1C (240 mA g^{-1}), respectively. *Operando* X-ray study confirms the improved structural stability in the Zr-modified one during the phase transition from the P3 to OP2 phase, which was from 10.2% for the bare and 7.5% for the Zr-modified one. The Zr-based surface layer significantly protects the cathode from HF attack and the dissolution of transition metals during cycling. These findings underscore the synergistic effects of Zr surface coating and bulk doping in enhancing the functionality of O3-type cathode materials.

Biography: Seung-Taek Myung is a Professor of Nano Engineering and Advanced Materials at Sejong University in Seoul, South Korea. His research specializes in electrode materials for rechargeable batteries, particularly high-energy and high-stability cathodes, and in studying battery electrochemistry and performance.



Thermal Stability Index of Sodium Layered Oxide Cathodes

Masashi OKUBO*

Okubo 3-4-1, Shinjuku-ku, Tokyo 169-8555, Japan

Department of Electrical Engineering and Bioscience, School of Advanced Science and Engineering, Waseda University

E-mail: m-okubo@waseda.jp

Keywords: cathode • layered oxide • DSC • safety

Abstract: Sodium layered oxides provide the best electrode performance for sodium-ion batteries with high gravimetric/volumetric energy and power densities. However, their safety issue should be addressed for gird-scale use. In the present work, we systematically quantify the thermal stability of layered oxide cathodes using thermial stability index (TSI), and demonstrate a rational strategy to improve it.

Biography: Masashi Okubo received a Ph.D. in coordination chemistry from the University of Tokyo in 2005. After working at Université Pierre et Marie Curie, National Institute of Advanced Industrial Science and Technology, and the University of Tokyo for 16 years, he was appointed as a professor at Waseda University, where he is now.

Fast-Ion Conducting Catholytes $A_xNbO_xCl_{5-x}$ (A = Na, Li) for Dual Electrolyte Solid-State Batteries

Aniruddh Ramesh,[1] Haowen Wu,[1] Max Avdeev,[2] and Stefan Adams[1*]

[1]Department of Materials Science and Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117575, Singapore

[2]Australian Centre for Neutron Scattering, New Illawarra Road, Lucas Heights, NSW 2234, Australia

E-mail: mseasn@nus.edu.sg

Keywords: ion transport in solids • fast-ion conducting oxyhalides • structure-property relationships • rational materials design • solid-state batteries

Abstract: Identifying solid electrolytes that combine fast ionic conductivity with electrochemical, chemical, and mechanical compatibility to high-voltage cathodes remains challenging. Among the promising candidates are glass-ceramic oxyhalides, which provide tunable lattice environments and structural flexibility for ionic transport. The recent finding that $LiNbOCl_4$ features an ionic conductivity of 10 mS/cm while being oxidation-stable and highly compressible inspired a search for an analogous Na^+ ion conductor $NaNbOCl_4$. Here, we mechanochemically synthesize and characterize glass-ceramic samples of both materials and regulate their composition to $A_xNbO_xCl_{5-x}$ ($x \leq 1$, A=Na, Li) to maximize ionic conductivity. Structural analysis of X-ray and neutron diffraction data reveal distinct tetragonal (A= Li) or orthorhombic (A= Na) structures that differ in the packing of $(NbCl_4O_{2/2})_\infty$ polyanion chains and the extent of cation disorder. Differential scanning calorimetry of the $ANbOCl_4$ glass ceramics reveal phase transition slightly above room temperature. Molecular dynamics simulations indicate for both phases high rotational mobility of $NbCl_4$ groups, explaining the materials' soft mechanical properties and fast ionic transport. Simulation findings are in line with Raman spectroscopic analyses of the vibrational characteristics. Rotational anion mobility also induces negative thermal expansion, while compression reduces conductivity by restricting anion reorientation. More in detail, the ion-tranport mechanisms for the Li^+ and Na^+ oxychlorides differ, with a paddle-wheel type 1:1 correlation between cation mobility and polyanion rotation for A = Na only. Our simulated energy landscapes for alkali ion transport align well with experimental measurements, which for A=Na lead to a low bulk activation energy of 0.15 eV, but a higher activation energy of 0.3 eV for total conductivity below room temperature. Despite the low-barrier Na^+ bulk ion transport channels, the total room temperature conductivity remains with 1 mS/cm an order of magnitude smaller than the 11.4 mS/cm for slightly off-stoichiometric $Li_{0.9}NbO_{0.9}Cl_{4.1}$. Combining $Li_{0.9}NbO_{0.9}Cl_{4.1}$ as a catholyte with NMC811, $Li_{1.97}(Si_{0.97}P_{0.03})S_3$ anolyte, and Li-In alloy, results in initial capacities of 191 mAh/g, demonstrating potential for future solid-state batteries.

Biography: After a Ph.D. from Saarbrücken/Germany, **Adams** worked at the Stuttgart Max-Planck Institute and habilitated from Göttingen University before joining National University of Singapore in 2005, where he is Assoc. Professor for Materials Science and Engineering. His research focuses on rational design of inorganic materials and interfaces with optimal transport properties for energy storage and conversion devices. To this end his group combines electrochemical, diffraction and NMR experiments with high-throughput computational design. Adams also serves as Vice-President of the Materials Research Society of Singapore, has been Secretary of the Asian Society for Solid State Ionics 2013-24 and is member of the editorial boards of several journals including Solid State Ionics, Int. Journal for Ionics and Batteries.

Enhancing Oxygen Redox Kinetics in Na-Layered Cathodes toward High-Power and High-Energy Sodium-Ion Batteries

Jongsoon Kim* [1 2]

[1]Department of Energy Science, Sungkyunkwan University, Suwon 16419, Republic of Korea

E-mail: jongsoonkim@skku.edu

[2]SKKU Institute of Energy Science and Technology, Sungkyunkwan University, Suwon 16419, Republic of Korea

Keywords: Na ion batteries • cathode • oxygen redox • layered oxide • high power

Abstract: The growing demand for sustainable and cost-effective energy storage technologies has led to increasing interest in sodium-ion batteries (SIBs) as alternatives to lithium-ion systems, particularly for grid-scale and stationary applications. Sodium is abundant, inexpensive, and shares similar electrochemical properties with lithium, making it attractive for large-scale deployment. Among the available cathode materials, Na-layered oxides are considered promising due to their high theoretical capacities. Importantly, their ability to utilize both transition metal and oxygen redox reactions offers a pathway to further enhance energy density beyond conventional limits.

However, the practical realization of oxygen redox in Na-layered cathodes remains challenging. The participation of lattice oxygen often induces sluggish kinetics, large voltage hysteresis, and irreversible structural changes during cycling. These issues are especially pronounced under high-rate conditions, where overpotentials and phase transitions degrade electrochemical performance. As a result, many oxygen-redox-active cathodes suffer from poor cyclability and limited power capability, which hinder their applicability in SIB systems.

In this study, we investigate Na-layered cathode materials designed to overcome these limitations and enable stable oxygen redox behavior even under fast discharging conditions. By optimizing the local structure and electronic environment, we suppress structural instabilities typically associated with oxygen activity and improve the overall reaction kinetics. The resulting materials demonstrate both high energy density and excellent fast discharing performance, with minimal voltage decay over prolonged cycling. Our findings provide insight into how oxygen redox can be harnessed more effectively in Na-layered oxides and point toward practical strategies for advancing high-performance SIB cathodes suitable for demanding energy storage applications.

Biography: Jongsoon Kim is an associate professor of Department of Energy Science in Sungkyunkwan University. He received B.Sc. and M.Sc. at Korea Advanced Institute of Science and Technology (KAIST). Then, He completed Ph.D. at the Seoul National University. His research laboratory focuses on development of novel cathode materials for Li- and Na-ion batteries first-principles calculations and advanced structural analyses.

Glassy Solid Electrolytes for All-Solid-State Na Batteries

Akitoshi Hayashi*, Kota Motohashi, Atsushi Sakuda

Department of Applied Chemistry, Graduate School of Engineering, Osaka Metropolitan University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka, 599-8531, Japan

E-mail: akitoshihayashi@omu.ac.jp

Keywords: solid electrolyte • glass • sulfide • chloride • all-solid-state battery

Abstract: All-solid-state rechargeable batteries have attracted attention because of their long cycle life, high safety even at high temperature, and high power/energy density. To realize all-solid-state Na batteries, inorganic solid electrolytes including sulfides and chlorides have been studied. Sodium-ion conducting sulfides are expected to have the advantages of high conductivity and deformability due to the weaker Lewis acidity of sodium ions [1]. The sodium ion conductivity in the sulfide system is equal to or greater than the lithium-ion conductivity in the LGPS-type sulfide electrolytes. Especially, crystalline $Na_{2.88}Sb_{0.88}W_{0.12}S_4$ showed the sodium-ion conductivity of over 10^{-2} S cm^{-1} at 25°C [2]. On the other hand, glass-based sulfide electrolytes exhibit moderate conductivity, along with enhanced formability and compatibility with electrode active materials. The Na_3PS_4 glass-ceramic electrolyte, characterized by a metastable cubic phase was embedded within amorphous domains, demonstrated a conductivity of 10^{-4} S cm^{-1} [3]. Furthermore, incorporating Na_3PO_4 into Na_3PS_4 significantly improved its electrochemical stability for Na metal negative electrodes [4]. The Na_3BS_3 glass exhibited superior Na plating/stripping performance, attributed to the formation of an electronically insulating, thin passivated interphase [5]. The chloride sodium-ion conductor $NaTaCl_6$ with oxidation tolerance serves as an effective solid electrolyte suitable for use with positive electrodes [6]. The addition of Ta_2O_5 to $NaTaCl_6$ promoted amorphization and increased conductivity, and the obtained oxychloride electrolytes exhibited the high conductivity of over 10^{-3} S cm^{-1} at 25°C [7].

Acknowledgements: This work was partially supported by JSPS KAKENHI (24H02204, 25H00904), MEXT Program: Data Creation and Utilization-Type Material Research and Development Project (JPMXP1122712807), and JST Adopting Sustainable Partnerships for Innovative Research Ecosystem (JPMJAP2313).

References:

[1]. A. Hayashi, Electrochem., 91 (2023) 101002.

[2]. A. Hayashi et al., Nat. Commun., 10 (2019) 5266.

[3]. A. Hayashi et al., Nat. Commun., 3 (2012) 856.

[4]. A. Nasu et al., ACS Appl. Mater. Interfaces, 14 (2022) 24480.

[5]. Y. Fujita et al., ACS Appl. Energy Mater. (2025) in press.

[6]. K. Motohashi et al., ACS Mater. Lett., 6 (2024) 1178.

[7]. K. Motohashi et al., Chem. Mater., 36 (2024) 9914.

Biography: **Akitoshi Hayashi** is a professor in the Department of Applied Chemistry at the Graduate School of Engineering, Osaka Metropolitan University, Japan. He earned his B.S., M.S., and Ph.D. from Osaka Prefecture University. His research focuses on developing lithium, sodium and potassium ion-conducting solid electrolytes—including sulfides, oxides, and halides—and their application in all-solid-state rechargeable batteries.

Pourbaix-Diagram-Enabled Design of Advanced Cathode Materials for Sodium-Ion Batteries

C.C. Sorrell and S. Mofarah

School of Materials Science and Engineering, UNSW Sydney, Sydney, NSW 2052

Email: c.sorrell@unsw.edu.au

Abstract: Sodium-ion batteries (SIBs) are emerging as a promising alternative to lithium-ion batteries for large-scale energy storage owing to the abundance, low cost, and broad distribution of sodium resources. However, the performance of SIBs often is limited by the cathode, where issues of phase instability, compositional inhomogeneity, and poor long-term structural retention hinder commercial progress. Conventional fabrication methods, typically involving high-temperature solid-state synthesis and the use of binders and conductive additives, provide limited control over local chemistry and often result in compromised electrochemical behaviour. To advance beyond these limitations, there is a need for predictive, thermodynamically guided, design strategies that can enable the rational synthesis of complex cathode materials.

One such strategy is the application of aqueous speciation and Pourbaix diagrams to guide electrode fabrication. These diagrams map the interplay of pH, potential, and ion concentration across multiple oxidation states, thereby identifying stability domains and feasible transformation pathways. This predictive capability allows the targeted synthesis of multivalent oxides and related frameworks while avoiding parasitic secondary phases or uncontrolled precipitation. Importantly, it transforms cathode development from empirical trial-and-error to a model-driven approach grounded in fundamental chemistry.

The feasibility of this approach has been demonstrated in systems using the modified anodic chronoamperometric electrodeposition (MACE) technique, where Pourbaix-diagram-guided conditions enable the formation of metal-based coordination polymers (MCPs) with unprecedented morphologies, such as nanosheets, honeycomb networks, and hollow frameworks. These results highlight the ability of Pourbaix-diagram-informed synthesis to stabilise novel phases, engineer defect chemistry, and achieve scalable and room-temperature fabrication. Translating these principles to sodium transition-metal oxides opens new avenues to create Na-rich layered cathodes with enhanced structural tunability and electrochemical potential.

Thus, by combining thermodynamic modelling with aqueous processing, this methodology establishes a versatile framework for next-generation sodium-ion cathodes. Beyond providing a route to improved battery performance, it offers a strategy for materials discovery, where speciation and Pourbaix diagrams act as blueprints for rational electrode design.

Biography: Sorrell education was in Ceramic Engineering and Ceramic Science. He has been an academic staff member of the School of Materials Science and Engineering, UNSW Sydney since 1987. His research activities are very broad, albeit generally underpinned by phase equilibria and processing approaches.

Li and F Co-Doping Enhances Oxygen Redox Stability in P2-Type Layered Oxide Cathodes for High-Performance Sodium-Ion Batteries

Elang Barruna[1,2], Hyung-Seok Kim[1,2,*]

[1]Energy Storage Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea

[2]Division of Energy & Environment Technology, KIST School, University of Science and Technology (UST), Seoul 02792, Republic of Korea

E-mail: hskim0227@kist.re.kr

Keywords: sodium-ion batteries • layered oxides • oxygen redox • F-doping

Abstract: Sodium-ion batteries (SIBs) have attracted attention as a cost-effective alternative to lithium-ion batteries (LIBs) for large-scale applications due to the abundance and low cost of sodium. However, their lower energy density remains a challenge. To address this, various strategies have been explored to boost cathode capacities. P2-type layered oxides offer high theoretical capacity, yet studies indicate that the capacity from transition metal redox nearly reaches the theoretical limit, leaving little room for further enhancement. Consequently, oxygen redox has been investigated as a means to provide additional capacity. Unfortunately, oxygen redox typically suffers from rapid capacity fading caused by structural ordering and oxygen release. By doping with the more electronegative F^- ions at oxygen (O^{2-}) sites, stronger bonding with transition metals is achieved, leading to improved structural stability and suppressed oxygen release during cycling. In this study, the compound $Na_{0.7}Li_{0.1}Mg_{0.15}Mn_{0.75}O_{1.9}F_{0.1}$ (NLMMOF) was synthesized via a solid-state method. NLMMOF exhibited a high discharge capacity of 191.96 mAh/g over a voltage range of 1.5–4.5 V and maintained 85.1% capacity retention after 100 cycles at 0.5 C. Combined analyses using ex-situ XPS, in-situ XRD, and in-situ DEMS confirmed that the improved electrochemical performance of the NLMMOF cathode originates from the suppression of the P2-to-O2 phase transition and the inhibition of oxygen gas release in the high-voltage region associated with oxygen redox. Additionally, GITT and CV measurements demonstrated that Li and F co-doping enhances the Na-ion diffusion coefficient, while DFT calculations revealed a higher oxygen redox onset potential, indicating a more stable oxygen redox process. This work presents a novel strategy for enhancing and stabilizing oxygen redox in P2-type layered oxide cathodes, offering promising insights for the design of advanced cathode materials in SIBs.

Biography: Hyung-Seok Kim received his Ph.D degree in Materials Science and Engineering from University of California, Los Angeles and he worked as a PTD engineer at Intel Corp. He is currently a principal research scientist in Energy Storage Research Center at Korea Institute of Science and Technology (KIST) and associate professor in Division of Energy & Environment Technology at Korea University of Science and Technology (UST). His current research interests include developing cathode materials for lithium/sodium ion batteries and zinc anode for aqueous zinc-ion secondary batteries.

Operando XAS Analysis during Synthesis of $ANiO_2$ (A = Li, Na) Cathode Materials

Kei Kubota*

Research Center for Energy and Environmental Materials (GREEN), National Institute for Materials Science (NIMS), Ibaraki, Tsukuba, 305-0044, Japan

E-mail: kubota.kei@nims.go.jp

Keywords: operando analysis • valence variation • material synthesis • layered oxides • cathode

Abstract: In situ measurement technology has developed in addition to performance improvement of rechargeable batteries. Real-time measurement of structural and electrical changes during charging and discharging is utilized to elucidate the reaction and degradation mechanisms of batteries. While such in situ measurement technology during battery operation is rapidly developing, there are very few in situ measurements that focus on the synthesis process of electrode materials, which determines the essential battery performance. Recently, layered oxides with low Co and high Ni content have been developed as inexpensive and high-capacity cathode materials for lithium-ion batteries for automotive applications, but in situ X-ray diffraction studies during the synthesis process were reported as recently as 2020 by Dahn and Bianchini groups. Our research since 2021 has focused on the development of high-temperature in situ/operando measurement techniques to elucidate the synthetic process, including the identification of unknown metastable intermediates. Focusing on the synthesis process of typical $LiNiO_2$ and $NaNiO_2$ cathode materials, the local structure and electrical structure changes around Ni are investigated using operando high-temperature X-ray absorption spectroscopy (XAS) at the synchrotron facility of Photon Factory, High Energy Accelerator Research Organization, Japan. The variation of Ni K-edge absorption energy was measured from room temperature to 900 °C by using a very thin pellet precursor, about 50 μm thick, without dilution with boron nitride. Regardless of the Li/Ni ratio, Ni is irreversibly reduced above 700 °C even under oxygen flow and that such irreversible reduction of the transition metal is not observed in $NaNiO_2$ even when heated up to 900 °C. Based on these operando results, the essential differences between Li and Na systems will be discussed.

Biography: Kei Kubota is a senior researcher at National Institute for Materials Science, NIMS. His main research focuses on the development of new materials for lithium-ion and sodium-ion batteries and the operando analysis of these materials during synthesis and during charge-discharge. He has published over 100 internationally refereed publications including in Advanced Materials, Chemical Reviews, Angewandte Chemie and so on, which have been cited over 17,000 times according to web of science with an H-index of 47. He also received several awards such as Young Researcher Award of the Electrochemical Society of Japan (Sano Award) and the Young Scientists' Award from the Minister of Education and Science (MEXT), Japan.

An Investigation of Local-Scale Distortions in Perovskite Solid Electrolytes via Neutron Total Scattering

Frederick P. Marlton*[1], Frederick Z.T. Yang[2], S. Michelle Everett[3], Joerg Neuefeind[3], Siegbert Schmid [2]

[1]Centre for Clean Energy Technology, School of Mathematical and Physical Sciences, Faculty of Science, University of Technology Sydney, Sydney, NSW, 2007, Australia

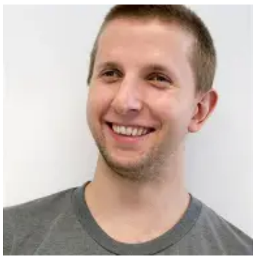
E-mail: Frederick.marlton@uts.edu.au

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

[3]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37731, USA

Keywords: perovskite • structure • neutron • pair distribution function • big-box modelling

Abstract: The perovskite structured oxides of composition ABO_3 are considered strong candidates for solid-state electrolytes in all-solid-state batteries due to their chemical and structural flexibility. However, further improvements must be made before they become commercially viable, and this requires a clear understanding of the structure-property relationships. In this study, the local structure of the perovskite sodium-ion solid electrolyte series $Na_{1/2-x}La_{1/2-x}Sr_{2x}ZrO_3$ (NLSZ, x = 1/4, 1/6, 1/8, 1/16) was investigated via neutron total scattering. Small-box modelling against the neutron pair distribution function with the orthorhombic Pbnm structure showed local-scale features that deviate from the average structure. Big-box modelling quantified significant differences between the bonding configurations of the different A-site cations, which impacts the ionic conductivity of the material. This study demonstrates how understanding local-scale disorder is important for tuning the structure property relationships of inorganic solid-state electrolyte materials in sustainable battery technologies.



Biography: Dr Marlton is a Chancellor's Research Fellow at the University of Technology Sydney. He received his BS and PhD from ANU and UNSW, respectively. He has postdoctoral experience from Aarhus University in Denmark and the University of Sydney and in 2024 conducted a 6 month Fulbright at Stanford University. He specialises in understanding structure-property relationships in functional inorganic materials with a focus on local structures and "hidden" disorder using total scattering methods.

Layered’ Transition Metal Oxides as Electrode Materials for Na-Ion Batteries: Composition - Structure - Environmental Stability - Electrochemical Behaviour/Performance

Amartya Mukhopadhyay

Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India

E-mail: amartya_mukhopadhyay@iitb.ac.in

Abstract: In the context of the upcoming Na-ion battery system, O3-structured ‘Layered’ transition metal (T_M) oxides are promising as cathode-active materials due to their inherently high initial Na-content (as compared to the P2 counterparts); but suffer from instabilities caused due to multiple phase transformations during Na-removal/insertion and sensitivity to air/moisture. Against this backdrop, by tuning the overall covalency of the cation-oxygen bonds in the T_M-layer (which, in turn, influences the Na-O bond) and also with the help of a dopant having d^0 electronic configuration (*viz.*, no OSPE), we have been able to tune the composition and structural features to suppress the phase transitions upon Na-removal/insertion and improve the air/water-stability in significant terms; so much so that long-term cyclic stability has been achieved with health/environment-friendly ‘aqueous processed’ electrodes (sans, usage of toxic/expensive chemicals like NMP and PVDF) [*J. Mater. Chem. A* **8** (2020) 18064, *Adv. Energy Mater.* **13**[19] (2023) 2204407, *J. Mater. Chem. A* **13** (2025) 5807]. The changes in structural features, which have led to such outstanding water-stability, include differential contraction/dilation of the Na-‘inter-slab’/T_M-‘slab’ spacing and partial occupancy of the dopant at tetrahedral sites of the structure. The former aspect has also been invoked to enhance the Na-transport kinetics and, hence, the rate-capability of the, otherwise, inherently sluggish O3-structured NaT_MO_2-based cathode material [*ChemComm* **59** (2023) 4332]. Furthermore, in the context of the more ‘rate-capable’ P2-structured ‘layered’ Na-T_M-oxide based cathode materials, but lacking in terms of having a lower starting Na-content (typically, 0.67-0.7 Na-ions *p.f.u.*), a universal strategy towards designing and developing high Na-containing P2-structured ‘layered’ Na- transition metal oxides has been evolved. This is based on increasing the average ‘charge:size’ ratio of the cation-combination in the T_M-layer and concomitant T_M-O bond covalency, resulting in lower effective negative charge on O-ions; and, in turn, rendering the prismatic coordination of O-ions around Na-ions more favourable even at higher Na-content. Accordingly, by careful selection of the combination of non-T_M-/T_M-ions in the T_M-layer, a high Na-containing (*viz.*, ~0.84 p.f.u.) P2-type Na-T_M-oxide has been developed, which, as a cathode material for Na-ion batteries, exhibits a high desodiation capacity of ~178 mAh/g (@ C/5; within 2-4 V vs. Na/Na^+), exceptional cyclic stability pertaining to ~98% capacity retention after 500 galvanostatic desodiation/sodiation cycles @ 2.5C and also stability upon exposure to air/water [*Chem. Mater.* **34** (2022) 10470].

Biography: Amartya Mukhopadhyay is a Professor in the Department of Metallurgical Engineering & Materials Science at IIT Bombay, where he leads the Advanced Batteries & Ceramics Laboratory. His research focuses on electrochemical energy storage materials (especially alkali-metal ion batteries such as Na-ion, Li-ion, K-ion), development of stable air/water tolerant cathodes, and the design of solid electrolytes and ceramics with high mechanical, chemical, and electrochemical performance.

Advanced Alloy Anodes for High Energy Density Sodium-Ion Cells

Martins Obialor[2], Matthew Garayt[1], Libin Zhang[1], Ian Monchesky[1], Meredith Tulloch[2], Svena Yu[2], J.R. Dahn[1,2], Michael Metzger[1,2] *

[1]Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Canada

[2]Department of Process Engineering and Applied Science, Dalhousie University, Halifax, Canada

Email: michael.metzger@dal.ca

Keywords: sodium-ion Cells, alloy negative electrodes, energy density

Abstract: Worldwide efforts to develop sodium-ion batteries have accelerated in recent years. There are several companies that are developing sodium-ion batteries, including CATL, HiNa, LiFUN, Natron, Tiamat, Faradion, and UNIGRID. Commercial sodium-ion cells are available at this time, but their energy density may not be sufficient for practical application. Now it is necessary to create sodium-ion cells with a volumetric energy density greater than that of LFP/graphite cells.

The volumetric capacity of typical sodium-ion battery negative electrodes like hard carbon is limited to less than 450 mAh/cm^3. Alloy-based negative electrodes such as phosphorus (P), tin (Sn), and lead (Pb) more than double the volumetric capacity of hard carbon, all having a theoretical volumetric capacity above 1,000 mAh/cm^3 in the fully sodiated state. [1] These alloy materials have massive volume expansion, with P expanding by almost 300% and both Sn and Pb expanding to about 400% of their initial volumes when fully sodiated. We will show that Sn and Pb have excellent half-cell cycling performance despite this large volume change, including high Coulometric efficiency. [2, 3] Pb experiences 387% volume expansion upon full sodiation, which leads to significant changes in the electrode morphology. We will track the morphology of Pb and Pb-hard carbon blended electrodes using SEM imaging. As well, each Na-Pb phase will be examined to analyze their physical properties. These analyses will show that the Pb particles restructure into ~1 µm particles (see Figure 1), even after just a single cycle, and surprisingly do not pulverize the hard carbon in a blended electrode. Single-walled carbon nanotubes appear to be necessary to maintain active material electrical connection. [4]

Furthermore, we will show how to improve the formulation of the Pb negative electrode and evaluate capacity retention in half- and full-cell configurations, while investigating the potential degradation mechanisms. The impact of oxide impurities on the cycling stability of Pb negative electrodes will be studied using a controlled heat treatment procedure. The irreversible formation of Na_2O, a side product of the sodiation reaction of Pb oxide, results in sodium inventory loss, decreased first cycle efficiency, and a detrimental impact on the cell's long-term cyclability. [5]

Additionally, the thermal stability of fully sodiated Pb in the presence of ether-based electrolyte will be investigated. The results suggest that Pb not only provides an energy density advantage, but is also marginally more stable at elevated temperatures compared to hard carbon under the same testing conditions. Overall, we aim to provide valuable insights into the cyclability, degradation mechanisms and thermal stability of Pb, offering useful guidance for its future commercialization and deployment in sodium-ion batteries. [6]

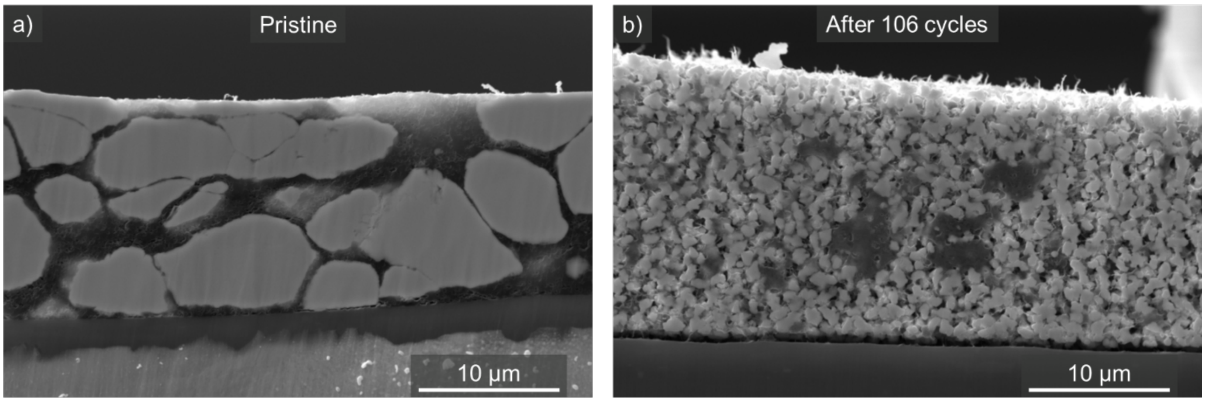


Figure 1. SEM images of an ion-mill cross-section of a pristine Pb electrode (a) and desodiated Pb electrode after 106 cycles (b).

References:

[1] V. Chevrier and G. Ceder *J. Electrochem. Soc.* **158** (2011).

[2] T. R. Jow and L. W. Shacklette *J. Electrochem. Soc.* **136** 1 (1989).

[3] M. Garayt,[=] L. Zhang,[=] Y. Zhang,[=] M. Obialor[=] et al. *J. Electrochem. Soc.* **171** 070523 (2024).

[4] M. Garayt et al. *J. Electrochem. Soc.* **171** 120521 (2024).

[5] M. Obialor et al. *submitted* (2025).

[6] M. Obialor et al. *manuscript in preparation* (2025).

Biography: Michael Metzger is the Herzberg-Dahn Chair and Assistant Professor in the Departments of Physics & Atmospheric Science and Process Engineering & Applied Science at Dalhousie University, Halifax, Canada. He holds a Diploma in Physics and a PhD from the Technical University of Munich (TUM), where his doctoral work included developing methods to study lifetime and aging in Li-ion batteries in collaboration with BASF and BMW. Before joining academia, he worked as a Senior Research Engineer at Bosch Research & Technology Center North America, focusing on solid-state lithium batteries and energy conversion technologies. His research group at Dalhousie works on energy-dense, safe, long-lasting, low-cost battery materials (including Li- and Na-ion), novel diagnostics for degradation mechanisms, and emerging battery applications such as desalination batteries.

Sodium-magnesium Dual-ion Flexible Gel Polymer Electrolyte with Diglyme as Solvent for Hybrid Battery Application

Pratibha Kumari and S.A. Hashmi*

Department of Physics and Astrophysics, University of Delhi, Delhi – 110007, India

E-mail: sahashmi@physics.du.ac.in

Keywords: dual-ion hybrid batteries • sodium-magnesium dual ion gel polymer electrolyte • diglyme • ionic conductivity • charge-discharge

Abstract: In recent few years, hybrid batteries based on dual-ions e.g. Mg-Li and Mg-Na have been reported as potential substitutes of single-ion battery technology [1]. Particularly, such dual-ion systems exhibit ability to overcome various limitations of magnesium-ion battery technology. In such hybrid battery configurations, Mg-metal sheet acts as anode and lithium/sodium-ion intercalating materials as cathode, separated by electrolyte containing dual Mg/Li or Mg/Na salts.

In this presentation, we report an electrochemically efficient dual ion gel polymer electrolyte (GPE) in the form of free-standing flexible thick films comprising a liquid electrolyte containing sodium and magnesium salts ($NaClO_4$ and $Mg(ClO_4)_2$) dissolved in diglyme (G_2), entrapped in a polymeric matrix of poly(vinylidene fluoride-co-hexafluoropropylene) (PVdF-HFP). The GPE-films have been optimized via various physical and electrochemical characterization methods for the application in Mg-Na hybrid battery (MNHB) configuration. The electrochemical properties namely; high ionic conductivity (~3.6 mS cm^{-1} at room temperature), wide oxidative stability window (~3.8 V versus Mg/Mg^{2+}) and high Mg^{2+} transport number (~0.75) make the optimized GPE-film for flexible and quasi-solid state MNHBs. The stripping-plating tests and EIS measurements ensure the long-term stability of the Mg@MWCNT (nanocomposite)/GPE interface. Performance of Mg/Na dual-ion GPE-film has been tested in MNHB configuration with Mg@MWCNT anode and $Na_3V_2(PO_4)_3$ (NVP)@MWCNT cathode via CV and galvanostatic charge-discharge cycles. The MNHB dual ion cell exhibits high initial capacity (~150 mAh g^{-1} at 0.1C) and high Coulombic efficiency (~98%). The post-mortem XPS studies of the electrodes indicate the co-intercalation of dual-ions (Na and Mg-ions) via NVP cathode and single-ion (Mg-ion) absorption-desorption at Mg/MWCNT nanocomposite anode in hybrid battery.

Reference:

[1]. S. Yagi, T. Ichitsubo, Y.Shirai, S. Yanai, T.Doi, K. Murase, E.A. Matsubara, J. Mater. Chem. A, 2 (2014) 1144-1149.

Biography: Prof. S.A. Hashmi is a Senior Professor in Department of Physics & Astrophysics, University of Delhi. His field of interest is Electroactive polymers for Batteries and Supercapacitors. His current interest is devoted towards the: (i) development of magnesium and sodium rechargeable batteries, (ii) development of solid-state and flexible supercapacitors based on carbonaceous materials and conducting polymer electrodes, and (iii) development of thermally and electrochemically stable polymer electrolytes for energy storage devices.

Prof Hashmi has published **Six** Edited Books/Journal on Electroactive Polymers/Solid State Ionics, **125 papers** in National and International journals and **15 Book chapters**. He visited De Montfort University, Leicester, UK, Tokyo University of Agriculture & Technology, Japan (three months, 2001), Max Planck Institute for Polymer Research, Mainz, Germany, University of Malaya, Kula Lumpur, Malaysia, in different academic activities.

Honours: -President, Indian Solid State Ionics Society (2017-2023)

Durable Layered Oxides for High-power Na-ion Batteries

Naoaki Yabuuchi* and Yosuke Ugata

Yokohama National Univ., 79-5 Tokiwadai, Hodogaya-ku, Yokohama, Kanagawa 240-8501, Japan

E-mail: yabuuchi-naoaki-pw@ynu.ac.jp

Keywords: layered oxide • sodium insertion • manganese • titanium

Abstract: The demand for cost-effective batteries is growing to realize the development of low carbon society. High-energy electrode materials with abundant Mn ions have been developed for Li-ion battery applications,[1-3] offering a promising system for high-energy density at a moderate cost. However, lithium, an essential element for Li-ion batteries, is itself regarded as a non-abundant element, making the development of Li-free, cost-effective batteries indispensable. O'3-type $NaMnO_2$, which is essentially isostructural with $LiCoO_2$ and $LNiO_2$, has been widely studied as a potential positive electrode material for Na-ion battery applications. Nevertheless, a practical issue lies in the high solubility of Mn ions into the electrolyte solutions during electrochemical cycling.[4] In contrast, P'2-type $Na_{2/3}MnO_2$ demonstrates excellent reversibility as an electrode material. Higher energy density with good capacity retention can be achieved by using highly concentrated electrolyte solutions.[5]

A major challenge for Na-ion batteries lies in the inferior electrode kinetics of hard carbon commonly used as the negative electrode material. Although their gravimetric energy density is limited, Ti-based layered oxides have emerged as attractive candidates for high-power battery systems.[6] In addition, Fe-based electrode materials are promising low-cost options for the negative electrodes of aqueous Na-ion batteries, due to the abundance of iron resoces.[7]

Based on these findings, the importance of layered Na insertion materials in the development of advanced and practical Na-ion battery applications is discussed in detail.

References

[1]. A. Kanno *et al.*, and N. Yabuuchi, *ACS Energy Letters*, **8**, 2753 (2023).

[2]. Y, Zhang *et al.*, and N. Yabuuchi, *Advanced Energy Materials*, **14**, 2304074 (2024).

[3]. Y. Miyaoka *et al.*, and N. Yabuuchi, *ACS Central Science*, **10**, 1718 (2024).

[4]. T. Sato *et al.*, and N. Yabuuchi, *Energy Material Advances*, **2021**, 9857563 (2021).

[5]. Y. Ugata, T. Kuriyama, and N. Yabuuchi, *Chemical Communications*, **61**, 338 (2025).

[6]. A. K. Pandey *et al.*, and N. Yabuuchi, *Advanced Functional Materials*, **35**, 2417830 (2025).

[7]. Y. Ugata, N. Hirakuni, and N. Yabuuchi, submitted.

Biography: Naoaki Yabuuchi is a professor at Yokohama National University. He completed his PhD at Osaka City University in 2006 and his postdoc at MIT, with research expertise in the development of new electrode materials and study on reaction mechanisms for high energy Li/Na batteries. He has over 130 publications in these areas. He is a fellow of the Royal Society of Chemistry and an associated editor of Energy Storage Materials. He is the recipient of First International Award, "Science Award Electrochemistry" by Volkswagen and BASF, The 2nd ISSI Young Scientist Award, and ISE Prize for Applied Electrochemistry, The Periodic Table of Younger Chemists (Niobium) from The International Union of Pure and Applied Chemistry (IUPAC) among other honors.

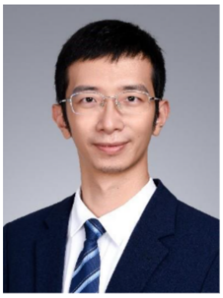
High Safety Electrolyte Design and Interfacial Chemistry for Sodium Metal Batteries and Beyond

Dong Zhou

Tsinghua Shenzhen International Graduate School, China

Email: zhou.d@sz.tsinghua.edu.cn

Abstract: The evolution trend of alkali metal-based batteries is from liquid-state to solid-state with energy density and safety merits. As a result, polymer electrolytes have attracted great interest due to their safety assurance and unique application benefits. In this talk, I will report the development of advanced polymer electrolytes and their applications in novel rechargeable alkali metal-sulfur batteries, including alkali metal-based batteries, room-temperature sodium-sulfur batteries, etc. The electrochemical performance and safety of these battery systems can be improved simultaneously through the molecularly design of polymer electrolytes and the optimization of electrode|electrolyte interfaces. Considering the rapidly growing academic and industrial interests in developing polymer electrolytes and solid-state alkali metal-based batteries, it is reasonable to expect important breakthroughs in the near future.



Biography: Dong Zhou is an associate professor and PhD supervisor at Tsinghua Shenzhen International Graduate School. His research topic mainly focuses on the design and synthesis of specialized solid polymer electrolytes and nano electrode materials for various advanced energy storage devices, and investigation of the interfacial mechanisms. As first/corresponding author, his research has resulted in more than 80 refereed journal articles with a total citation of >11,000 (Google scholar). He is the recipient of First Prize of Guangdong Natural Science in 2020, the Discovery Early Career Researcher Award (DECRA) and the Japan Society for the Promotion of Science (JSPS) Fellowship.

Multielectron Redox Chemistry in Alkali-Superrich Iron Oxides

Hiroaki Kobayashi*

Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan

E-mail: h.kobayashi@sci.hokudai.ac.jp

Keywords: cathode • Na vs. Li • cationic redox • anionic redox • tetrahedral unit

Abstract: Iron oxide-based materials are attractive cathodes due to their cost-effectiveness, and there have been efforts made for a long time to utilize Fe^{4+}/Fe^{3+} redox reactions at cathodes. Even in a well-known alkali iron binary oxide, AFeO$_2$ (A: Li, Na), the utilization of Fe^{4+}/Fe^{3+} one-electron redox is challenging; excess oxidation leads to O_2 evolution. Recently, we have focused on another stable phase of the A-Fe-O ternary system, and demonstrated that Alkali-superrich oxides A_5FeO_4, composed of tetrahedral FeO_4 units, exhibit two-electron redox reactions to achieve high reversible capacities (347 mAh g^{-1} in Li_5FeO_4 and 228 mAh g^{-1} in Na_5FeO_4).

Interestingly, the redox chemistry is different between Li_5FeO_4 and Na_5FeO_4. In Li_5FeO_4, reversible cationic Fe^{3+}/Fe^{4+} and anionic O^{2-}/O_2^{2-} redox reactions proceed under a semi-coherent structural transformation, enabled by cation disordering treatment.[1] The local structure change proceeds from tetrahedral FeO_4 (antifluorite) to octahedral FeO_6 (rocksalt) at the cationic oxidation, forming an anionic redox-active Li_2O byproduct. However, the irreversible O_2 evolution occurs competitively during the anionic oxidation, leading to poor capacity retention.

On the other hand, Na_5FeO_4 exhibits no local structure change during the two-electron redox, a different redox mechanism from Li_5FeO_4. Theoretical study supports the stability of the FeO_4 local structure in the oxidized phase of the Na-system, suggesting the topotactic two-electron redox reaction; in fact, Na_5FeO_4 shows superior cyclability to Li_5FeO_4. Alkali-superrich cathodes have the potential to hold both cost-effectiveness and high-capacity using topotactic multi-electron redox reactions.

References:

[1]. H. Kobayashi *et al.*, *Adv. Energy Mater.*, **13**, 2203441 (2023).

Biography:

2017: Ph. D. of Engineering, University of Tokyo, Japan

2017-2023: Assistant Professor, Tohoku University, Japan

2023-present: Associate Professor, Hokkaido University, Japan

Research interests: cathode materials, next-generation batteries

Regulating Redox Kinetics for Room-Temperature Sodium-Sulfur Batteries

Yun-Xiao Wang* [1]

[1]Institute of Energy Materials Science, University of Shanghai for Science and Technology
Shanghai 200093, China
Institute for Superconducting & Electronic Materials (ISEM), Australian Institute for Innovative Materials (AIIM), University of Wollongong (UOW)
E-mail: yunxiaowang@usst.edu.cn; yunxiao@uow.edu.au

Keywords: room-temperature sodium-sulfur batteries • S cathode • sulfur redox kinetics • reaction pathways • electrocatalysis

Abstract: Rechargeable room-temperature Na-S (RT-Na/S) batteries represent one of the most attractive technologies for stationary energy storage. Multi-electron S redox reactions offer a pathway to low-cost, high-energy-density Na-S batteries, yet face persistent challenges at room temperature: poor sulfur reactivity, sluggish kinetics, polysulfide shuttling, and limited reversibility**.** Understanding sulfur (S) redox chemistry and kinetics is critical for developing this rechargeable battery system. Effective regulation of S redox is thus essential to advance practical room-temperature Na-S batteries. Our group focuses on strategies to manipulate S redox kinetics for ambient sodium storage since 2016. With deepened understanding on electrochemical fundamentals, thermodynamics, and dynamic barriers governing S redox, we then systematically analyze strategies to enhance reaction efficiency, suppress shuttling, and lower energy barriers, including catalyst design, electrolyte engineering, and cathode host optimization. By linking theoretical insights to practical solutions, our research provides a roadmap for kinetically efficient S redox in RT-Na/S batteries, accelerating the development of high-energy-density storage technologies.

Biography: Yun-Xiao Wang is a Distinguished Professor and Vice Dean at the Institute of Energy Materials Science (IEMS), University of Shanghai for Science and Technology. She obtained her PhD in 2015 from the University of Wollongong, Australia. Her research focuses on advanced energy storage and conversion materials, especially novel battery systems (including room-temperature Na-S, Li-S, K-S, Li-air, Na-air, Li-CO_2 batteries), atomic-scale material synthesis, electrocatalysis, and probing electrochemical mechanisms. She has published over 110 papers in international journals, with more than 10,000 citations; many as first author or corresponding author in high-impact journals.

Phase Transitions Occurring During Sodium Intercalation and Deintercalation in Sodium Layered Oxides

Marie Guignard*, [1] and Claude Delmas [1]

[1]Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR 5026

87 avenue du Docteur Albert Schweitzer, 33600 Pessac, France

E-mail: marie.guignard@icmcb.cnrs.fr

Keywords: layered oxides • phase transition

Abstract: Sodium layered oxides with the general formula Na_xMO_2 (where x is comprised between 0 and 1 and M is transition metal) have been studied for more than 40 years as positive electrode materials in sodium and sodium-ion batteries. The structure of these materials is generally described as a stack of different layers: one layer $(MO_2)_n$, formed by edge sharing MO_6 octahedra, alternates with one layer of sodium ions. Whereas the environment of the transition metal within (MO_2)n layers is octahedral, the stacking of the $(MO_2)_n$ layers imposes an environment for the sodium ions which is either octahedral or trigonal prismatic. Depending on the sodium amount, x, and the synthesis conditions, the sodium layered oxides crystallize with different oxygen arrangements which give rise to the different environments for sodium ions.

During the electrochemical deintercalation and intercalation of sodium, structural rearrangements can occur that may or may not affect the cyclability of the positive electrode. These rearrangements include: sodium/vacancy ordering, layer gliding, transition metal migration. In this presentation, we will discuss the most common structural rearrangements observed in sodium layered oxides. They differ depending on the structure type of the layered oxides (O3, P3 or P2 structure type) and on the number and nature of the transition metal ions occupying octahedral sites in the $(MO_2)_n$ layers. The conclusions presented in the talk will be based on operando X-ray diffraction and pair distribution analysis experiments performed over the years on various sodium layered oxides.

Biography: Marie Guignard is an expert in the synthesis of novel oxides for use as positive electrode materials in lithium and sodium batteries, employing unconventional synthesis routes such as electrochemical, topochemical, high-pressure, and mechanochemical methods. Her research focuses on structural characterization using X-ray and neutron techniques, including diffraction and total scattering, to investigate both the average and local structure of these materials. With extensive experience in *operando* techniques (XRD, PDF, and XAS), she aims to unravel the structural and redox mechanisms occurring in electrode materials during battery operation.

Interphases stability and reliable electrochemical setup for Na-ion batteries

Alexandre Ponrouch[1]

[1]ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Catalonia, SPAIN

E-mail: aponrouch@icmab.es

Keywords: sodium • interphase • metal anode • half-cell • SEI

Abstract: Despite issues to develop viable and safe metal anodes, new material (positive and negative eelectrodes or electrolyte) testing commonly involves the use of an electrochemical setup called a half-cell in which metal counter and reference electrodes are used. While this protocol proved to be reliable in Li based cells, the requirements to obtain valid data using such setup in Na cells are not often met.[1-3] Here we first describe the different issues that become critical when moving away from Li. Workarounds are given, and a versatile setup is proposed to run reliable electrochemical tests for Na-ion battery materials in general, in a broad range of electrolyte compositions.[4]

One of the main parameter affecting plating and stripping and therefore the viability of metal electrodes as pseudo-reference or counter electrodes, is the passivation layer formed onto the metal after immersion in the electrolyte. Investigation on the impact of the electrolyte formulation on the composition and properties of such passivation layers is also presented.[5,6] Focus will be dedicated to highlighting the main differences, strengths and weaknesses of these different chemistries with respect to interfacial properties as well as presenting complementary characterization techniques enabling a better understanding of interphases.

References:

[1]. D. I. Iermakova, R. Dugas, M. R. Palacín, A. Ponrouch, *J. Electrochem. Soc.*, 162 (2015) A7060.

[2]. R. Mogensen, D. Brandell, Reza Younesi, *ACS Energy Lett.* 1 (2016) 1173.

[3]. D. S. Tchitchekova, D. Monti, P. Johansson, F. Bardé, A. Randon-Vitanova, M. R. Palacín, A. Ponrouch, *J. Electrochem. Soc.*, 164 (2017) A1384.

[4]. R. Dugas, J. D. Forero Saboya, A. Ponrouch, *Chem. Mater.*, 31 (2019) 8613.

[5]. R. Dugas, A. Ponrouch, G. Gachot, R. David, M. R. Palacin, J. M. Tarascon, *J. Electrochem. Soc.*, 163 (2016) A1.

[6]. J. Fondard, E. Irisarri, C. Courrèges, M. R. Palacín, A. Ponrouch, R. Dedryvère, *J. Electrochem. Soc.*, 167 (2020) 070526.

Biography: Alexandre Ponrouch received his Ph.D. in 2010 from the Institut National de la Recherche Scientifique (INRS-EMT, Canada) working on electrodeposition of metals, alloys, and oxides nanotubes and nanowires for application in fuel cells and supercapacitors.

He is currently staff researcher at Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC, Spain). His research is mainly focused on fundamental electrochemistry applied to the development of new electrolytes, interfaces, and interphases for post Li batteries, including Na-ion, Ca, and Mg.

Solvent Co-intercalation Chemistry in Sodium-Ion Batteries

Yanan Sun, * [1,2] Gustav Åvall, [2,3] Shu-Han Wu, [2] Guillermo A. Ferrero, [1,2] Annica Freytag, [1,2] Pedro B. Groszewicz, [4,5] and Philipp Adelhelm* [1,2]

[1]Joint research group CE-GOBA, Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), 12489 Berlin, Germany

[2]Institute of Chemistry, Humboldt-University Berlin, 12489 Berlin, Germany

[3]SEEL Swedish Electric Transport Laboratory, Säve Flygplatsväg 27, 423 73 Gothenburg, Sweden

[4]SE-ASPIN, Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), 12489 Berlin, Germany

[5]Department of Radiation Science and Technology, Delft University of Technology, Delft 2629JB, Netherlands

E-mail: philipp.adelhelm@hu-berlin.de; yanan.sun@helmholtz-berlin.de

Keywords: solvent co-intercalation • layered cathodes • sodium-ion batteries

Abstract: Solvent co-intercalation, i.e. the combined intercalation of ions and solvent molecules into electrode materials, is an additional but much less explored lever for modifying the properties of electrodes in metal-ion batteries (metal= Li, Na, Mg, …). So far, the knowledge on solvent co-intercalation is relatively scarce and largely limited to graphite anodes, for which in Na-ion batteries, the co-intercalation of glyme molecules is found to be very fast and highly reversible over many cycles. The use of co-intercalation in metal-ion batteries, however, still lacks a scientific breakthrough with respect to cathode active materials (CAMs). In this talk, we show for a series of Na-layered CAMs by experimental methods and theory, under which conditions solvent co-intercalation occurs and how this process impacts the phase behavior, electrode breathing, redox potential, and cycle life compared to “Na^+-only” intercalation. Solvent co-intercalation chemistry is discussed and compared at both the cathode and anode sides in sodium-ion batteries.

Biography: Yanan Sun is a battery materials scientist at the joint CE-GOBA group (HZB–Humboldt University of Berlin), focusing on sodium-ion batteries and operando characterization. Her research explores layered sulfide cathodes, Na-rich oxides, and intercalation/co-intercalation mechanisms, often using synchrotron-based X-ray techniques to uncover reaction pathways. She has co-authored influential works, including a Nature Materials study on solvent co-intercalation and a 2025 ChemRxiv preprint on high-capacity SnS anodes. Dr. Sun earned her PhD (2019) at the National Center for Nanoscience and Technology, CAS, after a BEng in metallic materials at Shandong University of Science and Technology and has been a postdoctoral researcher in Berlin since 2020.

Toward Stable Weberite-Type Sodium Metal Fluorides as High-Performance Sodium-Ion Cathodes

Hanna Z. Porter,[1,2] Emily E. Foley,[1,2] Sarasvati Satyanarayana,[1,2] Erick A. Lawrence,[1,2] Tianyu Li,[1,2] Euan N. Bassey,[1,2] and Raphaële J. Clément*[1,2]

[1]Materials Department, University of California Santa Barbara, California 93106, United States

[2]Materials Research Laboratory, University of California Santa Barbara, California 93106, United States

E-mail: rclement@ucsb.edu

Keywords: intercalation cathode • transition metal fluoride • phase stability • materials design • weberite

Abstract: Open-framework weberite-type sodium metal fluorides ($Na_2M^{2+}M'^{3+}F_7$) have emerged as potential high-performance Na-ion battery (NIB) cathode materials with theoretical energy densities higher than any known Na intercalation cathode material (*ca.* 600-800 Wh/kg) and the ability to accommodate a diverse set of battery-relevant transition and main group elements in the M^{2+} and M'^{3+} sites. Of the few weberite Na-ion cathodes studied to date, $Na_2Fe_2F_7$ exhibits excellent electrochemical performance, with reported capacities up to 184 mAh/g and energy densities up to 550 Wh/kg, motivating further investigation of the largely unexplored weberite phase space.[1] While many weberite phases can be readily synthesized with relatively high purity, they are often metastable and tend to decompose during the mechanochemical carbon-coating step needed to form sufficiently electronically conductive composite cathodes (this is the case for $Na_2Mn_xFe_{2-x}F_7$ and $Na_2Al_xFe_{2-x}F_7$ with $x > 0$), or undergo an irreversible phase transition during electrochemical cycling (e.g., Na_2FeF_7), as we have shown in our recent work.[2,3] This underscores the need to refine our design strategy toward practical weberite cathode materials. Here, we present a new computational framework for predicting the stability of weberite phases when exposed to typical battery electrode processing and cycling conditions, accelerating the experimental screening of weberite compounds in battery devices.[4] Furthermore, we determine key features underlying weberite phase stability, and identify, synthesize, and electrochemically test promising weberite compositions, including three entirely new compounds, and six compounds that had not yet been tested as battery cathodes. From this broad combined computational-experimental exploration of the weberite phase space, we provide guiding principles for the continued development of sodium metal fluoride intercalation cathodes.

Reference:

[1]. Park, H.; Lee, Y.; Myung, S.-T.; Kim, J., et al., *Energy Environ. Sci.* **2021**, *14* (3), 1469–1479.

[2]. Foley, E. E.; Wu, V. C.; Clément, R. J. *Chem. Mater.* **2023**, *35* (9), 3614–3627.

[3]. Porter, H. Z.; Foley, E. E.; Jin, W.; Chen, E.; Lawrence, E. A.; Bassey, E. N.; Clément, R. J. *ACS Mater. Au* **2025**, *5* (1), 170–181.

[4]. Porter, H. Z.; Foley, E. E.; Satyanarayana, S.; Lawrence, E. A.; Li, Ti.; Bassey, E. N.; Clément, R. J. **2025**. *In preparation*.

Biography: Hanna Porter is a fourth-year graduate student in Raphaële Clément's group and a Chancellor's Fellow at the University of California, Santa Barbara. She completed her B.S. in Chemistry at Harvey Mudd College in 2022. Her research interests lie in developing new chemistries for sodium ion battery (NIB) cathodes, with a particular focus on sodium metal fluorides (weberites).

Interface Regulation of Sodium-Ion Batteries

Weihua Chen[1]*, Mingrui Yang[1], Enhui Wang[1]

[1]Department of Chemistry, Zhengzhou University, No. 100 Science Avenue, High-tech Zone, Zhengzhou, Henan, 450001, P. R. China

E-mail: chenweih@zzu.edu.cn

Keywords: sodium-ion batteries • interface regulation • Na-ion transport

Abstract: The interface in sodium-ion batteries plays an important role in the efficient Na^+ ion transport and the structural stability of electrode materials, which determines the cycling stability and rate performance of both batteries and materials. However, compared to the extensive research on electrode materials, current understanding and regulation of interfaces in sodium-ion batteries remain limited. In this report, we will focus on the interface in sodium-ion batteries, via combining the electrode material structure, the interface design, the binder optimization and other strategies, to introduce the ideas of interfacial catalysis and the electric double-layer regulation of anions/cations. These efforts ultimately realize the construction of ultra-thin and efficient solid-state electrolyte membranes, the efficient sodium ion transport, the solid-solid interface contact enhancement and the dendrite deposition suppression. Finally, the coulombic efficiency, cycle life, rate performance, energy density and electrolyte compatibility of the electrode are improved, which lays the theoretical foundation for the assemble of sodium-ion battery devices as well as other battery systems.

Biography: Weihua Chen is a professor at Zhengzhou University. She was selected as a Young Scholar under the Ministry of Education's Changjiang Scholars Program, is a Fellow of the Royal Society of Chemistry (FRSC). She has been ranked among the top 0.05% of global scientists in 2024 and top 2% of global scientists in 2022, 2023, and 2024, and received the 2025 ACS Publications Award for Women Scientists in Surface and Interface Science. Her research focuses on high-performance, low-cost sodium-ion batteries, novel intergrated photo-rechargeable devices, and high-energy-density battery systems, with emphasis on the design, synthesis, and interfacial regulation of key electrode materials, separators, and electrolytes. She has published over 100 papers in journals including *Chem. Soc. Rev.*, *Nat. Commun.* (3), *Angew. Chem. Int. Ed.* (6), *J. Am. Chem. Soc.*, *Adv. Mater.* (3), *Chem* (2), *Matter*, *Mater. Today*, *Energy Environ. Sci.*, etc. with more than 14,000 citations and an H-index of 68. She has applied for 55 Chinese invention patents (31 authorized) and 3 PCT patents. She contributed a chapter in the *Handbook of Sodium-ion Batteries*. She has successively mastered more than 10 research projects, including the National Natural Science Foundation of China, subprojects of the National Key R&D Program, and industrial projects on key battery materials and interface compatibility. She also serves as a member of the Electrochemistry Professional Committee of the Chinese Chemical Society, a member of the Energy Storage Engineering Professional Committee of the Chinese Society of

Electrode and Interface Designs for Solid-State Batteries

Yijun Zhong*

[1]Curtin Centre for Advanced Energy Materials and Technologies, WA School of Mines: Minerals, Energy and Chemical Engineering (WASM-MECE), Curtin University, Perth, Western Australia, 6102, Australia.

E-mail: yijun.zhong@curtin.edu.au

Keywords: solid-state battery • lithium battery • proton battery • electrode • interface

Abstract: The development of new electric applications powered by batteries could further take advantage of Australia's abundant mineral resources (e.g., Li, Fe, Ni, Mn). Utilising solid-state electrolytes addresses the safety concerns of flammable organic liquid electrolytes in commercially available Li-ion batteries. In post-lithium batteries, e.g., proton batteries, solid-state electrolytes bring other benefits for better performance and stability. In recent years, my colleagues and I have dedicated ourselves to designing new electrode materials for solid-state batteries based on different battery chemistries. At this conference, I will present our recent works on the design of these electrodes and optimisation of electrode-electrolyte interfaces, focusing on rechargeable solid-state proton batteries[1] and solid-state lithium batteries[2,3].

References:

[1]. Y. Zhong, L. Zhao, D. Guan, Z. Wang, H. Wu, J. Liu, Z. Shao, *Natl. Sci. Rev.* 2025. In press. DOI: 10.1093/nsr/nwaf226

[2]. Y. Zhong, C. Cao, L. Zhao, M. O. Tadé, Z. Shao, *Green Carbon* 2024, *2*, 94.

[3]. Y. Zhong, C. Cao, M. O. Tadé, Z. Shao, *ACS Appl. Mater. Interfaces*, 2022 *14*, 38786.

Biography: Dr. Yijun Zhong is currently a research fellow at Curtin University. His research focuses on developing functional materials for highly efficient energy storage, e.g., proton batteries, Li(-ion) batteries, and zinc-based batteries. His primary interests lie in understanding the effect of structure, composition, and morphology on the electrochemical properties of these materials.

Structure and ion-exchange mechanisms of layered transition metal oxides

Govardhan Sontam [1], Aditha Rawal [1], Adam Best [2], Neeraj Sharma *[1]

[1]School of Chemistry, The University of New South Wales, Kensington, NSW 2052, Australia.

E-mail: neeraj.sharma@unsw.edu.au

[2]Research Way, Clayton, Victoria 3168, Australia

Keywords: • ion-exchange • structural evolution • NMR • Na [$Ni_xFe_yMn_z$] O_2

Abstract: Cathodes play a key role in the function of sodium-ion batteries. Understanding their structure and structural evolution under various processes is critical to develop better materials and superior battery performance, whether it be lifetime or capacity. In the present work, we investigate the ion-exchange mechanism of a commercially available Na [NixFeyMnz]O2 (NFM), an O3 type layered oxide. Specifically we are focused on the Li-Na ion exchange behaviour, trying to understand to how to control Na extraction and Li insertion. Using 7Li and 23Na NMR (solution and solid-state), we are able to determine the local chemical environments around these elements in Li/Na-NFM materials. These data are coupled with compositional changes determined using inductively coupled plasma optical emission spectroscopy (ICP-OES) and bulk structural changes using X-ray diffraction (XRD). The talk will highlight the work underway to observe the ion-exchange process in situ via a variety of characterization techniques.

Biography: Govardhan is a first year PhD student at UNSW working with Prof. Neeraj Sharma and Dr. Adam Best of CSIRO. Gova is trying to understand the ion-exchange mechanism of layered transition metal oxides to develop novel materials. Previously, worked as a manager, Electrochemical division at Relaince New Energy, and did masters thesis on iron-based cathodes for sodium-ion batteries from IIT Bombay.

High Entropy Design to Enhance the Electrochemical Performance of Fe-rich Cathode Materials for Na-ion Batteries

Eugene Bakker

Centre for Clean Energy Technology, University of Technology Sydney, 2007, Australia

Abstract: Fe-rich layered transition metal oxides (TMOs) are promising low-cost cathode materials that offer a balanced energy density and cycling stability for Na-ion battery grid storage applications. However, Fe-rich TMOs experience Fe migration, dissolution of Mn 3+ , and poor anionic oxygen redox stability at high voltages that constrain their electrochemical performance. To address these challenges, high entropy doping offers the capability of utilising complementary dopant synergies and emergent cocktail effects to concurrently manage multiple performance-limiting obstacles. The effective utilisation of high entropy doping requires the rational selection of compositions and concentrations considering the effects of dopants on phase transformations, electronic properties, and local environment structures.

Quasi-Solid-State Sodium Batteries Using Novel Single-Ion Polymer Electrolytes

Maider Zarrabeitia,*[1] Clemens Wunder[1] and Stefano Passerini*[1,2]
[1]Helmholtz Institute Ulm (HIU), 89081 Ulm, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany
E-mail: maider.ipina@kit.edu
[2]Austrian Institute of Technology (AIT), Center for Transport Technologies, Giefinggasse 2, 1210 Wien, Austria
E-mail: stefano.passerini@kit.edu

Keywords: single-ion polymer electrolytes • anionic center • safety • Prussian white • quasi-solid-state sodium batteries

Abstract: Sodium-ion batteries (SIBs) are proposed as a complementary technology to lithium-ion batteries (LIBs) for light electromobility and stationary applications due to their lower cost and higher sustainability, which is achieved by utilizing non-critical raw materials[1]. However, the SIBs are based on carbonate-based liquid electrolytes, which suffer from low thermal stability, high volatility, and high flammability. Therefore, developing advanced and safer electrolytes, specifically solid-state electrolytes (SSEs), is crucial for enhancing the performance and avoiding safety issues of sodium batteries. Among the SSEs, single-ion polymer electrolytes (SIPEs) are safe and non-flammable, and they can hinder dendrite growth and enhance the mechanical stability of the cell due to the anion is chemically bonded to the polymer backbone[2]. Despite all the advantages, only a limited number of reports related to SIPEs for SIBs can be found in the literature[3,4].

This work focuses on the design of SIPEs for manufacturing high-performing sodium batteries. The SIPE has been optimized through a deep investigation of the influence of the SIPE components' concentration, anionic center chemistry and mobility, and the chemistry of the polymer backbone[5,6]. Finally, the developed SIPEs have been tested in quasi-solid-state sodium metal cells as a proof of concept, using Prussian white as a cathode, demonstrating the transition from liquid-based to solid-state sodium technology.

References:

[1]. S. Isikli, K. M. Ryan. *Current Opinion Electrochem.* 21 (2020) 188-191.

[2]. S. Qianru, L. Xue, D. Qin, B. Du, J. wang, L. Chen. *J. Mater. Chem. A* 2 (2014) 15952-15957.

[3]. J. Li, H. Zhu, X. Wang, M. Armand, D. R. MacFarlane, M. Forsyth. *Electrochim. Acta* 175 (2015) 232-239.

[4]. X. Dong, X. Liu, H. Li, S. Passerini, D. Bresser. Angew. Chem. Int. Ed. 62 (2023) e202308699.

[5]. C. Wunder, T-L. Lai, E. Sic, T. Gutmann, E. De Vito, G. Buntkowsky, M. Zarrabeitia, S. Passerini. *J. Mater. Chem. A*. 12 (2024) 20935-20946.

[6]. C. Wunder, L. Graeber, D. Bresser, M. Zarrabeitia, S. Passerini. *ACS Appl. Polym. Mater.* 7 (2025) 4895-4907.

Biography: Maider Zarrabeitia has been the associated principal investigator and group leader of “*Beyond Li: materials and interphases*” at Helmholtz-Institute Ulm (HIU), Germany, since 2022. Her activities focused on electrode materials and solid-state electrolytes for sodium and potassium-based batteries, as well as understanding the electrode-electrolyte interphases for several battery technologies. She received her Ph.D. in Materials Science and Technology in 2016 from the University of the Basque Country (UPV/EHU, Spain) while being a researcher at CIC energiGUNE, including two research stages at the University of Camerino (Italy). She is a principal investigator of several national and international competitive research projects, and she is the author of >60 articles published in international high-impact journals, with >2500 citations, and co-author of 1 book chapter. Recently, she was awarded the Electrochemistry 2025 Group “Young Talents” Award from the Spanish Royal Society of Chemistry and Electrochemistry Group (RSEQ-GEE).

Structural Evolution Involving Anionic Redox in a Co-doped P2-type Layered Oxide Sodium Insertion Material

Prabeer Barpanda* [1]

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

E-mail: prabeer@iisc.ac.in

Keywords: sodium-ion batteries • cathode • P2-type oxide • anionic redox • rate kinetics

Abstract: To realize high energy density cathode materials, anionic redox processes have been exploited over the last decade. In addition to cationic redox, employing anionic redox activity can improve the energy density of sodium-ion batteries. While anionic redox activity offers enhanced capacity with oxygen redox activity at higher voltages, it comes with poor structural and cycling stability. It is particularly true for P2-type layered oxide cathode materials. The structural stability can be improved by doping to suppress any unwanted phase transition. However, the root cause of capacity fading and its relationship with the cycling conditions, structural transformation and surface processes remain unanswered. Here, a Co-doped P2-type $Na_{0.7}Mn_{0.6}Ni_{0.3}Co_{0.1}O_2$ cathode material has been examined to show that O-redox dominates the capacity observed above 4.2 V. While P2-O2 conversion is suppressed, faster cycling results in inhomogeneous desodiation, thereby forming a P″2 phase next to the P2 phase. Slower cycling allows for uniform P2-to-P″2 phase transformation. While both processes are reversible, the two-phase regime results in larger strain and degradation. The majority of capacity fading arise from partially reversible O-redox as seen in structural change, despite absence of O_2 evolution. The role of kinetics of phase transformation will be stressed as a key parameter to develop anionic redox-based high-energy density sodium insertion materials.

Biography: Prabeer Barpanda is currently an Associate Professor in the Materials Research Center at Indian Institute of Science (IISc), Bangalore. His research focuses on synthesis, structural, and electrochemical study of novel inorganic materials for secondary Li-ion/ Na-ion batteries. So far, he has published over 150 journal articles, 42 conference proceedings, 3 book chapters, and 3 world patents. He has received few awards including Shell Centenary British Chevening Fellowship (UK), C.G. Fink Fellowship (ECS, USA), H.H. Dow Award (ECS, USA), JSPS Postdoctoral Fellowship (Japan), ECS Young Investigator Award (ECS, USA), ISE Prize for Applied Electrochemistry (ISE, Switzerland), Ross Coffin Purdy Award (ACerS, USA), and Humboldt Fellowship for Senior Researchers (Humboldt Foundation, Germany). He directs the Faraday Materials Laboratory (FaMaL) at IISc.

Cost-Driven Engineering of Electrode Materials for High-Performance Sodium-Ion Batteries

Xin Guo[1,*], Guoxiu Wang[2] and Hui-Ming Cheng[1]

[1]Faculty of Material Science and Energy Engineering, Shenzhen University of Advanced Technology, Shenzhen 518107, Guangdong, China

[2]Centre for Clean Energy Technology, School of Mathematics and Physics, Faculty of Science, University of Technology Sydney, Broadway, Sydney NSW2007, Australia

E-mail: x.guo1@siat.ac.cn

Keywords: layer oxides • hard carbon • anode materials • high-entropy doping• interface engineering

Abstract: Sodium-ion batteries (SIBs) have emerged as a promising solution for cost-sensitive and sustainable energy storage, yet their commercial viability is still limited by the lack of competitive electrode materials. In this work, we present a cost-driven, co-engineering strategy targeting both cathode and anode development. On the cathode side, layered oxide materials were designed with dual-site doping. and high-entropy configurations, significantly enhancing structural stability and mitigating degradation [1, 2] The use of Ni- and Co-free chemistries further improves economic and environmental viability. On the anode side, we developed high-capacity alloy/carbon composites through nanoengineering and interface optimization, delivering improved reaction kinetics and structural robustness.[3-5] Additionally, we introduced a simplified, scalable synthesis method for biomass-derived hard carbon, effectively lowering production costs.[6, 7] Together, these advances establish a practical and scalable roadmap for electrode materials innovation, accelerating the path toward high-performance, low-cost sodium-ion batteries for next-generation energy storage.

Reference:

[1] Huang, Z.; Wang, S.; **Guo, X.***; Marlton, F.; Fan, Y.; Pang, W.K.; Huang, T.; Xiao, J.; Li, D.; Liu, H.; Gu, Q.; Yang, C.; Dong, C.; Sun, B.*; Wang, G.*, *Adv. Mater.* 2024, 36 (50), 2410857

[2] Xiao, J.; Gao, H.; Xiao, Y.; Wang, S.; Gong, C.; Huang, Z.; Sun, B.; Dong, C.; **Guo, X.***; Liu, H.*; Wang, G.*, *Chem. Eng. J.* 2025, *506*, 160010.

[3] Osman, S.; Hu, S.; Wei, Y.; Liu, J.; Xiao, J.; Yao, W.; Han, C.; **Guo, X.***; Liu, J.*; Tang, Y., *Adv. Energy Mater.* 2025, 15 (8), 2404685

[4] **Guo, X**.; Zhang, W.; Zhang, J.; Zhou, D.; Tang, X.; Xu, X.; Li, B.; Liu, H.; Wang, G., *ACS Nano* 2020, 14, 3651.

[5] Yang, J.; **Guo, X.***; Gao, H.; Wang, T.; Liu, Z.; Yang, Q., Yao, H., Li, J.; Wang, C.*; Wang, G.*, *Adv. Energy Mater.* 2023, 13, 2300351.

[6] Yuan X.; Zhang G.; Wei Y.; Xiao J.; Wei X.; Gao H.; **Guo X.***; Liu J.*; Cheng H.M.; *Sci. China Mater.* 2025, DOI: org/10.1007/s40843-025-3499-6.

[7] Li, J.; Hao, J.; Yuan, Q.; Wang, R.; Marlton, F.; Wang, T.; Wang, C.*; **Guo, X.***; Wang, G.*, *Carbon Energy* 2024, 6, e518.

Biography: Xin Guo is an assistant professor at the Faculty of Materials Science and Energy Engineering, Shenzhen University of Advanced Technology. He received his Ph.D. degree in 2019 from the University of Technology Sydney under the supervision of Prof. Guoxiu Wang. His research focuses on advanced materials for sodium-ion batteries, including layered oxide cathodes, alloy and carbon-based anodes, and functional additives.

Aging and SEI Stability in the Prussian White and Hard Carbon Cell System

Charles Aram Hall[1] and Reza Younesi[1]

[1] Department of Chemistry – Ångström Laboratory, Structural Chemistry, Lägerhyddsvägen 1, 75237 Uppsala

E-mail: charles-aram.hall@kemi.uu.se

Keywords: SEI • electrolyte • aging

Abstract: Though sodium-ion batteries (SIBs) have matured dramatically, there is still progress to be made in extending cycling life. Thus, a key challenge is to understand aging mechanisms in order to minimise their effect. Cells ustilising hard carbon (HC) negative electrodes and Prussian white (PW) positive electrodes have curiously been shown to degrade moreso when cycled only at a low state of charge (SoC; roughly 0 to 50% SoC) than at a high SoC (roughly 50 % to 100% SoC). [1] It is ambiguous whether this dervies from increasing polarisation of the high-spin iron or collapse of the PW structure, increasing resistance in the HC electrode or from an overall loss of sodium inventory, or a combination of all of these mechanisms.

This talk will discuss the observed aging in PW||HC cells cycled in different voltage ranges. [1] Likely aging mechanisms will be discussed, drawing on information *operando* X-ray diffraction (XRD) [2] and operando electrochemical mass spectrometry (OEMS). [3] The results of XRD suggest that though polarisation does increase in the PW positive electrode, it is difficult to link these effects to a structural degredation of the PW. It seems more likely instead that aging is due to a loss of sodium inventory, although it is difficult from XRD to pinpoint where this sodium inventory is lost. From OEMS, it seems possible that one route for sodium inventory loss is via oxidation of the solid electrolyte interphase (SEI) at the end of discharge, requiring a fresh SEI to be formed in the subsequent cycle. Another loss mechanism relates to SEI dissolution, which similarly requires a fresh SEI to be formed in the subsequent cycle. [4] Using this understanding, preliminary results in a model system will seek to test how the electrolyte choice affects the stability of the SEI.

References:

[1] Buckel, Hall, Ma, Colbin, Eriksson, Mogensen and Younesi, Batteries and Supercaps 2023, 7, 2, e202300533

[2] Nielsen, Hall, Mattsso, Younesi, Buckel, Ek and Brant, J. Mater. Chem. A 2024, 12, 17413-17421

[3] Misiewicz, Ulander, Melin, Hall and Berg, Advanced Materials Interfaces 2024, 12, 10, 2400854

[4] Ma, Buckel, Hofmann, Nyholm and Younesi, Advanced Science 2023, 11, 6, 2306771

Liquid and solid electrolytes for sodium-based batteries

Cristina Pozo-Gonzalo*, [1,2]

[1]Instituto de Carboquímica (ICB-CSIC), C/Miguel Luesma Castán, 4, 50018, Zaragoza, Spain.

[2]Institute for Frontier Materials, Deakin University, 221 Burwood Highway, Burwood, Victoria 3125, Australia.

E-mail: cpozo@csic.es

Keywords: quasi-solid-state battery (QSSB) • Na-O_2 battery • ionic liquids • phosphates • hybrid electrolytes.

Abstract: LIBs are ubiquitous in all portable devices (mobile phones, laptops and tablets) and, with on-going development realising higher energy density and power output, LIB is now the dominant technology for battery electric vehicles (EVs) and preferred for the rapidly developing market of grid-based storage. However, LIB batteries require the use of scarce, toxic and unethically resourced materials for their fabrication1, pushing the need to develop novel and improved technologies. Among the different energy technologies, Sodium-based battery has emerged as the safer and more sustainable technology that can complement lithium-ion battery in the global energy storage scenario.[1]This is due to the low-cost and abundance of sodium and cathode/anode materials necessary in the manufacturing process, and enhanced safety in comparison with LIB.

In all battery technologies, the electrolyte plays a critical role in their performance and safety. Hence, optimising electrolytes is important to increase the current density and improve the stability and safety of batteries.[2]In this work a series of liquid and solid electrolytes will be presented which has successfully being use for sodium-air batteries. For instance, a quasi-solid-state electrolytes based on polyamide (PA) and polyethylene oxide has been tested as a proof of concept in full Na–O_2 cells, delivering stable cycling performance. This new electrolyte offers enhanced safety, efficiency, and durability in comparison with common diglyme-based electrolytes.[3]Additionally, organic, hybrid and ionic liquid-based electrolytes will be discussed in this paper.

Biography: Pozo-Gonzalo is a CSIC Principal Researcher, working at the Carboquimica Institute (Spain) and an honorary Associate Professor at Deakin University (Melbourne). She received her PhD degree in from the University of Manchester (United Kingdom) on the electrochemical synthesis of Conducting Polymers. Her current research interest focuses on energy, recovery of critical raw materials from waste using safe and unexpensive methods, and redesign of materials for energy. During her research career, she has authored and co-authored 119 peer-review international publications, 3 book chapters and holds 5 patents, in the areas of electrochemistry, materials, circular economy and energy storage. She is an associate editor for the RSC Sustainability. She has supervised 11 Postdoctoral Research Fellows and 12 PhD students to completion. She has led a total of 38 projects, 14 of them with industry partners, and 5 prestigious European funded projects within different calls STRP-FP6, FP7-NMP, RISE, MSCA.

References:

[1]. N. Tapia-Ruiz et al., *J. Phys. Energy* **2021**, *3*, 031503.

[2]. F. Makhlooghi, et al., in Monconduit, L., Croguennec, L. (eds) (**2021**), *Na-ion Batteries*. ISBN 9781789450132.

[3]. Mohamed Yahia, Marina Enterría, Cristina Pozo-Gonzalo, Nagore Ortiz-Vitoriano, “Advanced Science, **2025**, e04490.

Exploring Promising Electrode Materials for Sodium-Ion Batteries: From Advanced Oxides to Amorphous Chalcogenides

Han-Yi Chen*, Chia-Ching Lin, Yu-Ming Chang, Jin-Wei Kang, Hsu-Chen Cheng, Hsiang-Jung Chen, Cheng-Yen Wu

Department of Materials Science and Engineering, National Tsing Hua University, 101, Sec. Kuang-Fu Road, Hsinchu 300044, Taiwan

E-mail: hanyi.chen@mx.nthu.edu.tw

Keywords: high-entropy oxide • oxygen-redox • operando XAS • operando XRD • bimetallic chalcogenide

Abstract: In pursuit of safe, high-energy, and low-cost rechargeable batteries, we present a series of advanced electrode materials tailored for sodium-ion batteries. First, a novel high-entropy O3-type layered oxide, $NaCu_{0.1}Ni_{0.3}Fe_{0.2}Mn_{0.2}Ti_{0.2}O_2$ (NCNFMT), was synthesized via the Pechini method and demonstrated excellent electrochemical stability with a reversible capacity of 130 mAh g^{-1} and 87% retention over 100 cycles. The high-entropy effect was confirmed to stabilize the O3-phase and delay phase transitions during cycling, as supported by operando synchrotron X-ray diffraction and X-ray absorption analyses. Quasi-solid-state cells with NCNFMT also showed promising performance, achieving 112 mAh g^{-1} with 78% retention after 100 cycles. We also developed an oxygen-redox active P2-type cathode, $Na_{0.61}Ca_{0.03}[Mg_{2/9}Cu_{1/9}Mn_{2/3}]O_2$, offering a high specific capacity of 205 mAh g^{-1} and remarkable rate performance (142 mAh g^{-1} at 2.5C). Ca doping acts as a structural pillar, and Cu substitution stabilizes oxygen anions, collectively suppressing voltage hysteresis and enhancing structural integrity. Operando X-ray absorption spectroscopy/X-ray diffraction, gas chromatography, and DFT calculations elucidated the reaction mechanisms and full-cell tests with hard carbon achieved an energy density of 250.7 Wh kg^{-1}. Furthermore, to overcome the conductivity limitations of phosphate-based cathodes, Mo was introduced into $Na_4MnV(PO_4)_3$. The Mo-doped material exhibited significantly enhanced rate capability (up to 46.4 mAh g^{-1} at 20C) and cycling stability, retaining 78.8% capacity after 300 cycles. Spectroscopic and neutron analyses confirmed the preferential Mo substitution at phosphate sites and a reduced band gap, which facilitates improved electronic transport. For anode studies, an amorphous bimetallic chalcogenide, $MoSnSe_{1.5}S_{1.5}$ (MSSS), was designed to address volume expansion issues commonly observed in transition metal sulfides/selenides. MSSS delivered high capacities of 526 mAh g^{-1} in sodium-ion batteries, with outstanding rate tolerance up to 20 A g^{-1}. In situ X-ray absorption spectroscopy and transmission x-ray microscopy studies revealed its dominant pseudocapacitive charge storage and structural robustness. These results collectively demonstrate how rational design from atomic-level composition control to structural amorphization can drive next-generation sodium-ion battery performance.

Biography: Han-Yi Chen is a professor in the Department of Materials Science and Engineering at National Tsing Hua University in Taiwan. Her research centres on electrode and solid-electrolyte materials for energy storage devices (lithium-, sodium-, zinc-ion batteries, supercapacitors), high-entropy oxide materials, ceramics and carbon materials, and she employs operando / in situ measurement techniques to elucidate charge-storage mechanisms. She has also been recognized with multiple young scholar and distinguished researcher awards in Taiwan.

Understanding the charge transfer effects for Na-S batteries

Yaojie Lei,[1] and Guoxiu Wang* [2]

[1]Centre for Clean Energy Technology, University of Technology Sydney, 2007, Australia

E-mail: Guoxiu.Wang@uts.edu.au

Keywords: sodium-sulfur batteries • sulfur cathode • charge transfer • reaction pathway

Abstract: Efficient electron transport within bulk electrodes is critical for achieving high-performance batteries. However, the inferior conductivity of sulfur molecules results in a high barrier for electrons to traverse the electrode structure, which leads to incomplete reactions and the formation of metastable products. To improve electrode performance, it is important to introduce alternative charge units to accelerate the fragmentation of sulfur molecules and enhance the selectivity towards stable products during charge and discharge. Here, we developed a charging strategy to address the electron transport issue in bulk sulfur electrodes. The establishment of a synergistic effect between adsorption models and electron transfer helps us achieve high selectivity towards desirable short-chain sodium polysulfides in practical battery tests. Furthermore, the charge transfer process can accelerate sodium ion kinetics through electrostatic forces. These will result in superior electrochemical performance for room-temperature sodium-sulfur batteries.

Biography: Yao-Jie Lei is a Research Associate working under the supervision of Prof. Guoxiu Wang at the Centre for Clean Energy Technology, University of Technology, Sydney. He received his bachelor of science major in chemistry from Lanzhou University, and research master degree from the University of Sydney. He obtained his PhD from the University of Wollongong. His research interests include the synthesis of nanostructured materials for room-temperature Na–S batteries.

Crystal Chemistry of Sulfates for Sodium-Ion Batteries: From Mineral-Inspired Structures to Functional Electrode Materials

Vadim M. Kovrugin [1,2,]* and Valérie Pralong [1,2]

[1]CRISMAT, ENSICAEN, Université de Caen Normandie, CNRS UMR 6508, 14000 Caen, France

E-mail: vadim.kovrugin@ensicaen.fr

[2]RS2E, FR CNRS 3459, 80039 Amiens Cedex 1, France

Keywords: Na-ion • electrode material • sulfate • crystal structure • mineral

Abstract: Polyanionic sulfate compounds have emerged as a promising class of electrode materials for sodium-ion batteries (SIBs) primarily due to their high redox potentials induced by the strong inductive effect of the SO_4^{2-} group. In this study, we explore the crystal chemistry of sulfates as Na^+-intercalation hosts through both historical developments and recent advances, with the objective of unveiling key structure-property relationships essential for the rational design of novel electrode materials. A central theme of our work is the intrinsic connection between synthetic sulfate phases and naturally occurring minerals. Minerals have long served as a powerful source of inspiration in materials science, with several commercial electrode materials, such as, *e.g.*, LFP directly derived from mineral structures (*triphylite* $Li(Fe,Mn)PO_4$ of the *olivine* group). Similarly, the most investigated and best-performing sulfate-based electrodes for SIBs are those related to the *alluaudite*,[1] *triplite*,[2] and *eldfellite*[3] mineral families. Hence, adopting this mineral-inspired perspective, we build upon our previous works on sulfates for SIBs[4–6] to conduct a comprehensive analysis of the diversity of reported sulfate electrode materials, highlighting their close crystallographic parallels with naturally occurring minerals. Special attention is given to the geological formation conditions of these minerals, which may offer invaluable guidance for developing new synthetic strategies for battery electrodes based on sulfates. Given that over 650 sulfate mineral species are recognized by the *International Mineralogical Association*, this family of compounds remains vastly underexplored in the context of energy storage. Our findings emphasize the substantial potential of sulfate-based phases as electrode materials to deliver competitive energy densities, while also offering access to previously unexplored structural motifs favourable for Na^+ ionic conduction. This crystal chemical investigation sets the foundation for the rational design of next-generation SIBs electrode materials based on Earth-abundant and structurally versatile sulfate compounds.

Reference:

[1]. S. Li, W. Wang, Y. Jia, H. Xu, R. Liu, Z. Wang, Z. Xie, L. Zhang, R. He, L. Wang, *Small Methods* **2025**, 2402110.

[2]. M. Kim, D. Kim, W. Lee, H. M. Jang, B. Kang, *Chem. Mater.* **2018**, *30*, 6346–6352.

[3]. S. Singh, D. Singh, R. Ahuja, M. Fichtner, P. Barpanda, *J. Mater. Chem. A* **2023**, *11*, 3975–3986.

[4]. M. Gnanavel, O. I. Lebedev, P. Bazin, B. Raveau, V. Pralong, *Solid State Ionics* **2015**, *278*, 38–42.

[5]. V. M. Kovrugin, D. O. Nekrasova, O. I. Siidra, O. Mentré, C. Masquelier, S. Y. Stefanovich, M. Colmont, *Cryst. Growth Des.* **2019**, *19*, 1233–1244.

[6]. S. Singh, A. Neveu, K. Jayanthi, T. Das, S. Chakraborty, A. Navrotsky, V. Pralong, P. Barpanda, *Dalt. Trans.* **2022**, *51*, 11169–11179.

Biography:

V. Kovrugin, Assistant Professor ENSICAEN

V. Pralong, Senior CNRS Researcher CRISMAT

Utilising Acoustic Techniques to Improve Understanding of the Formation Process in Sodium-Ion Batteries

Arthur Fordham[1,3], Dylan Wee [2,3], Tongjun Luo[4], Tianqi Jia[4], James Robinson[1,3,6], Rhodri Jervis[1,3*] and Wesley M Dose[4]*

[1]Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, London, WC1E 7JE

E-mail: rhodri.jervis@ucl.ac.uk

[2]Department of Mechanical Engineering, Imperial College London, London, SW7 2BX

[3]The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, UK, OX11 0RA

[4]School of Chemistry, The University of Sydney, Camperdown, NSW 2006, Australia

E-mail: wesley.dose@sydney.edu.au

[6]Advanced Propulsion Lab, Marshgate, 7 Sidings Street, University College London, London, UK, E20 2AE

Keywords: sodium-ion batteries • acoustic emission • ultrasonic testing • formation cycles • solid electrolyte interphase • electrolyte additives • X-ray CT

Abstract: Sodium-ion batteries (NIBs) offer a more sustainable and cost-effective alternative to lithium-ion batteries (LIBs) due to the absence of materials such as cobalt and the greater global abundance of sodium.[1] However, key challenges remain underexplored, particularly the crucial formation process and the impact of electrolyte additives on the properties of the solid electrolyte interphase (SEI) and overall cell performance.[2,3] Existing diagnostic techniques for monitoring SEI formation are often prohibitively expensive, limiting their widespread adoption. Acoustic techniques, including Acoustic Emission (AE) and Ultrasonic Testing (UT), have emerged as promising operando monitoring tools due to their cost-effectiveness and non-invasive nature.[4–6] These methods enable real-time diagnostics by detecting physical and electrochemical changes within cells.

This study employs the first application of AE and UT as a combined diagnostic tool to monitor SEI formation in $NaMn_{0.39}Fe_{0.31}Ni_{0.22}Zn_{0.08}O_2$/hard carbon (HC) pouch cells with four electrolyte chemistries: a baseline of 1 M $NaPF_6$ in 1:1 EC:DMC, and formulations with 5 wt.% fluoroethylene carbonate (FEC), vinylene carbonate (VC), and a FEC+VC blend. SEI development was tracked during formation cycles using AE and UT, and correlated with findings from gas analysis, X-ray CT, and electrochemical measurements.

To determine the origins of acoustic activity, three-electrode *dQ/dV* profiles were correlated with AE events, enabling identification of the specific reduction processes and corresponding electrode contributions. Bespoke machine learning algorithms were used to classify acoustic signals based on their features, helping to assign physical origins - such as gas evolution, or intercalation - within the battery.[7] This revealed distinct acoustic signatures associated with additive reduction and SEI formation at the negative electrode.[8] Notably, the data highlights the greater difficulty in passivating hard carbon compared to graphite in LIBs, with continued gas evolution and irreversible capacity loss observed across all electrolyte chemistries, even after three formation cycles.[9]

The behaviour observed during formation was reflected in the long-term cycling results, where FEC emerged as the most effective additive, delivering 90% capacity retention after 250 cycles. In contrast, VC alone was less effective, with only 68% retention. Cells without additives displayed the lowest performance, underscoring the critical role of additive chemistry. This work demonstrates that AE and UT provide a viable, cost-effective method for real-time SEI monitoring in NIBs and, when coupled with three-electrode electrochemistry, can offer mechanistic insights previously accessible only through more expensive and complex techniques.

References:

[1]. Vaalma, C., Buchholz, D., Weil, M., and Passerini, S., Nat. Rev. Mater., 3, 18013 (2018).

[2]. Song, X., Zhou, X., Zhou, Y., Deng, Y., Meng, T., Gao, A., Nan, J., Shu, D., and Yi, F., ChemElectroChem, 5, 2475 (2018).

[3]. Peled, E., and Menkin, S., J. Electrochem. Soc., 164, A1703 (2017).

[4]. Majasan, J.O., Robinson, J.B., Owen, R.E., Maier, M., Radhakrishnan, A.N.P., Pham, M., Tranter, T.G., Zhang, Y., Shearing, P.R., and Brett, D.J.L., J. Phys. Energy, 3 (3), 032011 (2021).

[5]. Fordham, A., Milojevic, Z., Giles, E., Du, W., Owen, R.E., Michalik, S., Chater, P.A., Das, P.K., Attidekou, P.S., Lambert, S.M., Allan, P.K., Slater, P.R., Anderson, P.A., Jervis, R., Shearing, P.R., and Brett, D.J.R., Joule 7, 2622 (2023).

[6]. Dreyer, S.L., Zhang, R., Wang, J., Kondrakov, A., Wang, Q., Brezesinski, T., and Janek, J., J. Phys. Energy, 5 (3), 035002 (2023).

[7]. Fordham, A., Joo, S., Owen, R.E., Galiounas, E., Buckwell, M., Brett, D.J.L., Shearing, P.R., and Jervis, R., J. Electrochem. Soc., 171 (7), 070521 (2024).

[8]. Noll, L., Mrowetz, J., Kretschmer, K., and Schröder, D., J. Power Sources, 629, 235978 (2025).

[9]. Fondard, J., Irisarri, E., Courrèges, C., Palacin, M.R., Ponrouch, A., and Dedryvère, R., J. Electrochem. Soc., 167, 070526 (2020).

Biography: Wesley M. Dose is a Senior Lecturer, ARC DECRA Fellow, and Sydney Horizon Fellow in the School of Chemistry at the University of Sydney. His research interests are in energy storage materials for applications in current and emerging battery chemistries including lithium-ion, sodium-ion, and other ‘beyond lithium’ battery chemistries. He is particularly focused on the chemistry and electrochemistry of sustainable and high-energy materials and understanding the interfacial chemistry at electrode-electrolyte interfaces.

Poster Abstracts

#1

The Role of Oxygen Redox in Enhancing the Performance of 'Layered' Na-Transition Metal Oxide Cathode Materials for Na-ion Batteries

Adrija Goswami a, Bachu Sravan Kumar a, Velaga Srihari b, Himanshu K. Poswal b, Amartya Mukhopadhyay a*

a Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai 400076, India

c High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Center, Mumbai 400085, India

d Department of Chemical Engineering, Indian Institute of Technology Bombay,

Mumbai 400076, India

* Corresponding author's e-mail-id: amartya_mukhopadhyay@iitb.ac.in

Keywords: Anionic Redox • Sodium-ion Batteries • Cathode • Layered Transition metal oxides • Energy Storage

Abstract:

The growing demand for high energy density Li-ion and Na-ion batteries has led to significant impetus towards the development of 'layered' or even cation-disordered Li-/Na- transition metal (TM) oxide cathode materials that can utilize 'anionic redox' as an additional charge compensation mechanism beyond the TM-redox. However, the stability of 'anion redox' still remains unsatisfactory, with the mechanisms associated with this phenomenon poorly understood [1]. Against this backdrop, our work looks into the correlations between the compositional-structural-electrochemical aspects of 'layered' Na-TM-oxide based cathode materials, starting with our high Na-containing P2-structured $Na_{0.84}([]_{0.06}Li_{0.04}Mg_{0.02}Ni_{0.22}Mn_{0.66})O_2$ [as reported in Chem Mater (2022), 34(23), 10470-10483][2] and generating a few logical variations of the same. While Na-extraction/insertion takes place via solid-solution pathway and primarily N2+/4+ redox within a potential window of 2-4 V vs. Na/Na+, phase transformation(s), yielding either OP4/O2, is/are observed beyond 4 V, with 'anionic redox' primarily supporting the electrochemical Na-extraction/insertion, leading to reversible specific capacities of 161, 164, and 193 mAh g^{-1} upon cycling within 2–4.2, 2–4.3, and 2–4.5 V, respectively. A combination of XPS, in-situ Raman, in-situ XANES, ex-situ soft XAS, magnetic measurements and DFT-based simulations reveal a complex interplay between O-redox and transition metal over-oxidation/reduction when going beyond 4 V; thus, throwing new insights into the 'anion redox' mechanism of such 'layered' transition metal oxide-based cathode materials.

References:

[1] McColl, et al., (2022). Nature communications, 13(1), 5275.
[2] Kumar, et al.; (2022). Chemistry of Materials, 34(23), 10470-10483.

Biography:

I, Adrija Goswami am a 3rd Year PhD student in the department of Metallurgical Engineering and Materials Science Department in Indian Institute of Technology, Bombay (IIT Bombay). My area of interest lies in energy storage specifically focusing on Sodium-ion Battery cathodes. I have previously done my Bachelor and Masters degree in Physics.

#2

A Systematic Study of the P2/O3/P3 Sodium-ion Layered Oxide Cathode Materials, $Na_{1-2x}Ni_{1/2-x}Mn_{1/2+x}O_2$ ($0 < x \leq 1/6$)

Arthur Fordham[1,2,3], Zoë H Wright[2,3], Joseph Paul Baboo[2,4], Thomas J Wood[2,4], Jake M Brittain[4*], and William IF David[2,3,4*]

[1] Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, London, WC1E 7JE

[2]The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, UK, OX11 0RA

[3]Inorganic Chemistry Laboratory, University of Oxford, S Parks Rd, Oxford OX1 3QR, United Kingdom

[4]ISIS Neutron and Muon Spallation Source, STFC Rutherford Appleton Laboratory, Harwell, Oxford OX11 0QX, United Kingdom

*Corresponding authors: bill.david@stfc.ac.uk, jake.brittain@faradion.co.uk

Keywords: sodium-ion batteries; cathodes; temperature-dependence; electrochemistry; synchrotron; X-ray diffraction; Rietveld refinement

Abstract:

The development of efficient sodium-ion batteries is critical for advancing sustainable energy storage, with cathode materials playing a central role in determining performance. Sodium-ion cathodes offer a cost-effective and resource-abundant alternative to lithium-based systems, addressing economic, environmental and supply concerns.[1]

This study presents a comprehensive structural and electrochemical investigation of the prototypic layered sodium-ion cathode system $Na_{1-2x}Ni_{1/2-x}Mn_{1/2+x}O_2$ ($0 < x \leq 1/6$).[2,3] Synchrotron high-resolution X-ray powder diffraction was used to characterise 29 synthesised compositions across a wide stoichiometric and thermal landscape. Detailed Rietveld refinement revealed complex multiphase behaviour between the P2 ($Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$, $P6_3/mmc$) and O3 ($NaNi_{1/2}Mn_{1/2}O_2$, $R\text{-}3m$) end members.[4,5] Orthorhombic and monoclinic variants of P2 and O3 structures were frequently observed, with some compositions exhibiting up to four coexisting phases. [6,7] Diffraction peak broadening and volcano-shaped profiles suggest significant local strain induced by sodium ordering.

The study is structured in three parts. First, samples synthesised at 900 °C were analysed, identifying five principal phases across the stoichiometry range. The P2 hexagonal phase was found only in pure P2 compositions; in all other cases, symmetry was lowered to orthorhombic, and a broad mixed-phase region was identified. Second, the effect of synthesis temperature was explored, revealing new low-temperature phase preferences. Notably, sodium-rich samples favoured P3 phases (trigonal prismatic Na coordination) over the O3 phase (elongated octahedral Na coordination), due to the energetic accessibility of multiple low-energy trigonal prismatic sites under disordered conditions. Third, electrochemical testing of a selected subset of cathodes in full-cell configurations showed that mixed-phase compositions outperformed single-phase materials, demonstrating enhanced capacity and stability.

Overall, this work provides the first comprehensive high-resolution structural analysis of all phases in the undoped $Na_{1-2x}Ni_{1/2-x}Mn_{1/2+x}O_2$ materials between P2 and O3 endmembers, revealing key structure–property relationships. It highlights the performance advantages of mixed-phase cathodes and the vital role of synthesis conditions, offering valuable guidance for the design of next-generation sodium-ion batteries.

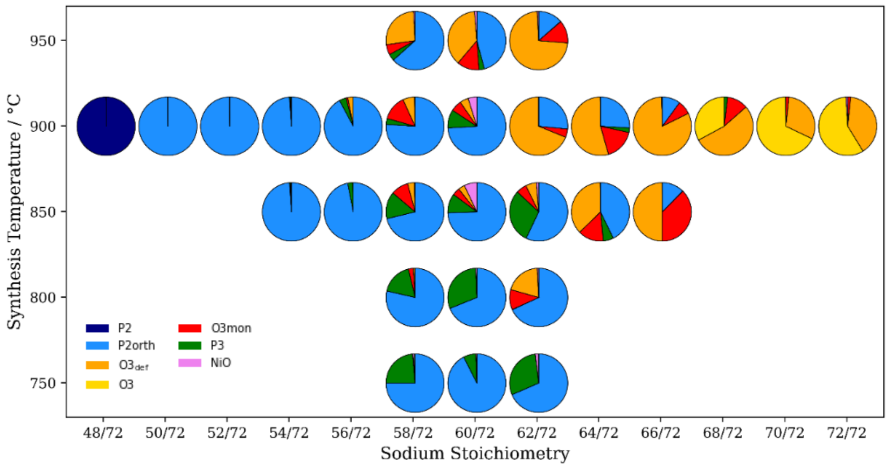


Figure 1. **Pie-chart phase diagram illustrating the structural phases inside the 29 synthesised cathode materials, in the $Na_{1-2x}Ni_{1/2-x}Mn_{1/2+x}O_2$ system, as a function of synthesis temperature and stoichiometry temperature.**

References

1. Zhao, L., Zhang, T., Li, W., Li, T., Zhang, L., Zhang, X., and Wang, Z. (2023). Engineering of Sodium-Ion Batteries: Opportunities and Challenges. Engineering *24*, 172–183. 10.1016/j.eng.2021.08.032.

2. Han, M.H., Gonzalo, E., Singh, G., and Rojo, T. (2015). A comprehensive review of sodium layered oxides: Powerful cathodes for

Na-ion batteries. Energy Environ. Sci. *8*, 81–102. 10.1039/c4ee03192j.

3. Khan, M.A., Han, D., Lee, G., Kim, Y. Il, and Kang, Y.M. (2019). P2/O3 phase-integrated Na0.7MnO2 cathode materials for sodium-ion rechargeable batteries. J. Alloys Compd. *771*, 987–993. 10.1016/j.jallcom.2018.09.033.
4. Komaba, S., Yabuuchi, N., Nakayama, T., Ogata, A., Ishikawa, T., and Nakai, I. (2012). Study on the reversible electrode reaction of Na 1-xNi 0.5Mn 0.5O 2 for a rechargeable sodium-ion battery. Inorg. Chem. *51*, 6211–6220. 10.1021/ic300357d.
5. Delmas, C, Fouassier, C , Hagenmuller, P. (1980). STRUCTURAL CLASSIFICATION AND PROPERTIES OF THE LAYERED OXIDES. 1–22.
6. Li, R., Liu, Y., Wang, Z., and Li, J. (2019). A P2/O3 biphasic cathode material with highly reversibility synthesized by Sn-substitution for Na-ion batteries. Electrochim. Acta *318*, 14–22. 10.1016/j.electacta.2019.06.020.
7. Zeng, Z., Li, Q., Liu, W., Li, L., Song, C., and Yang, J. (2025). Comparative study of Na 0 . 95 Ni x Mn 1-x O 2 cathode materials for sodium ion batteries based on phase structure modulation. *107*, 1–10. 10.1016/j.est.2024.114923.

Biography:

Arthur is a final-year PhD researcher at University College London, with a Master's in Chemistry from the University of Oxford. He spent five months at UNSW with Dr Wesley Dose through a lab exchange. His research develops advanced diagnostic techniques - such as acoustic analysis and operando methods - to understand and mitigate degradation in next-generation batteries. He is particularly focused on sodium-ion systems, combining electrochemical analysis with structural techniques like XRD to study cathode evolution and improve long-term stability.

#3

‘Layered’ Transition Metal Oxide Cathodes for Sodium-Ion Batteries: Controlled Phase Formation via Transition Metal-Oxygen Bond Covalency Tuning.

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

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

*Email: amartya_mukhopadhyay@iitb.ac.in

Keywords: layered Na- transition metal oxide • phase evolution • cathode • O-P intergrowths • Na-ion battery • Energy storage

Abstract:

This work introduces a universal strategy towards facilitating and controlling the formation of biphasic P2/O3 structures, along with other preferred structural types (P-type and O-type), in ‘layered’ Na- transition metal (TM) oxides. Building on our previous study[1], where we revealed that it is the overall degree of covalency of the cation-oxygen bonds in the TMO_2-‘slab’, as governed by the overall average charge:size ratio (C:S) of the cation-combination in the TM-layer (*viz.*, electronegativity), that tilts the balance between P2 vs. O3 phase formation for a given Na-content, we reveal here the possibility of facilitating and controlling the P2 + O3 (*i.e.*, bi-phasic/single phase) content in ‘layered’ Na-TM-oxide based on the same concept. Using a predominantly Ni-Mn-based composition, we systematically modulated the overall covalency of the TM–O by substituting a low-electronegativity cation (Ti^{4+}, having a lower “charge:size” ratio ~6.5 Å^{-1}) into the transition metal (TM) layer for Mn^{4+} (having a higher “charge:size” ratio of ~7.5 Å^{-1}). This reduction in covalency enhanced the relative stability of the O3 phase over that of the P2 phase for the original composition, enabling a controlled phase formation/content for the mixed phase (*i.e.*, O3 + P2) and then eventually in phase pure O3. The effects of the phase assemblage on the electrochemical behaviour have also been studied in Na ‘half’ cells. These findings offer insights into the design of mixed-phase (O3/P2) cathode materials by precisely tuning the covalency of the TM-O bond and following the map reported in our previously published work[1] (*viz.*, the C:S corresponding to the TM-layer relative to the stoichiometric Na content), enabling optimized structural stability and improved electrochemical performance as cathodes for sodium-ion batteries.

References

1. Kumar, Bachu Sravan, Rahul Kumar, Anagha Pradeep, Amardeep Amardeep, Velaga Srihari, Himanshu K. Poswal, Abhijit Chatterjee, and Amartya Mukhopadhyay. "Fundamental principles toward designing high Na-containing P2-structured “layered” Na-transition metal oxides as high-performance cathode materials for Na-ion batteries." *Chemistry of Materials* 34, no. 23 (2022): 10470-10483.

Biography:

Brijesh presently, pursuing his PhD from IITB-Monash Research Academy(A joint venture between IIT Bombay and Monash University, Australia). His current research interest lies investigating Electrolytes & Electrode materials for Alkali Metal-ion Batteries(Na, Li, K). He completed his bachelor's master’s in chemistry from University of Delhi.

#4

Structure and ion-exchange mechanisms of layered transition metal oxides

Govardhan Sontam 1, Aditha Rawal 1, Adam Best 2, Neeraj Sharma *1

1School of Chemistry, The University of New South Wales, Kensington, NSW 2052, Australia.

*E-mail: neeraj.sharma@unsw.edu.au

2 Research Way, Clayton, Victoria 3168, Australia

Keywords: • Ion-exchange • structural evolution • NMR • Na [NixFeyMnz] O2

Abstract:

Cathodes play a key role in the function of sodium-ion batteries. Understanding their structure and structural evolution under various processes is critical to develop better materials and superior battery performance, whether it be lifetime or capacity.

In the present work, we investigate the ion-exchange mechanism of a commercially available Na [NixFeyMnz]O2 (NFM), an O3 type layered oxide. Specifically we are focused on the Li-Na ion exchange behaviour, trying to understand to how to control Na extraction and Li insertion.

Using 7Li and 23Na NMR (solution and solid-state), we are able to determine the local chemical environments around these elements in Li/Na-NFM materials. These data are coupled with compositional changes determined using inductively coupled plasma optical emission spectroscopy (ICP-OES) and bulk structural changes using X-ray diffraction (XRD). The talk will highlight the work underway to observe the ion-exchange process *in situ via* a variety of characterization techniques.

Biography:

Govardhan is a first year PhD student at UNSW working with Prof. Neeraj Sharma and Dr. Adam Best of CSIRO. Gova is trying to understand the ion-exchange mechanism of layered transition metal oxides to develop novel materials. Previously, worked as a manager, Electrochemical division at Relaince New Energy, and did masters thesis on iron-based cathodes for sodium-ion batteries from IIT Bombay.

#5

Fe–Mn Substitution-driven P2/P3 Phase Modulation in Layered Transtion Metal Oxides for Sodium-Ion Storage

Heramba V. S. R. M. Koppisetti, 1 and Amartya Mukhopadhyay* 1

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

* Corresponding author's e-mail-id: amartya_mukhopadhyay@iitb.ac.in

Keywords: Sodium ion batteries • Biphasic • Iron manganese cathodes • Layered oxides • Energy storage

Abstract:

Sodium ion batteries are sustainable electrochemical energy storage systems due to the lower cost and higher abundance of precursors, as compared to the already commercialized Li-ion bateries. The 'layered' Na- transition metal (TM) oxide cathode materials are important towards bestowing high energy density to Na-ion batteries, but usually suffer from cyclic instability. Heterostructure engineering is one of the avenus towards mitigating multiple phase transitions, TM-dissolution, in a bid to induce better structural-cum-cyclic stability and facilitate Na+ transport kinetics. In this regard, a major emphasis has been on tuning of P2/O3 phase by carefully choosing the cation-combination in the TM-layer based on cation charge-to-size ratio (as reported in a previous work from our group [1]). However P2/P3 modulation is seldom reported, which we report herein based on tuning the ratio of earth abundant elements like Mn and Fe. The so far optimized P2/P3 heterostructure, based on a Mn:Fe ratio of ~1.7 deliverd an initial discharge capacity of 152 mAh/g @ 15 mA/g and 94 mAh/g @ 150 mA/g, out performing both the pure P2 (based on Mn:Fe ~3.1) and P3 (based on Mn:Fe ~1.2) counterparts. The biphasic oxide based cathode also retained ~82% of its initial capacity after 100 cycles @ 30 mAh/g. The improved electrochemical performance has been attributed to the enhanced stablility of the structure and efficient Na+ transport between the prismatic Na-sites. These findings offer a stragety and a cost-effective route towards designing high-performance sodium-ion cathodes with reduced reliance on critical minerals.

Reference:

1. Kumar, et al.; (2022). *Chemistry of Materials*, **34**(23), 10470-10483.

Biography:

I, Heramba Koppisetti, am currently a postdoctoral fellow in the Department of Metallurgical Engineering and Materials Science Department in the Indian Institute of Technology Bombay (IIT Bombay). My areas of interest includes electrochemical energy storage, *i.e.*, rechargeable alkali metal-ion batteries and supercapacitors. I have completed my doctoral studies from the Indian Institute of Science Education and Research, Kolkata. I have also worked as overseas visiting doctoral fellow at Purdue university, USA during my tenure as a PhD student.

#6

Investigations of Charge Storage Mechanism on Cu and F Doped $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ Layered Oxide as Cathode Material for Sodium-Ion Batteries

Hsiang-Jung Chen, and Han-Yi Chen*

Department of Materials Science and Engineering, National Tsing Hua University, 101, Section 2, Kuang-Fu Road, Hsinchu 300044, Taiwan

*E-mail: hanyi.chen@mx.nthu.edu.tw

Keywords: F-doping • sodium-ion batteries • cathode materials •layered transition metal oxides • P2-type

Abstract:

Sodium-ion batteries (SIBs) offer comparable performance to lithium-ion batteries (LIBs) at a lower cost. Here, layered transition metal oxides (LTMOs, Na_xTMO_2; TM = Cu, Mn, Fe, Ti, Cr, Ni, etc.) are promising cathodes due to LIB-based maturity. P2-type Ni/Mn-based LTMO (e.g., $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$) delivers high capacity (ca. 173 mA h g^{-1}) with eco-friendly elements but suffers from poor stability due to P2−O2 phase transition above 4.2 V, low rate performance, and air/moisture sensitivity. To address these issues, we apply a facile cation-and-anion dual-doping strategy to enhance both structural stability and electrochemical performance for improved SIB cathode development. Therefore, a Cu and F dual-doped $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ (NNCMOF) cathode material is developed, featuring high structural stability and rate capability. Cu doping stabilizes the P2−O2 phase transition, improves moisture resistance, and adds capacity via Cu^{2+}/Cu^{3+} redox (~3.8 V vs. Na/Na^+). F doping enhances Na^+ kinetics by expanding interlayer spacing and activates Mn redox by lowering Mn^{4+} valence through charge compensation.

In this work, the successful synthesis of NNCMOF through a facile sol-gel method was confirmed by X-ray diffraction, scanning electron microscope, and energy dispersive spectroscopy. Also, F doping was proved applicable comprehensively by X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, F K-edge soft X-ray absorption spectroscopy (XAS), wavelet-transformed extended X-ray absorption fine structure, ^{19}F solid-state nuclear magnetic resonance spectroscopy, and time-of-flight secondary ion mass spectrometry. In addition, the NNCMOF//Na cell shows the best comprehensive electrochemical performance in this research. At the current density of 1 C, a capacity > 100 mA h g^{-1} was maintained after 100 cycles (retention rate of about 85%). At a high current density of 30 C, it can still possess a capacity of ca. 60 mA h g^{-1}, showing predominant rate performance.

Furthermore, synchrotron-based operando hard/soft XAS, and ex-situ XPS were conducted to study the behavior of transition metal ions and oxygen ions, explaining the underlying charge storage mechanism upon Na ion intercalation/deintercalation. Moreover, operando synchrotron XRD was also used to analyze the structural change during charging and discharging, which demonstrated the enhanced cycling stability of NNCMOF. Also, Na ion diffusion coefficient estimation has been done, showing that D_{Na^+} of NNCMOF has a high value between 10^{-9} and 10^{-11} $cm^2\ s^{-1}$, confirming the improved rate performance. In practice, The NNCMOF//hard carbon full cell achieves ca. 270 W h kg^{-1} and 77% retention after 50 cycles, confirming the practical potential of fluorine-based dual-doped layered cathodes for next-generation SIBs.

Biography:

Hello, I am Hsiang-Jung Chen from Taiwan. I am currently a first-year Ph.D. student in the Department of Materials Science and Engineering at National Tsing Hua University (NTHU), Taiwan. My research focuses on cathode materials for sodium-ion batteries, particularly layered oxides, which I began exploring during my master's studies. Through this work, I developed a strong passion for designing high-performance, practical materials for energy storage applications, with a keen interest in understanding their underlying fundamental mechanisms. I am especially honored to utilize synchrotron-based techniques in my research. Attending ICNaB offers a valuable opportunity to engage with the broader research community and gain insights into cutting-edge developments in the field. I am truly looking forward to the conference.

#7

Redox Stability Engineering of P2-Type Layered Oxides for Sodium-Ion Storage via Li, Ni, and Cu Triple Doping

Hye-Jin Kim, [1] and Seung-Taek Myung* [2]

[1] *Hybrid Materials Research Center, Department of Nanotechnology and Advanced Materials Engineering & Sejong Battery Institute, Sejong University, 98 Gunja-dong, Gwangjin-gu, Seoul 05006, South Korea*

E-mail: hyejink@sju.ac.kr

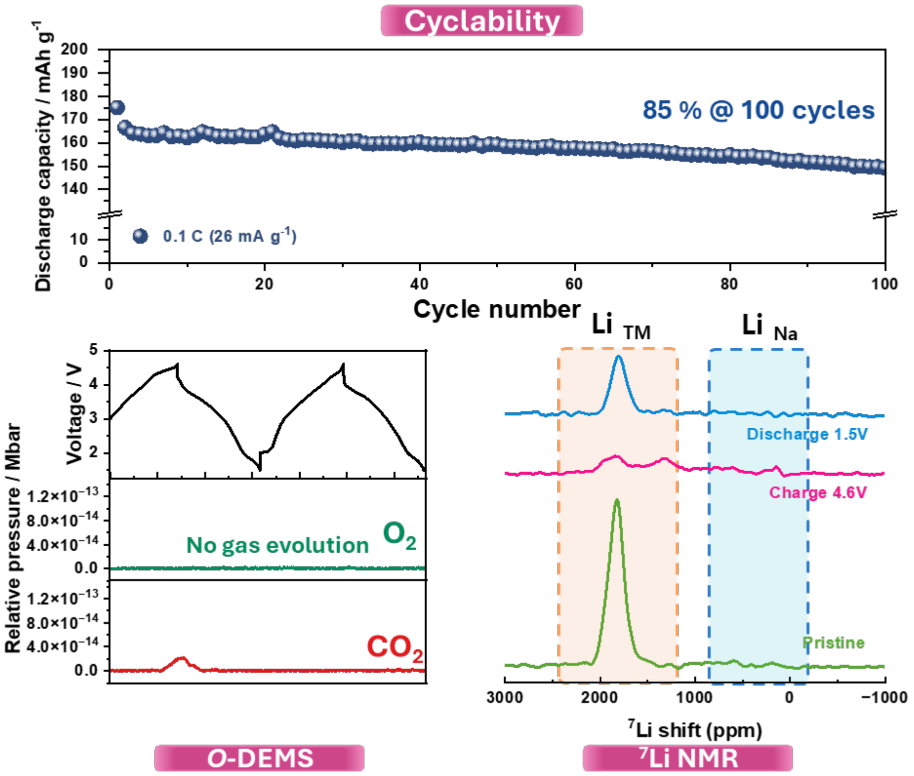
[2] *Hybrid Materials Research Center, Department of Nanotechnology and Advanced Materials Engineering & Sejong Battery Institute, Sejong University, 98 Gunja-dong, Gwangjin-gu, Seoul 05006, South Korea*

E-mail: smyung@sejong.ac.kr

Keywords: Sodium-ion batteries • Cathode • Oxygen redox

Abstract:

P2-type sodium-deficient layered oxides exploit their Na–O–A (A = Li, Mg, Zn, vacancy) defect configuration to activate high-capacity oxygen redox, yet they suffer from irreversible Oxgyen redox, O_2 evolution, structural distortion, and rapid capacity fade. In this work, we address these limitations by introducing Li/Ni/Cu triple doping into $Na_{0.7}[Li_{0.1}Ni_{0.1}Cu_{0.1}Mn_{0.7}]O_2$. *Operando* X-ray diffraction, neutron powder diffraction, and X-ray absorption analysis were employed to monitor Na insertion/extraction and the real-time redox states of Ni, Cu, and Mn during cycling. ^{7}Li NMR revealed a pronounced depletion of Li in the TM layer upon charging and complete recovery upon discharging, confirming a fully reversible Li migration pathway. ToF-SIMS demonstrated dynamic Li redistribution within the SEI layer, while combined XAS analyses verified stable Ni^{2+}/Ni^{4+}, Cu^{2+}/Cu^{3+}, Mn^{3+}/Mn^{4+} cation redox alongside reversible $O^{2-}/(O_2)^{n-}$ anion redox at elevated potentials. Crucially, *O*-DEMS up to 4.6 V detected no O_2 evolution, evidencing truly reversible oxygen redox without gas release. As a result, the triple-doped P2 cathode delivers an initial discharge capacity of 175 mAh g^{-1} at 0.1 C and retains 85 % of its capacity after 100 cycles, while securing additional high-voltage capacity via oxygen redox. This work provides a strategic framework for the design of high-capacity, oxygen-redox active P2 cathodes in sodium-ion batteries.



#8

Molten-Salt Synthesis of Pore-Free Single Crystalline Particles for Durable Na-Ion Battery Cathodes

Hyokyeong Kang, [1] and Jang-Yeon Hwang* [2]

[1,2] Department of Energy Engineering, Hanyang University, Seoul 04763, Republic of Korea

E-mail: jangyeonhw@hanyang.ac.kr

Keywords: *sodium-ion batteries, single-crystalline particles, polycrystalline particles, NaNCM cathodes, microcracking*

Abstract:

The increasing demand for lithium-ion batteries (LIBs) is challenged by the limited lithium reserves and high material costs, prompting the exploration of sodium-ion batteries (SIBs) as cost-effective alternatives. Owing to their similar intercalation chemistry, SIBs have gained significant attention; however, polycrystalline cathode materials suffer from mechanical degradation during Na^+ (de)intercalation, leading to interparticle pulverization, microcrack formation, and detrimental electrolyte–electrode interfacial reactions. Single crystalline cathodes offer improved structural integrity but conventionally require high-temperature calcination, especially problematic for O3-type $NaNi_xCo_yMn_zO_2$ (O3-NCM) cathodes, where NiO phase formation and particle aggregation occur due to Ni solubility constraints at elevated temperatures. In this study, a pore-free single crystalline O3-type $Na[Ni_{0.6}Co_{0.2}Mn_{0.2}]O_2$ (SC-NCM) cathode is developed via a molten-salt method at a relatively low calcination temperature. The dissolution–recrystallization mechanism inherent to the molten-salt process promotes efficient metal ion diffusion, enabling the formation of single crystalline particles irrespective of the precursor's initial morphology. Furthermore, this synthesis strategy simplifies the overall procedure by eliminating the need for a co-precipitation step and lowering the calcination temperature, thereby reducing both processing time and complexity.

1. *ACS Appl. Mater. Interfaces* ***2018**, 10*, 17850−17860
2. *Chem. Soc. Rev.* **2017***, 46*, 3529−3614
3. *Adv. Energy Mater.* **2023**, *13*, 2301975

Biography:

Hyokyeong Kang is presently a Ph.D. candidate under the supervision of Prof. Jang-Yeon Hwang in the Department of Energy Engineering at the Hanyang University. Her current research interests focus on the design of cathode materials and their application in alkali-ion batteries.

#9

O3/P2 Layered Oxide Hybridisation as a Tool for Enhancing Capacity via Intergrowth Formation

Jose-Enrique Rodriguez-Fernandez*[1], and Maider Zarrabeitia[1]

[1] Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany

*E-mail: enrique.rodriguez@kit.edu

Keywords: Hybrid layered oxides • O3/P2 intergrowths • Ni/Mn ratio • Synergistic phase effect •

Abstract:

Sodium-layered oxides are promising candidates as cathode materials for the commercialisation of Na-ion batteries (NIBs). According to Delmas' notation, these layered oxides can be classified as, e.g., P2 or O3-type materials depending on their unit cell. The structure of this cathode material will have a direct impact on the final electrochemical performance of the NIBs [1]. Regarding kinetics, P2-type materials have been demonstrated to be superior [2]. Nevertheless, O3-type ones typically have higher Na content than P2, which translates into higher capacities [3] but suffers from poorer stability. As a strategy to combine the advantages of both, a series of hybrid layered oxide materials with the formula $Na_xMn_{0.60-y}Ni_{0.12+y}Fe_{0.08}Mg_{0.09}Zn_{0.11}O_2$ has been proposed. Here referred to as P2-Na0.72, O3/P2-Na0.88, and O3/P2-Na0.92, depending on their initial Na concentration. These systems resulted in P2 with O3 intergrowth structure, offering not only enhanced electrochemical behaviour due to the presence of both phases but also unique properties arising from the intergrowth itself. During the selection of materials, the effect of the Mn/Ni ratio on the final phase composition was studied. Moreover, the reported increase in discharge capacity is significant and attributed to the synergistic effect of the two phases. For example, the O3/P2-Na0.88 material exhibits an increase in capacity, which is 100% higher compared to P2-Na0.72 and 20% higher compared to O3/P2-Na0.92 (see **Figure 1**). Overall, the combination of O3 and P2 phases in an intergrowth crystal structure demonstrates promising results. These findings suggest that careful tuning of the Mn/Ni ratio and phase composition can lead to significant performance enhancements. As such, the O3/P2-Na0.88 layered oxide cathode material represents a strong candidate for future development of NIBs.

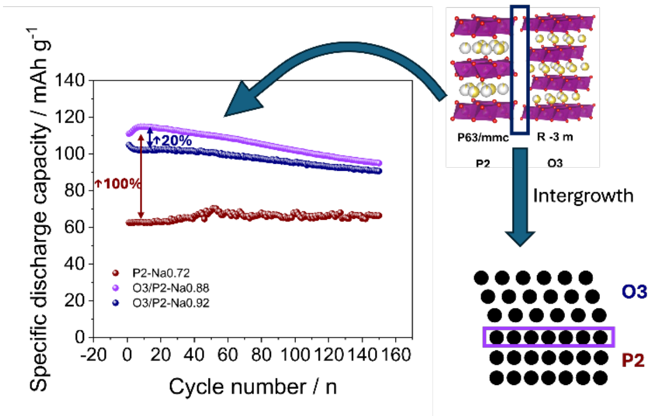


Figure 1. Specific discharge capacities for the P2-Na0.72, O3/P2-Na0.88 and O3/P2-Na0.92

References:

[1] GRÉPIN, Elisa, et al. Rational selection of sodium layered oxides for high performance Na-ion batteries: P2 vs O3 vs P2-O3 intergrowths. Journal of The Electrochemical Society, 2023, vol. 170, no 8, p. 080510.
[2] GUO, Shaohua, et al. A layered P2-and O3-type composite as a high-energy cathode for rechargeable sodium-ion batteries. *Angewandte Chemie International Edition*, 2015, vol. 54, no 20, p. 5894-5899.
[3] GUO, Yu-Jie, et al. Sodium layered oxide cathodes: properties, practicality and prospects. *Chemical Society Reviews*, 2024.

Biography:

José Enrique is currently a Ph.D. student at the Karlsruhe Institute of Technology and Helmholtz Institute Ulm under the supervision of Dr. Maider Zarrabeitia, where he focuses on the development of novel cathode materials and solid-state electrolytes for next-generation sodium-ion batteries. He holds a Bachelor's degree in Chemistry from the Autonomous University of Madrid, where he completed his thesis in the Department of Applied Physical Chemistry. He later pursued a Master's degree in Electrochemistry through an interuniversity program jointly offered by the University of Alicante, the Autonomous University of Madrid, and the University of Barcelona. His Master's thesis involved studying lignin as an additive in PEM-type cells to enhance hydrogen production by partially substituting the oxygen evolution reaction in water electrolysis.

#10

Unraveling Mechanism for Microstructure Engineering toward High-Capacity Nickel-Rich Cathode Materials

Lili Lin, [1] Lihan Zhang, * [2] Zhiqiang Fu, [1] Jiatao Lou, [1] Ziyao Gao, [1] Junru Wu, [1] Chenglei Li, [1] Cuiping Han, [3] Dong Zhou, [1] * Ziqiang Wang, [1] * and Baohua Li [1] *

[1] Institute of Materials Research, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen 518055, China

E-mail: zhou.d@sz.tsinghua.edu.cn; wangziqiang@sz.tsinghua.edu.cn; libh@sz.tsinghua.edu.cn

[2] Beijing Key Laboratory of Microstructure and Properties of Solids, Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing 100124, China

E-mail: zhanglh06@bjut.edu.cn

[3] Faculty of Materials Science and Energy Engineering/Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen 518055, China

Keywords: capacity enhancement • coherent spinel twin boundaries • microstructure engineering • nickel-rich cathodes • tungsten modification

Abstract:

Nickel-rich layered oxides (NRLOs) are the most promising cathode materials for lithium-ion batteries. Recent studies have demonstrated that incorporating high-valence elements can significantly improve the capacity of NRLOs without compromising cycling stability. However, the underlying mechanism behind this enhancement remains unclear.

In this work, we uncover that the formation of coherent spinel twin boundaries plays a critical role in boosting the capacity of NRLOs. As a demonstration model, we introduce W into NRLO (W-Ni83) to modulate the micro and nano structure of NRLOs. The as-developed W-Ni83 shows a significant discharge capacity enhancement of about 14 $mAh \cdot g^{-1}$ at the first cycle. High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) reveals that W doping induces the formation of coherent spinel twin boundaries within the bulk phase. These twin boundaries significantly enhance Li^+ transport kinetics by facilitating deeper lithium insertion/extraction into the bulk structure, as further supported by theoretical modeling and electrochemical analysis. Beyond bulk-phase modification, W doping also forms a dense LiW_xO_y coating layer on both primary and secondary particles of W-Ni83. This protective layer mitigates detrimental side reactions with the electrolyte, thereby improving cycling stability.

Our findings present a simple yet effective strategy to simultaneously enhance capacity and cycle life through microstructure engineering. This work provides a new design principle for developing high-capacity, long-life battery materials via targeted microstructure control.

Biography:

Lili Lin is a Ph.D. candidate in Materials Science and Engineering at Tsinghua Shenzhen International Graduate School, specializing in nickel-rich cathode materials for lithium-ion batteries. Her research focuses on microstructural engineering and performance optimization of nickel-rich layered oxide cathode materials for next-generation high-energy lithium-ion batteries.

#11

Refining Testing Conditions for Comparative Evaluation of O3-$NaCoO_2$ and P2-$Na_{2/3}CoO_2$ Electrodes

Mika Takemura,[1] Kodai Moriya,[1] Sho Toriumi,[1] Shinichi Kumakura,[1] Shinichi Komaba[1]

[1] e, 1-3 Kagurazaka, Shinjukuku, Tokyo 162-8601, Japan

E-mail: Komaba@rs.tus.ac.jp

Keywords: Cathode・layered oxides・polymorphs・morphology・electrode formuration

Abstract:

Layered oxides Na_xTMO_2 (TM = transition metal) are promising cathode materials for next-generation Na-ion batteries, offering diverse compositions and polymorphs. O3-type (Na/TM = 1) and P2-type (Na/TM = 2/3) materials are particularly well-studied in electrochemical reactivity and structural points of view.[1] On the other hand, since the electrode is consisted of a complicated composite, the impact of crystallographic differences on battery performance is not fully understood. The typical battery performance is compared based on the total mass loading of as-prepared electrodes. However, it might cause overestimation of reversible capacity for P2-type materials than O3-type because mass of 1/3 mole Na deficiency is not considered for capacity calculation. Furthermore, a difference on the particle morphology between O3-type and P2-type materials[2] causes an impact on Na dffusivity in the electrode level. This study therefore optimized synthesis conditions for comparative evaluation of O3-type and P2-type Na_xCoO_2 as model materials to achieve uniform particle morphologies. By comparing their electrochemical properties under the refined test-condition, we discuss cycle characteristics and Na diffusivity between these polymorphs.

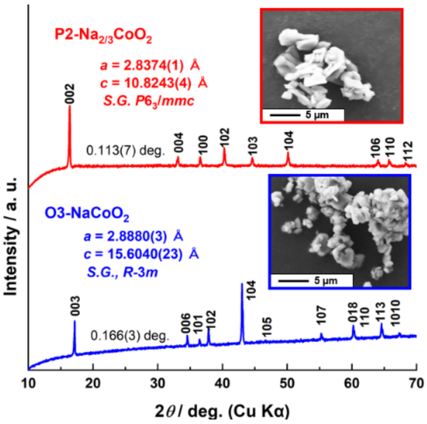


Fig. 1 XRD patterns and SEM images of Na_xCoO_2

Na_xCoO_2 were synthesized by solid-state reaction using NaOH and Co_3O_4. Characterization involved XRD, SEM, particle size distribution, and galvanostatic charge-discharge tests using coin-type half-cells with a fixed ratio of active material, conductive agent (AB), and binder (PVdF) on an Al foil working electrode and a Na metal counter electrode.

Fig. 1 shows particle size control of P2/O3-Na_xCoO_2 by adjusting calcinating condisions. P2-$Na_{2/3}CoO_2$ was obtained by firing in air at 750 °C, while O3-$NaCoO_2$ was obtained in O_2 atmosphere at 500 °C, The two samples exhibited comparable crystallinity and particle size distribution. For P2/O3 comparison, in addition to conventional composite electrodes prepared based on mass, we also prepared composite electrodes based on equimolar concentrations of the active materials.

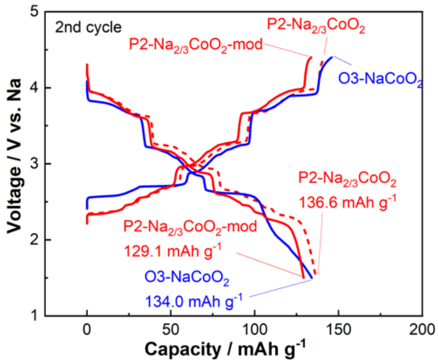
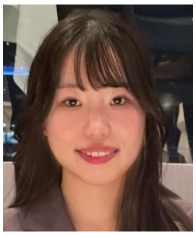


Fig. 2 Charge/discharge curve for the 2nd cycle of Na_xCoO_2.

Fig. 2 shows 2nd cycle charge/discharge curves. P2-$Na_{2/3}CoO_2$-mod (equimolar concentrations) achieved a capacity of 129.1 mAh g^{-1}, allowing for the equalization of the weight ratio at full discharge. We will compare the cycle characteristics of O3-type and P2-type materials obtained by optimizing synthesis conditions and adjusting electrode blend conditions, and additionally discuss the differences in Na diffusivity.

(1) N. Yabuuchi, S. Komaba, *et al.*, *Nat. Mater.*, **11**, 512 (2012).
(2) Y. Lei, G. Ceder, *et al.*, *Chem. Mater.*, **26**, 18, 5288 (2014).

Biography:



Mika Takemura is a master's student in the Department of Applied Chemistry at Tokyo University of Science, Japan. She joined Komaba group in 2024. Her research focuses on sodium layered oxides and the electrochemical performance of Na-ion rechargeable batteries. She presented her work at the 2025 Annual Meeting of The Electrochemical Society of Japan.

#12

Accelerating solid-state synthesis for sodium layered oxide cathodes via in situ formed molten salt

Qinzhe Liu,[1] Yixiao Qiu[1] and Chao Xu[1,*]

[1] School of Physical Science and Technology, ShanghaiTech University, Shanghai, China.

E-mail: xuchao1@shanghaitech.edu.cn

Keywords: Anionic redox; O3-type layered oxides; Atmosphere-controlled synthesis; *Operando* characterization

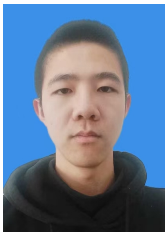
Abstract:

Energy enhancement through oxygen anionic redox (OAR) is present in both lithium and sodium batteries.[1] However, research on the latter, especially the O3-type OAR cathodes, is still insufficient, mainly due to the difficulty of synthesising these materials.[2-3] Our recent work demonstrates that the synthesis of O3-type sodium anion-redox cathodes involves a complex reaction scheme that necessitates precise control of atmosphere modulation.[4] Herein, we further advance the understanding of the synthesis reaction for O3-type sodium anion-redox cathodes by studying the impact of reactants. Using a variety of characterisation techniques such as in-situ and ex-situ X-ray diffraction, thermogravimetric analysis, and electron microscopy, we have found that the use of nitrate provides a molten environment for the calcination process and that the inter-transformation of nitrate with other phases makes the reaction process much simpler, resulting in high purity O3 phases under simpler conditions. This study not only provides fundamental mechanistic insights into the evolutionary processes and interactions of the components during the synthesis process, but also guides the synthesis of next-generation OAR cathodes for high-energy density sodium-ion batteries.

Reference

[1] Priti, S.; Mudit, D. Opportunities and Challenges in the Development of Layered Positive Electrode Materials for High-Energy Sodium Ion Batteries: A Computational Perspective. *Langmuir* **2023**, *39*, 28-36.
[2] Zhao, C.; Wang, Q.; Yao, Z.; Wang, J.; Sánchez-Lengeling, B.; Ding, F.; Qi, X.; Lu, Y.; Bai, X.; Li, B.; et al. Rational design of layered oxide materials for sodium-ion batteries. *Science* **2020**, *370*, 708-711.
[3] Wang, Q.; Mariyappan, S.; Rousse, G.; Morozov, A. V.; Porcheron, B.; Dedryvere, R.; Wu, J.; Yang, W.; Zhang, L.; Chakir, M.; et al. Unlocking anionic redox activity in O3-type sodium 3d layered oxides via Li substitution. *Nat Mater* **2021**, *20*, 353-361.
[4] Qiu, Y.; Liu, Q.; Tao, J.; Yan, P.; Tan, G.; Liu, F.; Wang, D.; Yu, N.; Zhang, N.; Yang, Y.; et al. Enabling the synthesis of O3-type sodium anion-redox cathodes via atmosphere modulation. *Nature Communications* **2025**, *16*, 2343.

Biography:



Qinzhe Liu received his B.Sc. (2023) from Tianjin University. He is currently a PhD student at ShanghaiTech University. His research focuses on anionic-redox-active layered oxides for sodium-ion battery cathodes.

#13

Surface Modification of O3-type Sodium Layered Oxides for Improvement of Safety of Sodium-Ion Batteries

Shaofan LYU, [1] Chia-Ching LIN, [2] Denis Y.W. YU, [2] Satoshi KAJIYAMA, [1] Masashi OKUBO* [1]

[1] Department of Electrical Engineering and Bioscience, Waseda University, Tokyo 169-8555, Japan

E-mail: m-okubo@waseda.jp

[2] Research Center for Energy and Environmental Materials (GREEN), National Institute for Materials Science, Tsukuba 305-0044, Japan

Keywords: Layered oxides • cathode materials • surface modification • thermal stability

Abstract:

Sodium-ion batteries (SIBs) have been considered as one of the most promising alternatives to lithium-ion batteries (LIBs). While sodium layered oxides provide the best electrode performance among all the candidates of cathode materials for SIBs, their poor cycle stability and safety issue should be addressed, for example, by improving a surface structure as well as an electrode fabrication procedure. In particular, the surface residual alkali species at surface of sodium layered oxides, either from the synthesis process or exposure to moisture, cause both the gelation of slurry and safety issues during charge-discharge process.[1] In the present work, we demonstrate a facile way to modify the surface structure of O3-type sodium layered oxides, which enhances both the cycle life and thermal stability.

Surface modification of sodium layered oxide materials was conducted by the acid treatment with phosphoric acid of O3-$NaNi_{0.5}Mn_{0.5}O_2$ synthesized by a convention sol-gel process. Further surface treatment was conducted by calcination at 500 °C after the acid treatment. Thermal behaviour of pristine and surface modified materials with electrolyte was examined at pristine and charged states using differential scanning calorimetry. To better comparing the thermal stability of each sample, thermal stability index (TSI) was calculated. [2]

As shown in Fig. 1, the TSI value of O3-$NaNi_{0.5}Mn_{0.5}O_2$ present high value (> 9) when charged to 180 mAh/g. While both acid and heat treatments lower the TSI (<5), even at high charge states, indicating enhanced thermal stability. These results highlight the critical role of surface modification in improving thermal stability of sodium layered oxide cathodes.

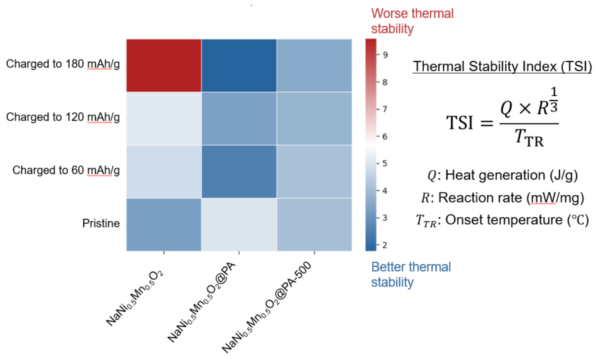


Fig.1 Heat map of the thermal stability index (TSI) as a function of the cathode materials and capacity.

References

[1] T. Zhao *et al.*, *ACS Energy Lett.* **2023**, *8*, 4753−4761.
[2] Cui, Z *et al. Nat Energy* **10**, **2025,** 490–501

Biography:

Shaofan Lyu is currently a PhD student in the Okubo lab at Waseda University. His research is mainly focused on the characterization of O3-type sodium layered oxides, especially their thermal stability.

#14

Unveiling lattice defect-driven electrochemical behavior in corrugated layered NaMnO$_2$

Shinichi Kumakura, [1] Kei Kubota, [2] and Shinichi Komaba* [1]

[1] Tokyo University of Sience, 1-3 Kagurazaka, Shinjukuku, Tokyo 162-8601, Japan

[2] Research Center for Energy and Environmental Materials (GREEN), National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

E-mail: Komaba@rs.tus.ac.jp

Keywords: Mn oxide • Corrugated layer • Stacking fault • Positive electrode • DFT calculation

Abstract:

The Na-Mn-O ternary system has received increasing attention in both academic and industrial fields because of its diverse crystallographic and physical properties. In particular, layered Na$_y$MnO$_2$ is of paramount interest for studying two-dimensional features in solid state chemistry[1] and its application as a cathode material in rechargeable batteries since Delmas *et al.* first reported reversible electrochemical Na extraction/insertion for layered Na$_y$MnO$_2$ polymorphs.[2] Understanding of Mn(III/IV) redox reaction and its associated structural changes in the layered oxides is of critical importance for realizing Na-ion technology while it remains to be understood due to its structural complexity derived from Jahn-Teller actitivy of Mn(III) ions.

In this study, we demonstrate the new positive electrode material, i.e. corrugated layered sodium manganese oxide, so-called β-NaMnO$_2$ as polytype of a planar layered a-NaMnO$_2$. The assessment of the prospects of this material as a cathode material for Na-ion battery is hindered by the insufficient understanding of its solid-state chemistry owing to its stacking faults (SFs). To overcome the challenges posed by the SFs in the crystal structure of β-NaMnO$_2$, we first succeeded in modulating the amount and distribution of SFs in β-NaMnO$_2$ through partial replacement of Mn ions with Jahn-Tellar active Cu(II), and non-active Zn(II) ions. The scanning transmission electron microscopy (STEM) revealed that non-doped sample contains the ordered domain of a- and b- phases. Cu doping effectively removes SFs and Zn doping induces random distribution of SFs. These differences in the lattice defect provide significant impact on the electrochemical behavior, such as the cycle stability shown in Figure 1d. SF-free Cu doped sample shows superior cycle stability to the other samples. SF triggers the formation of a-domain and accerelates the capacy fading. In the presentation, the structural change during 1st cycle will be also discussed with in-situ and ex-situ XRD results, and DFT calculation.

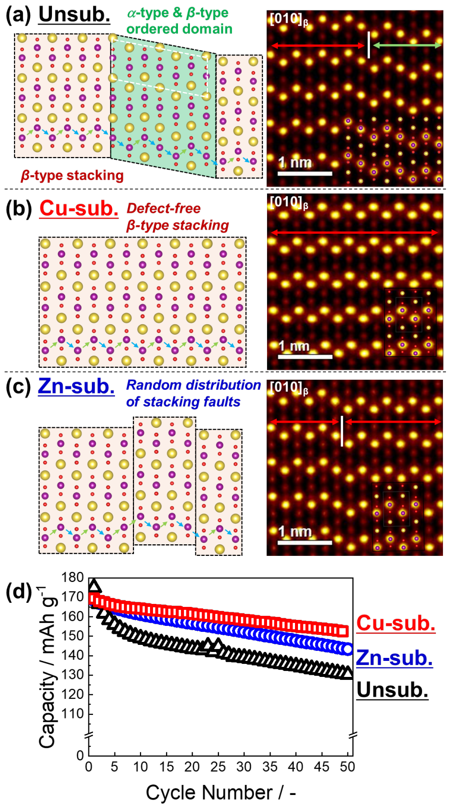


Fig. 1 STEM images for (a) non-doped, (b) Cu doped, and (c) Zn doped β-NaMnO$_2$. (d) Cycle stability comparison for the obtained materials.

Reference:

1. A. Mendiboure, C. Delmas, P. Hagenmuller, *J. Solid Sate Chem.* **1985**, *57*, 323.
2. J. Billaud *et al.*, *J. Am. Chem. Soc.* **2014**, *136*, 17243.

Biography:

Shinichi Kumakura obtained his PhD from the Komaba lab at the Tokyo University of Science in 2017. Then, he developed advanced battery materials at Umicore N.V. where he is a coinventor of 30 published patents related to battery material technologies. Since 2024, he has been a project scientist at the Tokyo University of Science. His research is focused on cathode materials for both Li-ion and Na-ion batteries, as well as those for all-solid batteries.

#15

Magnesium Cation Substitution to Optimize Capacity Retention of Na0.67Mn1-xFexO2 Layered Oxides for Sodium-Ion Batteries

Thilini Rathnayaka Mudiyanselage, Dmitri Golberg1 and Deepak Dubal* 1

1Centre for Material Science, School of Chemistry and Physics,Queensland University of Technology,Brisbane,QLD 4000, Australia E-mail: deepak.dubal@qut.edu.au

Keywords: Na ion batteries • Layered oxides • Mg doping • Na0.67 Mn1-x FexO2 • Capacity retention

Abstract:

The development of high-performance, cost-effective cathode materials is crucial for advancing sodium-ion battery (SIB) technology as a sustainable alternative to lithium-ion batteries. Among the various cathode candidates, layered sodium transition metal oxides with a general formula Na0.67Mn1-xFexO2 (NMF) have attracted attention due to their earth-abundant, environmentally friendly constituents and relatively high theoretical capacities. However, these materials suffer from poor structural stability and rapid capacity fading during prolonged cycling, primarily due to the Jahn -Teller distortion of Mn^{3+} and irreversible phase transitions. In this study, we report a systematic investigation into the effect of magnesium (Mg2+) cation substitution on the structural, electrochemical, and cycling stability of Na0.67 Mn1-x FexO2 layered oxides. Mg^{2+}, a non-redox-active and electrochemically inactive cation with strong metal-oxygen bonding, was partially substituted at the transition metal sites to suppress Mn3+-induced distortion, stabilize the layered framework, and improve sodium diffusion kinetics. A series of Na0.67Mn1-x-yFexMgyO_2 compositions were synthesized via a conventional furnace calcination and microwave assisted calcination using solid state method. Synthesized materials were characterized followed by extensive structural characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). Electrochemical properties were assessed using galvanostatic charge–discharge testing and cyclic voltammetry (CV) in the voltage window of 2.0-4.2 V vs. Na^+/Na. The results reveal that moderate Mg substitution significantly enhances cycling stability and capacity retention over 100 cycles. The Mg-doped samples exhibit reduced voltage hysteresis and improved structural reversibility during Na^+ intercalation/deintercalation. The improved performance is attributed to suppressed phase transitions and enhanced structural integrity of the P2-type layered framework due to Mg incorporation. This study highlights the critical role of aliovalent doping strategies in tailoring the physicochemical properties of layered sodium cathodes. The findings provide a promising pathway to engineering stable, high-capacity cathode materials for next-generation sodium-ion batteries.

Biography:

Thilini Rathnayaka Mudiyanselage is a PhD candidate in the School of Chemistry and Physics at the Queensland University of Technology (QUT), Australia. She began her postgraduate journey at QUT as a Master of Philosophy (MPhil) student, where she focused on the recovery and repurposing of critical materials from spent lithium-ion batteries. Building on this foundation, her current PhD research centers on the development and optimization of high-performance cathode materials for sodium-ion batteries, with an emphasis on transition metal doping strategies to enhance electrochemical performance and structural stability. Thilini holds a Bachelor of Science Honours degree in Polymer Chemistry from the University of Sri Jayewardenepura, Sri Lanka, and brings valuable industrial experience from her time at Ansell Lanka. Her research is supported by the QUT–Centre for Materials Science Linkage Spark Program Scholarship and the QUT Postgraduate Research Award.

#16

Investigation of Synthesis Mechanisms of O3-type Sodium Anion-Redox Cathodes via Atmosphere Modulation

Yixiao Qiu,[1] Qinzhe Liu,[1] Jiangwei Tao[1] and Chao Xu[1,*]

[1] School of Physical Science and Technology, ShanghaiTech University, Shanghai, China.

E-mail: xuchao1@shanghaitech.edu.cn

Keywords: Anionic redox; O3-type layered oxides; Atmosphere-controlled synthesis; *Operando* characterization

Abstract:

O3-type layered sodium transition metal oxides capable of oxygen anionic redox (OAR) reactions hold great promise as high-capacity cathodes for sodium-ion batteries (SIBs).[1-3] However, the synthesis of phase-pure O3-type OAR cathodes remains a major challenge due to complex reaction pathways and insufficient understanding of the role of oxygen partial pressure. In this work, we unravel the critical influence of oxygen chemical potential on the synthesis mechanism of O3-$Na[Li_{1/3}Mn_{2/3}]O_2$ using comprehensive *operando* techniques, including X-ray diffraction, thermogravimetric analysis, and gas chromatography.[4] Our findings reveal that a moderate oxygen environment (1-2% O_2 in Ar/N_2) is necessary to balance the redox states of manganese a nd to avoid undesirable Mn-based impurities. A dynamic controlled atmosphere (DCA) strategy is proposed, which starts with an oxidizing environment and transitioning to an inert one at high temperatures, in order to guide the reaction toward the formation of phase-pure O3-type materials. This method enables the successful synthesis of O3-$Na[Li_{1/3}Mn_{2/3}]O_2$ and a series of Ti-substituted derivatives $NaLi_{1/3}Mn_{2/3-x}Ti_xO_2$ ($x = 1/18, 1/9, 1/6$), all exhibiting reversible capacities exceeding 190 mAh g^{-1}. This study not only provides fundamental mechanistic insight into the interplay of oxygen dynamics and phase evolution during synthesis but also offers a versatile and scalable route toward high energy density OAR cathodes for next-generation SIBs.

Reference

[1] Wang, Q.; Mariyappan, S.; Rousse, G.; Morozov, A. V.; Porcheron, B.; Dedryvere, R.; Wu, J.; Yang, W.; Zhang, L.; Chakir, M.; et al. Unlocking anionic redox activity in O3-type sodium 3d layered oxides via Li substitution. *Nat Mater* **2021**, *20*, 353-361
[2] Cao, Y.; Xiao, M.; Sun, X.; Dong, W.; Huang, F. Recent Advances on High-Capacity Sodium Manganese-Based Oxide Cathodes for Sodium-ion Batteries. *Chemistry* **2023**, *29*, e202202997
[3] Jin, J.; Liu, Y.; Pang, X.; Wang, Y.; Xing, X.; Chen, J. A comprehensive understanding of the anionic redox chemistry in layered oxide cathodes for sodium-ion batteries. *Science China Chemistry* **2020**, *64*, 385-402
[4] Qiu, Y.; Liu, Q.; Tao, J.; Yan, P.; Tan, G.; Liu, F.; Wang, D.; Yu, N.; Zhang, N.; Yang, Y.; et al. Enabling the synthesis of O3-type sodium anion-redox cathodes via atmosphere modulation. *Nature Communications* **2025**, *16*, 2343

Biography:

Yixiao Qiu received his B.Sc. (2022) from Wenzhou University. He is currently a PhD student at ShanghaiTech University. His research focuses on anionic-redox-active layered oxides for sodium-ion battery cathodes.

#17

SYNTHESIS OF HIGH-ENTROPY OXIDES (HEOs) AS CATHODES FOR SODIUM-ION BATTERIES (NIBs)

Yueyue Luo, [1] Govardhan Reddy Sontam, [2] Dr. Sajjad Seifi Mofarah, [1] Prof. Charles Christopher Sorrell, [1] Prof. Neeraj Sharma, [2] A/Prof. Pramod Koshy* [1]

[1] School of Materials Science and Engineering, Faculty of Science UNSW Sydney, 2033, Australia

E-mail: yueyue.luo@unsw.edu.au, koshy@unsw.edu.au

[2] School of Chemistry, Faculty of Science UNSW Sydney, 2033, Australia

E-mail: g.sontam@unsw.edu.au

Keywords: sodium-ion batteries • cathodes • high-entropy oxides

Abstract:

Sodium-ion batteries (NIBs) are gaining research interest in electrochemical energy storage industry. The cathode is an important component of NIBs since it accommodates sodium ions for charging-discharging and plays a major role in determining the battery operating voltage and energy density. Layered sodium transition-metal oxides are commonly applied as cathodes, owing to their high average specific capacity and relatively simple synthesis process. However, such materials typically undergo irreversible phase transformations and volume changes during cycling process, which deteriorates capacity and rate performance.

High-entropy design offers a promising solution to the aforementioned limitations, by incorporating at least five principal cations into the oxide to generate a high configurational entropy greater than 1.5R to form high-entropy oxides (HEOs). HEOs exhibit entropy-stabilisation where a high entropy favours the formation of a single-phase material regardless of the number of elements present. Due to the mismatch between ionic radii of incorporated cations, the lattice of HEOs is severely distorted and the ionic diffusion is hindered, which minimizes the long-range ordered structural transformations and volume changes. Also, the synergistic effect of multiple cations generates various properties, including enhanced electrochemical activity and ionic conductivity.

This work fabricates HEOs via ball milling followed by heat treatment, aiming to understand the interplay between precursor types, synthesis conditions and air/air-free handling on product composition and properties. Single-element, multi-element and high-entropy compositions of oxide materials are fabricated into coin cells to examine the electrochemical properties, and their mechanisms of performance are elucidated.

Biography:

Yueyue Luo is a second-year PhD candidate at the University of New South Wales. Her research focuses on the cathode of sodium-ion batteries, especially the high-entropy transition-metal-based layered cathodes. She applies a scalable synthesis process to fabricate cathode materials and studies the effect of processing parameters on cathode composition and performance.

#18

Synthesis of $Na_{1+x}[Fe_{0.5}Mn_{0.5}]O_{2+0.5x}$ including sodium-excess phase for all-solid-state batteries

Miyu Kurebayashi, Daiki Hiraoka, Kota Motohashi, Atsushi Sakuda*, Akitoshi Hayashi

Department of Applied Chemistry, Graduate School of Engineering, Osaka Metropolitan University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan.

E-mail: saku@omu.ac.jp

Keywords: positive electrode • layered oxide • sodium-excess • low-cost materials • all-solid-state battery

Abstract:

Fe- and Mn-based layered oxides are candidates as positive electrode active materials because of their environmental and economic benefits. P2-type Fe- and Mn-based materials such as P2-type $Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$[1] show high electrode performance for sodium batteries. Na-deficient P2-type compounds require Na compensation from external Na sources in the negative electrode to achieve large reversible capacity. Compared with P2-type materials, O3-type Fe- and Mn-based materials have a higher sodium content, which increases the choice of negative electrode in the construction of full cells. In terms of mass production, it is preferable to use stable negative electrode such as hard carbon, tin, and phosphorus. However, O3-type $NaFe_{1/2}Mn_{1/2}O_2$[1] delivers a smaller reversible capacity than P2-type materials. To obtain large capacity in the high sodium content region, we have focused on sodium-excess materials. In Na_2RuO_3, honeycomb-type cation ordering enhanced reversible capacity based on the oxygen redox, leading to a 30% extra capacity than disordered Na_2RuO_3[2]. Metastable sodium-excess oxides $Na_{1.14}Mn_{0.57}Ti_{0.29}O_2$ showed a large reversible capacity originating from reversible redox reactions of cationic Mn^{3+}/Mn^{4+} and anionic O^{2-}/O^{n-} redox[3]. In this study, sodium-excess Fe- and Mn-based oxides $Na_{1+x}[Fe_{0.5}Mn_{0.5}]O_{2+0.5x}$ were prepared as positive electrode materials for all-solid-state batteries.

Sodium-excess Fe- and Mn-based oxides were prepared via classical solid-state reaction of Na_2CO_3, Fe_2O_3, and Mn_2O_3 at 800 ºC for 12 h. XRD patterns of the obtained samples were mainly indexed to the O3-type layered structure. Quantitative analysis of the prepared samples by ICP indicated that the content of sodium to transition metal was almost in agreement with the nominal composition. Cross-sectional SEM-EDX image of the sodium-excess samples showed that the samples were divided into two phases of sodium-excess one and sodium-deficient one. The all-solid-state sodium cells with $Na_{1.5}[Fe_{0.5}Mn_{0.5}]O_{2.25}$ positive electrode, Na_3PS_4 glass-ceramic solid electrolyte[4], and $Na_{15}Sn_4$ negative electrode showed an initial reversible capacity of 159 mAh g^{-1} at 25 ºC.

References

[1] N. Yabuuchi *et al.*, *Nat. Mater.*, **11** (2012) 512.
[2] B. Mortemard de Boisse *et al.*, *Nat. Commun.*, **7** (2016) 11397.
[3] T. Kobayashi *et al.*, *Small*, **16** (2020) 1902462.
[4] A. Hayashi *et al., Nat. Commun.*, **3** (2012) 856.

Biography:

Miyu Kurebayashi is a graduate student in the Department of Applied Chemistry at Osaka Metropolitan University, Japan. Her research focuses on positive electrode active materials for sodium batteries.

#19

Octahedral Tilt and Distortion Engineering in Prussian White Cathode $Na_{1+x}Fe[Fe(CN)_6]$ via Mg-doping for Enhanced Electrochemical Performance in Na-ion Batteries

Ashwani Tyagi [a], and Sreeraj Puravankara [a*]

[a] School of Energy Science & Engineering, IIT Kharagpur,

Kharagpur -721302, West Bengal, India

[a]Email: ashwani.tyagi@iitkgp.ac.in

[a*]Email: sreeraj@iitkgp.ac.in

Keywords: Prussian Blue analogues, Sodium-ion batteries, Distortions, Octahedral Tilts

Abstract

Prussian blue analogues (PBAs) are an exceptional and cost-effective choice for Na-ion battery cathodes, leveraging their robust open framework structure and efficient synthesis techniques. While Prussian white (PW) boasts a higher sodium content and fewer defects, it currently falls short in reversible capacity. This limitation arises from the restricted involvement of low-spin Fe and suboptimal Na-ion diffusion, which is hindered by the existing octahedral tilts. In this study, we decisively enhance the electrochemical performance of PW by optimizing the octahedral tilts through effective Mg doping. The pristine compound $Na_{1.8}Fe[Fe(CN)_6 \cdot 2.75H_2O$ exhibits a reversible capacity of 127 mAh/g, with notable capacity retention of 69% after 250 cycles. On the contrary, our 10% Mg-doped variant, $Na_{1.81}Mg_{0.09}Fe_{0.81}[Fe(CN)_6] \cdot 2.58H_2O$, significantly improves this performance to 138.2 mAh/g and achieves 85% capacity retention over the same cycle count at a C/10 rate. By incorporating Mg into the $Na_{1+x}Fe[Fe(CN)_6]$ framework and replacing Fe atoms, we effectively increase the electron density throughout the Fe-CN-Fe-NC chain, thus weakening the strong CN ligand field. This strategic alteration promotes greater participation of low-spin Fe in the electrochemical reactions. The open framework sodium-rich PBAs undergoes octahedral tilt distortion due to interaction between the A-site alkali metal and cyanide anion; therefore, the symmetry of the PBA changes from cubic to monoclinic. If the distortion is too high, which reduces the A-site pore size and hinders Na-ion diffusion, it can negatively impact the performance of the cathode. Furthermore, Mg doping provides critical structural stability by minimizing distortion and optimizing the octahedral tilt angle, greatly enhancing diffusion kinetics. The perovskite ABX_3 like PBA crystal structure helps us utilize the goldsmith tolerance factor to quantify distortions in PBA cathode materials. The application of distortion engineering can play a critical role in designing high-performance PBA cathodes.

References

[1] A. Tyagi, S. Puravankara, 2025, 202500045, DOI 10.1002/batt.202500045.

[2] J. Cattermull, M. Pasta, A. L. Goodwin, J. Am. Chem. Soc. 2023, 0–4.

#20

Synthesis and Electrochemical Properties of Dehydrated Phase of $Na_2Co[Fe(CN)_6]$ Prussian Blue Analogue

Daisuke Igarashi, [1] Kosei Watanabe,[1] Hitomi Nakazawa,[1] and Shinichi Komaba* [1]

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

E-mail: komaba@rus.tus.ac.jp

Keywords: Na-ion batteries • Prussian blue analogues • Cathode • Phase transition • Dehydration

Abstract:

Prussian blue analogues, $Na_2M[Fe(CN)_6]\cdot nH_2O$ is a promising candidate for the positive electrode material for Na-ion batteries, and their electrochemical properties are known to dramatically change depending on 3d transition metal species, M, and the crystalline water content, n.[1] For the case of M = Co, the electrochemical properties of dehydrated phase, $Na_2Co[Fe(CN)_6]$, has hardly studied, while that of hydrated $Na_2Co[Fe(CN)_6]\cdot 2H_2O$ are well known.[2] In this study, we successfully prepare the dehydrate phase and studied its electrochemical behaviour as a positive electrode material for Na-ion batteries. Although $Na_2Co[Fe(CN)_6]$ contains Co and therefore is not a practical electrode material, we believe that the fundamental research of this material will contribute to understanding the essence of the electrochemistry and practical application of Prussian blue analogues.

$Na_2Co[Fe(CN)_6]\cdot 2H_2O$ was synthesized via precipitation method using $Na_4Fe(CN)_6$ and Co^{2+}–EDTA complex as Na, Fe, and Co sources, respectively. The dehydrated phase, $Na_2Co[Fe(CN)_6]$, was prepared by vacuum drying of the hydrated sample at 160–170 °C. Figure 1 shows the X-ray diffraction (XRD) patterns of $Na_2Co[Fe(CN)_6]\cdot nH_2O$. The pattern of $Na_2Co[Fe(CN)_6]\cdot 2H_2O$ was consistent with that reported in some literatures.[2,3] and the pattern of $Na_2Co[Fe(CN)_6]$ matched that of dehydrated $Na_2Mn[Fe(CN)_6]$ and $Na_2Fe[Fe(CN)_6]$.[1]

Figure 2 shows the charge–discharge curves of $Na_2Co[Fe(CN)_6]\cdot nH_2O$. $Na_2Co[Fe(CN)_6]\cdot 2H_2O$ exhibited the two plateaus at 3.3 V and 3.8 V vs. Na^+/Na corresponding to the $Co^{3+/2+}$ and $Fe^{3+/2+}$ redox, respectively.[2] In contrast, $Na_2Co[Fe(CN)_6]$ exhibited a single plateau at 3.2 V vs. Na^+/Na across all composition ranges from x = 0 to 2, which indicated the absence of intermediate $Na_1Co^{III}[Fe^{II}(CN)_6]$ phase and simultaneous redox of $Co^{3+/2+}$ and $Fe^{3+/2+}$ associated with a direct phase transition from $Na_2Co^{II}[Fe^{II}(CN)_6]$ to $Co^{III}[Fe^{III}(CN)_6]$. Although this electrochemical behaviour of $Na_2Co[Fe(CN)_6]$ is very similar to that of $Na_2Mn[Fe(CN)_6]$ [4] and theoretically predicted by Guo et al.,[5] it was experimentally demonstrated for the first time, to our knowledge, in this study.

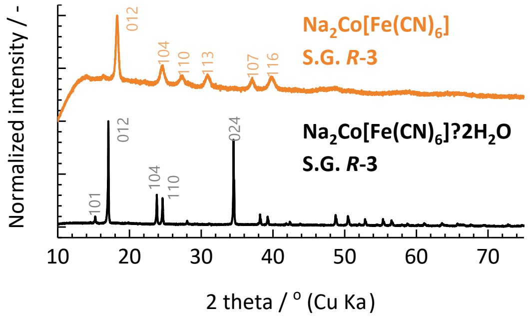


Figure 1. XRD patterns of $Na_2Co[Fe(CN)_6]\cdot nH_2O$

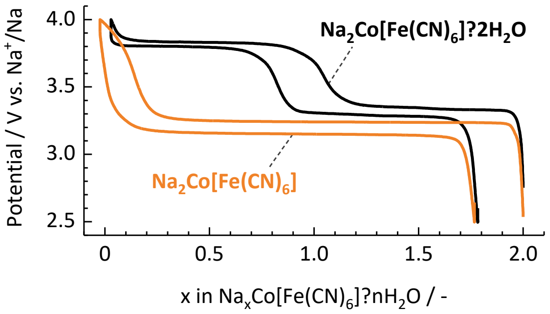


Figure 2. Charge–discharge curves of $Na_2Co[Fe(CN)_6]\cdot nH_2O$

[1] K. Sada et al., *Small*, **20**, 2406853 (2024). [2] X. Wu et al., *ACS Appl. Mater. Interfaces*, **8**, 5393 (2016). [3] J-H. Lee et al., *ACS Nano*, **18**, 1995 (2024). [4] J. Wu et al., *J. Am. Chem. Soc.*, **139**, 18358 (2017). [5] X. Guo et al., *Chem. Mater.*, **31**, 5933 (2019).

Biography:

#21

Operando X-ray Studies of Quaternary Prussian blue Analogs as Cathode Materials for Sodium-Ion Batteries

Hao-Hsiang Chang and Han-Yi Chen*

[1] Department of Materials Science and Engineering, National Tsing Hua University, 101, Sec. 2, Kuang-Fu Road, Hsinchu 300044, TAIWAN

E-mail: hanyi.chen@mx.nthu.edu.tw

Keywords: Sodium-ion batteries, Cathode materials, Prussian blue analogs

Abstract:

Sodium-ion batteries are promising candidates for large-scale energy storage systems due to the abundance and wide distribution of sodium sources. In the composition of sodium-ion batteries, the energy density and retention depend on the properties of the cathode material. Among the current research and commercial development, Prussian blue analogs ($Na_xTM^I[TM^{II}(CN)_6] \cdot y\ H_2O$, TM^I = Mn, Fe, Co, Ni, etc., TM^{II} = Mn, Fe, Co, etc.) have been extensively studied and commercialized owing to the cost-effectiveness of its fabrication process. Besides, its inherent open framework structure contributes to the diffusion pathway of sodium ions, and the composition of transition metals can vary widely, further enhancing its performance. However, in an aqueous synthesis environment, the unavoidable presence of coordinated water and interstitial water can influence the structural stability and storage sites of sodium ions. Additionally, the composition of transition metal elements is also a key factor influencing the performance characteristics of the cathode materials.

In this study, quaternary Prussian blue analogs, $Nax[MnFeNiCo]\ [Fe(CN)_6] \cdot z\ H_2O$, were fabricated by the co-precipitation method as a cathode material for Na-ion batteries. The material characteristics were confirmed by X-ray diffraction, field-emission scanning electron microscope, and energy dispersive spectroscopy. Operando synchrotron X-ray analyses were utilized to investigate the material. By extended X-ray absorption fine structure analysis, we confirmed that the positions of the doped elements within the structure align with our design intentions. The valence change and structure transformation during the charging/discharging process were investigated by X-ray absorption near-edge structures. The electrochemical properties were measured by galvanostatic charge-discharge, cyclic voltammetry, and rate performance testing. The results confirmed that the coexistence of these four metals can balance both capacity and stability, providing Prussian blue analogs a way to enhance the electrochemical performance.

Biography:

Hao-Hsiang Chang is currently a Ph.D. student in the Department of Materials Science and Engineering at National Tsing Hua University, Taiwan. His research focuses on cathode materials for sodium-ion batteries, with expertise in material characterization, electrochemical analysis, and in-situ synchrotron techniques for battery studying reaction mechanisms.

#22

Ion Exchange Synthesis of $Na_2Co[Fe(CN)_6]$ for Sodium-Ion Batteries

Kosei Watanabe, [1] Tomooki Hosaka, [1] and Shinichi Komaba* [1]
[1] Tokyo University of Sience, 1-3 Kagurazaka, Shinjukuku, Tokyo 162-8601, Japan
E-mail: Komaba@rs.tus.ac.jp

Keywords: Cathode • Prussian bule analogues • Ion exachange • Vacancy • High capacity

Abstract:

Prussian blue analogues (PBAs, $A_xM1[M2(CN)_6]_y \cdot nH_2O$, A : alkali metal, M1, M2 : transition metal, $x \leq 2$, $y \leq 1$) are promising cathode materials for sodium-ion batteries (SIBs). In order to improve electrochemical performance, $[Fe(CN)_6]^{4-}$ anion vacancy needs to be reduced. K-PBAs tend to have a smaller number of the anion vacancies than Na-PBAs.[1] Thus, synthesis of Na-PBAs from K-PBAs by ion exchange would reduce the number of anion vacancies. In this study, we synthesized $Na_xCo[Fe(CN)_6]_y$ (NaCoHCF), which shows high energy density [2], by ion exchange synthesis.

Ion exchange sample (IE-NaCoHCF) was synthesized through K/Na ion exchange from $K_xCo[Fe(CN)_6]$ (KCoHCF). First, KCoHCF was synthesized by the precipitation method.[1] After centrifuged and vacuum dried at 60 °C, the sample was placed into a saturated NaCl solution and stirred for 24 h. Finally, IE-NaCoHCF was centrifuged and vacuum dried at 60 °C overnight. The directly synthesized sample (NaCoHCF) was also synthesized by the same method as KCoHCF.

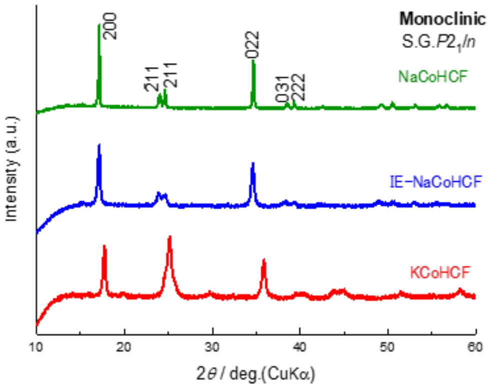


Fig.1 XRD patterns of NaCoHCF, IE-NaCoHCF and KCoHCF.

Fig. 1 shows X-ray diffraction patterns of synthesized samples. Both IE-NaCoHCF and NaCoHCF had the monoclinic structure with a space group of $P2_1/n$. From inductively coupled plasma-atmic emission spectrometry, the compositions of NaCoHCF and IE-NaCoHCF were estimated to be $Na_{1.54}Co[Fe(CN)_6]_{0.89}$ and $Na_{1.85}K_{0.03}Co[Fe(CN)_6]_{0.97}$, respectively, showing that K/Na ion exchange synthesis successfully reduces the number of anion vacancies.

The IE-NaCoHCF showed higher discharge capacity (145 mAh g^{-1}) than NaCoHCF (138 mAh g^{-1}), as shown in Fig. 2. In detail, IE-NaCoHCF exhibited larger capacity in the higher voltage plateau, which corresponds to the Fe^{2+}/Fe^{3+} redox reaction, because of the less $[Fe(CN)_6]^{4-}$ anion vacancies. In the presentation, rate capbility of NaCoHCF and IE-NaCoHCF will also be discussed.

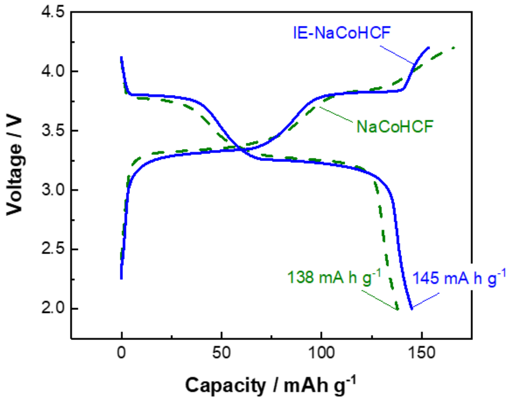


Fig.2 Charge/discharge curves of NaCoHCF and IE-NaCoHCF in Na cells.

Reference

1. T. Hosaka, S. Komaba *et al.*, ChemSusChem, **14**, 1173 (2021).
2. X. Wu, H. Yang *et al.*, *ACS Appl. Mater. Interfaces*, **8**, 5396 (2021).

Biography:

#23

Structural evolution of Prussian White powder for sodium-ion cathodes depending on air exposure and transition metals nature

Léna PINEAU1, David PERALTA1, Irina PROFATILOVA1, Quentin JACQUET2, Jakub DRNEC3, Valentin VINCI3, Loïc SIMONIN1

1Université Grenoble Alpes, CEA, LITEN, 17 Avenue des Martyrs, Cedex 9, Grenoble 38054, France E-mail: lena.pineau@cea.fr

2Université Grenoble Alpes, CEA, IRIG, 17 Avenue des Martyrs, Cedex 9, Grenoble 38054, France

3ESRF, ID31, 71 Avenue des Martyrs, 38000 Grenoble, France

Keywords: Prussian White • Sodium-ion • Hydration •

Abstract

Manganese-based Prussian Whites (PW) Na2Mn[Fe(CN)6] for sodium-ion batteries are developed nowadays as electrode materials thanks to their many advantages.[1] PW show an interest in order to overcome the utilisation of critical material. Furthermore, the PW diversity of composition depending on synthesis conditions, their intercalation properties and electrochemical performances make them promising candidates as a positive electrode material.[2] However, structure transformations are observed depending on the water amount and the nature of transition metals inside the lattice. Several studies have already demonstrated structural evolution in PW material. A sample dehydrated by heat treatement exhibits a different structure from a hydrated sample after synthesis, and the amount of water may affect electrochemical performances.[3], [4] Transition metals nature can also lead to material structure distortions (doped material). In this study, we report Na2-xMn1-yTMy[Fe(CN)6] compounds (TM represents a metal transition such as Zn, Ni,…) synthesized with a co-precipitation method. The Manganese-based PW Na2-xMn[Fe(CN)6] (y=1) presents a rhombohedral structure (R3) after a drying process at 180°C under strong vacuum. Its structure transforms after almost 30 minutes to a disordered monoclinic structure (P21/n) during air exposure (XRD and FT-IR). Since these structure observations were demonstrated in a recent report, the absorption of the water was followed through synchrotron experiment on a PW Na2-xMn[Fe(CN)6] under controlled humidified atmosphere. The results exihibits structural distortions, with a expansion of the volume cell, which would be explained by a lower amount of water. Indeed, TGA analyses showed that the sample capture a lower amount of water when it undergoes several dehydration and rehydration cycles. The dehydrated manganese-based compound PW demonstrates a first discharge capacity of 145 mAh/g obtained at a C/10 rate in a voltage range of 2.5 - 4 V, corresponding to 84% of the theoretical capacity (172 mAh/g). Doped compounds were synthesized in order to minimize structural degradations during the cycling process, and thus improve the cycling performances.[5], [6] Several transition metal dopants were used, such as Zn, Ni, etc. These dopants lead to different morphologies with a modification of cell parameters and electrochemical performances.

References:

[1] C. D. Wessells, Chapter 7 in *Les batteries Na-ion*, ISTE editions., p. 297-347 (2021)
[2] J. Song *et al.*, *J. Am. Chem. Soc.*, vol. 137, p. 2658-2664, doi: 10.1021/ja512383b (2015)
[3] L. Hartmann *et al.*, *J. Electrochem. Soc.*, vol. 170, p. 030540, doi: 10.1149/1945-7111/acc6f5 (2023)
[4] A. Clavelin *et al.*, *ACS Materials Lett.*, vol. 6, p. 5208-5214, doi: 10.1021/acsmaterialslett.4c01833 (2024)
[5] M. Wang *et al.*, *Electrochimica Acta*, vol. 462, p. 142711, doi: 10.1016/j.electacta.2023.142711 (2023)
[6] J. Peng *et al.*, *ACS Nano*, vol. 18, p. 19854-19864, doi: 10.1021/acsnano.4c07021 (2024)

Biography:

Léna is a second year PhD student in battery materials field at CEA Grenoble (38). She studies the effect of water on crystal structure and the reversibility of phase changes (drying and rehydration cycles), and tries to understand relationships between structures and electrochemistry as a function of structural water quantity and the nature of transition metals.

After a Preparation entry into the French Graduate School system, she joined the Engineering school ENSCBP in Bordeaux (France). She attended « Chemistry – Physical engineering » courses and she made a third year specialisation on Energy storage and conversion. She completed two internships at SAFT company (France) on zinc-ion batteries and at University of Turku (Finland) on redox-flow batteries, where she could improve her english skills. She learned to synthesize and shape active material, produce electrodes, and carry out physicochemical (SEM, XRD…) and electrochemical characterizations (performance measurements). She improved her technical skills by assembly redox flow batteries, and realize electrochemical characterizations (OCV, CV, performances measurements…).

#24

Controlling Crystallization of Prussian Blue Analogues for Sodium Ion Battery Cathode Materials

Rino Ichikawa, Yuta Igarashi, Kosuke Kawai, Atsushi Okazawa, Masashi Okubo*

Okubo 3-4-1, Shinjuku-ku, Tokyo 169-8555, Japan

E-mail: m-okubo@waseda.jp

Keywords: Prussian blue analogues• crystallization • cathode materials • full cell

Abstract:

Prussian blue analogues (PBA: $Na_2M_N[M_C(CN)_6]\cdot nH_2O$) is one of the cathode materials for sodium ion battery, which is synthesized in aqueous process. Defects and sodium contents in crystal structure, and morphology of PBA vary largely depending on synthetic conditions, and their structural factors influence the electrode performance. Chelation to metal ions in reaction solution is an effective approach to control the crystal growth of PBA.[1,2]

In the present study, PBA $Na_xMn[Fe(CN)_6]_y\cdot nH_2O$ was synthesized with changing sodium concentration and chelating ligands in reaction solution to examine the chelating effects on the crystallization. The structure and chemical composition of PBAs were analyzed using X-ray diffraction and inductively coupled plasma measurements. Scanning electron microscopy was used for morphological observation. The particle size and contents of sodium ions in the crystal structure varies depending on the synthesis conditions.

For the evaluation of electrode performance, synthesized PBA materials ware coated with conductive carbon and poly(vinylidene fluoride) binder on an aluminium foil. Galvanostatic charge/discharge measurements of half cells with sodium metal as a counter electrode and 1M $NaPF_6$ in EC-DEC (1:1 v/v) electrolyte were conducted to evaluate electrode performance of PBAs, especially delivering discharge capacities. Effects of particle size were observed and PBAs with mean particle size > 1 µm deliver a capacity of > 130 mAh/g. The electrode performance of synthesized PBA was evaluated using coin full cell with a commercial hard carbon anode (Fig.1). The assembled coin full cell stably operates with an areal cathode capacity of > 1.5 mAh/cm^2 with an average discharge voltage of 3.16 V at 0.067C.

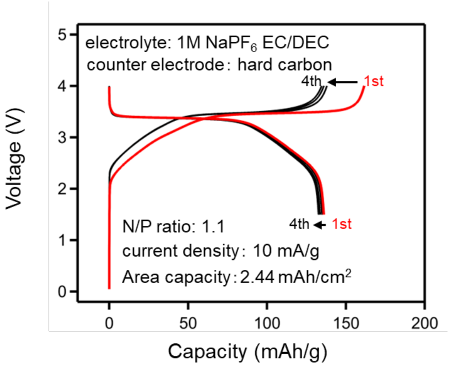


Fig. 1 Galvanostatic charge–discharge curves of a coin full cell using a PBA cathode. Capacity and current density are based on the weight of PBA.

References:

[1] F. Peng *et al.*, *J. Mater. Chem. A*, 2019, **7**, 22248–22256.
[2] Z. Shen *et al.*, *ACS Sustainable Chem. Eng.*, 2018, **6**, 16121–16129.

Biography:

Rino Ichikawa is a first-year PhD student working on the development of materials related to sodium-ion batteries in the School of Advanced Science and Engineering at Waseda University.

#25

Effect of Dehydration of $Na_2Cu[Fe(CN)_6]$ on Its Electrochemical Properties in Na Cell

Hitomi Nakazawa, [1] Daisuke Igarashi,[1] Satoshi Yasuno,[2] and Shinichi Komaba*[1]

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

E-mail: Komaba@rs.tus.ac.jp

[2]Japan Synchrotron Radiation Research Institute (JASRI), Hyogo 679-5198, Japan

Keywords: Na-ion batteries • Cathode • Prussian blue analogues • Dehydration • Phase transition

Abstract:

In this study, we focused on a Prussian blue analogue (PBA), $Na_2Cu[Fe(CN)_6]\cdot nH_2O$ (CuHCF), as a cathode material for Na-ion batteries. Although the structure and electrochemical property of PBAs was significantly changed by the presence of crystalline water, the dehydrated phase of CuHCF has not been studied unlike other PBAs such as $Na_2Mn[Fe(CN)_6]$ and $Na_2Fe[Fe(CN)_6]$.[1,2] Herein, we synthesized the dehydrated CuHCF (CuHCF-dehyd) and compared its structural and electrochemical properties with those of the hydrated CuHCF (CuHCF-hyd) to clarify the effect of crystalline water.

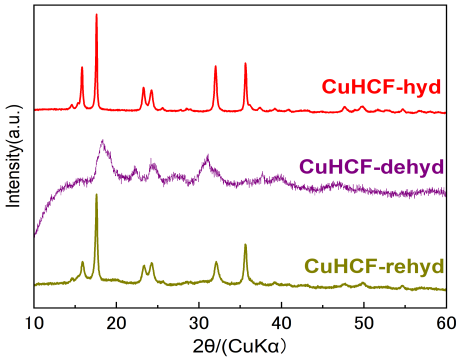


Fig. 1 XRD patterns of CuHCF-hyd, CuHCF-dehyd, and CuHCF-rehyd.

CuHCF-hyd were synthesized via precipitation method.[3] CuHCF-dehyd was obtained by vacuum drying CuHCF-hyd at 100 °C. To investigate the reversibility of dehydration, the re-hydrated sample (CuHCF-rehyd) was prepared by exposing CuHCF-dehyd to air for one day.

Fig. 1 shows the X-ray diffraction (XRD) patterns of CuHCF-hyd, CuHCF-dehyd, and CuHCF-rehyd. The main diffraction peaks of CuHCF-hyd were consistent with previous reports.[4] The pattern of CuHCF-dehyd exhibited small diffraction intensities and significant peak broadening. Rehydration of CuHCF-dehyd restored the original hydrated structure, indicating reversible dehydration behavior. The retention of CN groups and absence of H_2O after dehydration was confirmed by infrared spectroscopy, suggesting that the PBA framework remained intact despite structural changes.

Fig. 2 shows the initial charge–discharge curves of CuHCF-hyd and CuHCF-dehyd. The reversible capacity of CuHCF-hyd was 80 mAh g^{-1}, in good agreement with the $Fe^{3+/2+}$-based theoretical capacity of 75 mAh g^{-1}. In contrast, CuHCF-dehyd exhibited a reversible capacity of 107 mAh g^{-1}, beyond the $Fe^{3+/2+}$-based theoretical limit (83 mAh g^{-1}). These results suggest that crystalline water may activate the additional redox acitivity of Cu. In the presentation, the oxidation state changes of both Cu and Fe will also be discussed based on spectroscopic analyses.

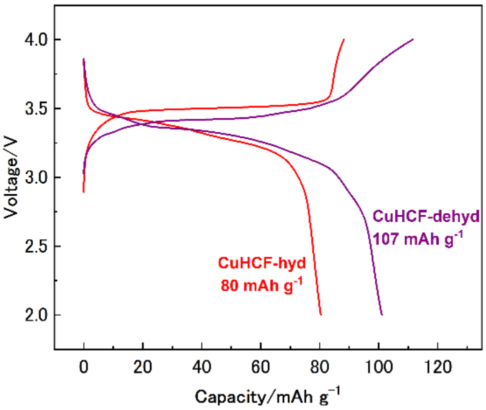


Fig. 2 First charge-discharge curves of CuHCF-hyd and CuHCF-dehyd.

Reference:

[1] J. Song, J. B. Goodenough, et al., *J. Am. Chem. Soc.*, **137**, 2659 (2015). [2] L. Wang, Y. Lu et al., *J. Am. Chem. Soc.*, **137**, 2548 (2015). [3] T. Hosaka, S. Komaba et al., *ChemSusChem*, **14**, 1166 (2021). [4] Y. Xu, J. Han et al., *Energy Storage Mater.,* **33**, 435 (2020).

Biography:

Hitomi NAKAZAWA is a first-year master's student in the Department of Applied Chemistry at the Tokyo University of Science, Japan. She is currently conducting research on cathode materials for sodium-ion batteries.

#26

Manipulation of Electrochemically (In)Active Elements Enhancing the Longevity of NASICON-type Cathodes for Sodium-Ion Batteries

Vaiyapuri Soundharrajan,*[1] Jung Ho Kim,[2] Chunjoong Kim*[1]

[1] Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea.

E-mail: soundharrajan@o.cnu.ac.kr, ckim0218@cnu.ac.kr

[2] Institute for Superconducting and Electronic Materials (ISEM), Faculty of Engineering and Information Sciences, University of Wollongong, North Wollongong, New South Wales, 2500 Australia.

Keywords: keyword 1 • keyword 2 • keyword 3 • keyword 4 • keyword 5

Abstract:

The practical deployment of sodium superionic conductor (NASICON)-type $Na_3V_2(PO_4)_3$ (NVP) cathode in sodium-ion batteries (SIBs) is hindered by toxicity and high cost of vanadium, despite NVP's excellent structural stability and sodium storage capability. To address, this we employed a materials engineering strategy to reduce vanadium content by partially substituting it with earth abundant, non-toxic elements particularly magnesium and titanium. This approach led to design of two new NASICON-structured compounds: $Na_3VMg_{0.5}Ti_{0.5}(PO_4)_3$ ($N_{3.0}$VMTP) and $Na_{3.5}V_{0.5}MgTi_{0.5}(PO_4)_3$ ($N_{3.5}$VMTP). The $N_{3.0}$VMTP and $N_{3.5}$VMTP materials have been synthesized using polyol-based solution-combustion technique in which the polyol forms the in situ carbon coating which is favourable for the electronic conductivity. The carbon coated cathode $N_{3.0}$VMTP/C and $N_{3.5}$VMTP/C exhibited stable soidum storage performance over 500 charge/discharge cycles at 150 mAg^{-1} with high capacity retention. In situ XRD analysis validated that NASICON cathodes will undergo the sequential SS (lower voltage range) and T-P (higher voltage range) reactions during (de)sodiation with only minor differences in the degree of lattice interface displacement, which accounts for the superior electrochemical performance.

Biography:

Vaiyapuri Soundharrajan is a postdoctoral research fellow in the professor Chunjoong Kim group in Department of Materials Science and Engineering, Chungnam National University, South Korea. He received his B.Tech. degree (2013) from Central Electrochemical Research Institute (CECRI), India. He completed his integrated (M.S.-Ph.D) program in 2021 under the supervision of Professor Jaekook Kim's group at the Department of Materials Science and Engineering, Chonnam National University. His research focuses on the design of electrode materials for Sodium, Zinc, Manganese, and Lithium-based batteries.

#27

Preparation of Structurally Optimized $NaFePO_4$

Jinkwang Hwang*, Fumiyasu Noazaki, Shaoning Zhang, Keita Yamasaki, Kazuhiko Matsumoto

Graduate School of Energy Science, Kyoto University, Yoshida, Sakyo-ku, Kyoto 606-8501, Japan

E-mail: hwang.jinkwang.5c@kyoto-u.ac.jp

Keywords: sodium ion battery • electrolyte additive • oxalate

Abstract:

Sodium-ion batteries offer significant promise as next-generation energy storage systems, particularly when leveraging abundant and low-cost raw materials. Among various positive electrode candidates, triphylite $NaFePO_4$ (olivine-type) stands out for its excellent structural stability, high theoretical capacity (155 mAh g^{-1}), and lack of rare metal dependency [1,2]. However, its practical application is hindered by thermal metastability during synthesis and suboptimal electrochemical performance [3].

To address these limitations, we design a closed-loop process. We introduce a sustainable, oxygen-powered synthesis method for heterosite $FePO_4$, which is the fully delithiated form of $LiFePO_4$. Here, oxygen acts as the oxidizing agent, and lithium is recovered in the form of lithium acetate, enabling cost-effective regeneration of $LiFePO_4$ from recycled lithium [4]. This circular approach not only mitigates raw material cost but also aligns with sustainable battery production goals. Moreover, we explore the substitution of iron with manganese in the $NaFePO_4$ lattice. Our investigation demonstrates that appropriate levels of manganese substitution significantly enhance the intrinsic kinetic properties of materials. Furthermore, we propose a novel charged-state metal battery configuration designed to improve cyclability in metal-free systems while maintaining high energy output.

References

[1] S.-M. Oh, S.-T. Myung, J. Hassoun, B. Scrosati and Y.-K. Sun, *Electrochem. Comm.*, 2012, **22**, 149.
[2] W. Tang, X. Song, Y. Du, C. Peng, M. Lin, S. Xi, B. Tian, J. Zheng, Y. Wu, F. Pan and K. P. Loh, *J. Mater. Chem. A*, 2016, **4**, 4882.
[3] M. Avdeev, Z. Mohamed, C. D. Ling, J. Lu, M. Tamaru, A. Yamada and P. Barpanda, *Inorg. Chem.*, 2013, **52**, 8685.
[4] F. Nozaki, S. Zhang, M. H. Petersen, J. Hwang, J. H. Chang, J. M. G.-Lastra, K. Matsumoto, *Energy Envron. Sci.,* 2025, **18**, 1408.

Biography:

Jinkwang Hwang received his Master's and Ph.D. degrees in Energy Science from Kyoto University. He was awarded a research fellowship for young scientists by the Japan Society for the Promotion of Science (JSPS). In 2020, he was appointed Assistant Professor at the Graduate School of Energy Science at Kyoto University. His current research interests focus on developing new electrode materials and electrolytes for Li and Na secondary batteries, as well as investigating their electrochemical and physical properties

Generation of Tripylite-$NaFePO_4$ Cathodes for Na-ion batteries

#28

Ramtin Hessam*[1], Matthew Boot-Handford[2], Montserrat Galcerán[3], Maria Forsyth[1], Patrick C Howlett[1], Youssof Shekibi[1], and Robert Kerr[1]

[1] Institute for Frontier Materials (IFM), Deakin University, Burwood, Victoria 3125, Australia.

[2] Calix Limited, 71 Rowsley Road, Maddingley, Victoria 3340, Australia

[3] Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Alava Technology Park, Albert Einstein 48, 01510, Vitoria-Gasteiz, Spain

r.hessam@deakin.edu.au

Keywords: Tripylite-$NaFePO_4$, $LiFePO_4$, Polyanion materials, Sodium-ion batteries

Abstract:

In response to the growing demand for energy storage in vehicles and renewable energy systems, the production of Li-ion batteries has increased due to their impressive energy density, durability, and fast-charging capability. Unfortunately, this growth in battery production will lead to the accumulation of large volumes of spent batteries, which pose a serious environmental concern. Recycling Li-ion batteries is proposed as an effective solution to address these environmental issues and recover critical elements such as Li, Co, and Ni. This work has investigated the effect of sodium persulfate and acetic acid as oxidizing agents on the delithiation of $LiFePO_4$ cathode material, followed by the sodiation of the resulting powder using two different sodiating agents: sodium thiosulfate and sodium iodide. The results have shown that there is no significant difference in the delithiation efficiency between sodium persulfate and acetic acid; however, the latter results in greater iron removal from $LiFePO_4$. Furthermore, the insertion of sodium into the delithiated sample using sodium thiosulfate and sodium iodide was examined. Elemental analysis revealed that more sodium (12%) was inserted using sodium iodide compared to sodium thiosulfate (4.5%). Electrochemical testing showed that $LiFePO_4$, with a capacity of 155 mAh/g (93% of its theoretical capacity of 167 mAh/g), was successfully transformed into an $NaFePO_4$ cathode with a capacity of 127 mAh/g (82% of its theoretical capacity of 154 mAh/g), demonstrating the effectiveness of the proposed method for repurposing spent $LiFePO_4$ cathodes.

Biography:

I began my academic journey in materials science with a master's degree from Shiraz University, Iran, where my research focused on the preparation and characterization of photoanode materials for photoelectrochemical water-splitting cells. Following my graduation, I continued working in the field of energy storage, contributing to research on the synthesis and characterization of anodes for lithium-ion batteries.

Driven by a strong interest in clean energy production and storage technologies, I commenced my PhD at Deakin University in 2023. My current research focuses on the investigation of advanced cathode materials for sodium-ion batteries. I am conducting this work under the supervision of A/Prof. Robert Kerr, Prof. Maria Forsyth, A/Prof. Youssof Shekibi at Deakin University, in collaboration with Dr. Matt Boot-Handford from Calix Limited as industry partner.

#29

Exploration of High-Energy Sodium Iron Oxide Cathode Using Multi-Electron Redox

Ayano Kuroda, Akira Nasu, Masaki Matsui, and Hiroaki Kobayashi*

Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan

E-mail: h.kobayashi@sci.hokudai.ac.jp

Keywords: sodium-ion batteries • Na-rich cathode materials •Multi electron redox • Na_5FeO_4 • Iron-based cathodes

Abstract:

Lithium-ion batteries, widely used today, face increasing risks related to high costs and unstable supply chains due to the limited availability and geographically concentrated distribution of key elements such as lithium and cobalt. As an alternative, sodium-ion batteries (SIBs) are gaining attention for their resource advantage, as sodium is an earth-abundant element. However, due to the heavy atomic weight of sodium compared to lithium, improving energy density remains a major challenge. To address this issue, sodium-rich transition metal oxides capable of multi-electron redox reactions have emerged as promising candidates. In this study, we focused on iron as an earth-abundant and cost-effective transition metal element, and synthesized three stable phases of sodium-rich iron oxides—Na_3FeO_3, Na_5FeO_4, and $Na_8Fe_2O_7$—via solid-state reaction for comparative electrochemical evaluation.

The sodium-rich iron oxides were prepared by calcination of β-$NaFeO_2$ and Na_2O mixture at the stoichiometric ratios under an argon atmosphere. Cathodes were fabricated by mixing the active material with acetylene black and polytetrafluoroethylene. A two-electrode cell was assembled using Na metal anode and 1M $NaPF_6$ electrolyte.

X-ray diffraction patterns suggest that Na_3FeO_3, Na_5FeO_4, and $Na_8Fe_2O_7$ were successfully synthesized as the stable phase. Among the samples, Na_5FeO_4 exhibited the highest reversible capacity of approximately 230 mAh g^{-1}, corresponding to a two-electron redox process. In contrast, Na_3FeO_3 and $Na_8Fe_2O_7$ showed lower capacities of around 100 mAh g^{-1} and 180 mAh g^{-1}, respectively; these capacities correspond to single-electron reactions, and cycling performances are poor compared to Na_5FeO_4. Fe *K*-edge XAFS measurements suggest the reversible redox reaction of Fe in Na_5FeO_4. These results highlight Na_5FeO_4 as the most promising candidate among the Na-Fe-O ternary system.

Biography:

Ayano Kuroda is a first-year Master's course student at Hokkaido University. She belongs to the inorganic chemistry laboratory. Her research focuses on cathode materials for sodium-ion batteries. Research interest is in increasing the energy density of SIBs using earth-abundant elements.

#30

AN UNEXPLORED LONG CYCLE SODIUM STORING CAPABILITY OF V_4O_9 CATHODE

Chandrasekar M Subramaniyam,[1*] Alois Kuhn,[1] Ester García-González,[2] Ignacio J. Villar-García,[1] Enrique Rodríguez-Castellón,[3] François Fauth,[4] Carlos Escudero,[4] Vlad Martin-Diaconescu,[4] Ajeet K Srivastav,[5] Flaviano García-Alvarado[1]

[1] Department of Chemistry and Biochemistry, Facultad de Farmacia, Universidad San Pablo-CEU, CEU Universities, Boadilla del Monte, 28668 Madrid, Spain.

[2] Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Madrid 28040, Spain.

[3] Departamento de Química Inorgánica, Facultad de Ciencias, Instituto Interuniversitario de Investigación en Biorrefinerías I3B, Universidad de Málaga, 29071 Málaga, Spain.

[4] CELLS-ALBA Synchrotron, Cerdanyola del Vallès 08290, Spain.

[5] Department of Metallurgical and Materials Engineering, Visvesvaraya National Institute of Technology Nagpur, India.

[*]Email: mayandi@ceu.es

Keywords: V_4O_9 Nanoflakes * Solvothermal synthesis * Sodium-ion cathode * *Operando/Ex-situ* synchrotron techniques

Abstract:

In this work, we introduce an unexplored 3D V_4O_9 as a novel sodium storing cathode material capable of delivering a reversible capacity of 127.7 mA h g^{-1} at 250 mA g^{-1} for 5000 cycles and 55.9 mA g^{-1} at the end of 10000 cycles upon cycling between 1.0 – 3.5 V. V_4O_9 nanoflakes exhibit an excellent rate capability at various current densities maintaining a stable capacity of 158.7 mA h g^{-1} at 50 mA g^{-1} at the end of 100 cycles. *Operando* synchrotron powder diffraction and *ex situ* spectroscopic data (x-ray photoelectron spectroscopy, x-ray absorption spectroscopy) indicate that the charge-storage mechanism in V_4O_9 is based on surface redox controlled pseudocapacitive behaviour. The V_4O_9 nanoflakes are synthesized in one-pot using an optimised solvothermal route which has great potential for scale up production. The combination of high capacity/high rate and unprecedented cycling stability make~~s~~ V_4O_9 a great candidate for building cost-effective and sustainable sodium-based high energy density storage devices for off-grid appliances and short-range electric vehicles.

Biography:

My interdisciplinary research includes the synthesis of nanomaterials for electrochemical storage devices, more importantly, for metal-ion battery applications. Li-ion battery is the topic of my PhD dissertation at University of Wollongong, Australia, under the supervision of Prof. HuaKun Liu and Prof. ShiXue Dou and at The University of Texas at Austin under the supervision of Nobel Laureate Prof. John B Goodenough (Co-Inventor of lithium-ion battery). Currently, I´m working as “Investigador Colaborador” at FUSP CEU, after completing a 2 years’ MSCA-IF contract. My research is focused on synthesis and characterization of mixed-anion compounds for building sustainable metal-ion batteries.

#31

Evaluation of the capacity degradation behavior of Na2FeS2 with cation-anion redox

Riki Miyamoto, 1 Akira Nasu*, 1,2 Hiroaki Kobayashi, 1,2 and Masaki Matsui 1,2

1 Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Hokkaido 060-0810, JAPAN

E-mail: nasu@sci.hokudai.ac.jp

2 Faculty of Science, Hokkaido University, Sapporo, Hokkaido 060-0810, JAPAN

E-mail: nasu@sci.hokudai.ac.jp

Keywords: Sulfide material • Cation-anion redox • Sulfur catenation • Sulfur dissolution • Transition metal migration

Abstract:

In positive electrode materials, the activation of anionic redox is expected to provide high capacities. However, anionic redox can cause irreversible structural changes associated with the formation of anionic dimers. Therefore, highly reversible positive electrode materials with anionic redox are required. To suppress dimer formation and improve reversibility, analyzing the electrochemical behavior of materials is necessary. We focused on Na2FeS2 as the model material exhibiting Fe and S redox1). In this material, the effect of S redox on structural changes remains unclear. In this study, we analyzed the structural changes and electronic state changes during charge/discharge reaction in cells with organic electrolyte to reveal the cause of irreversible reactions and improve reversibility.

All of the procedures were conducted in a dry Ar atmosphere. Na2FeS2 was synthesized by a conventional solid-state process. Na2S (Nagao Co., 98%), Fe (Kojundo Chem., 99.9%), and S (Kojundo Chem., 99.99%) were mixed in a stoichiometric ratio, and calcined at 700 °C for 5 hours. A twoelectrode cell was fabricated using synthesized Na2FeS2 for the positive electrode, a Na metal foil for the counter electrode, and a 1 mol L–1 sodium bis(fluorosulfonyl)amide/diglyme electrolyte. The electrodes after charge/discharge were analyzed by powder X-ray diffraction (XRD) measurement and X-ray Absorption Spectroscopy (XAS).

The charge/discharge behavior showed capacity degradation when two electrons contribute to the reaction. XRD patterns after two electrons charging showed irreversible structural changes. Furthermore, S2p XAS spectra showed absorption derived from the π* orbital of sulfur dimer. The formation of sulfur dimer is considered to cause the irreversible structural change and capacity degradation.

References:

1) A. Nasu *et al.*, *Small*, **18** (2022) 2203383.

Biography:

Riki Miyamoto is a graduate student at Hokkaido University, Japan, majoring in inorganic chemistry. His research focuses on sodium secondary batteries, particularly sulfide-based cathode materials. He is interested in the structural and e lectrochemical properties of these materials for next-generation energy storage systems.

#32

Sacrificial Additive Strategies for Na-Deficient Positive Electrodes in Na-Ion Batteries

Changhee Lee,1 Masayoshi Shimizu,1 Ryoichi Tatara,1 Tomooki Hosaka,1 and Shinichi Komaba*1

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

E-mail: komaba@rs.tus.ac.jp

Keywords: P2-Na2/3Ni1/3Mn2/3O2 • Na2CO3 sacrificial salt • aqueous binder • Coulombic efficiency

Abstract:

Sodium-ion batteries have recently gained attention as a promising next-generation secondary battery owing to their low cost and the abundance of sodium resources. Among various cathode candidates, P2-type layered oxides, which exhibit high discharge capacity and operating voltage, are particularly attractive. However, the inherent sodium deficiency in P2-type oxides (Na content ≈ 0.67) necessitates additional sodium compensation when paired with sodium-free anodes for practical full-cell configurations. To address this challenge, pre-sodiation strategies—particularly the incorporation of sacrificial sodium-based additives—have been widely investigated. These additives decompose at high voltage (>3.5 V vs. Na/Na^+), supplying Na^+ ions to compensate for sodium deficiency in full-cell systems. Our recent work demonstrated that the use of Na2CO3 as a sacrificial salt effectively mitigates Na off-stoichiometry, improving the electrochemical performance of P2-Na2/3[Fe1/2Mn1/2]O2 positive electrodes in full-cell configurations with HC negative electrodes.1

Herein, we applied sacrificial electrode additives to uniquely designed systems to maximize their effectiveness and elucidate their decomposition mechanisms in NIBs, systematically evaluating their impact on electrochemical performance across three key systems:

Na2CO3-added P2 (P'2)-Na2/3MnO2 positive electrodes, which exhibit ultrahigh discharge capacity but suffer from Mn dissolution and poor cycle stability.

Water-soluble sacrificial salts combined with aqueous binders for water-stable P2- Na2/3Ni1/3Mn2/3O2 (P2-NiMn) positive electrodes.

Diverse electrolyte environments, including carbonate-based organic solvents, ionic liquids, and highly concentrated electrolytes.

As shown in **Figure 1**, representatively, Na2CO3 incorporation in P2-NiMn positive electrodes significantly enhances initial charge capacity and dis- /charge capacity balance (~1), and increases energy density based on the weight of the active material. These findings highlight the potential of combining water-soluble sacrificial salts with aqueous processing as a viable approach for optimizing Na-deficient positive electrodes in NIBs. We anticipate that these strategies will provide deeper insights into their role in mitigating sodium deficiency and enhancing the long-term stability of full-cell configurations, which can advance the practical adoption of P2-type positive electrodes for NIBs.

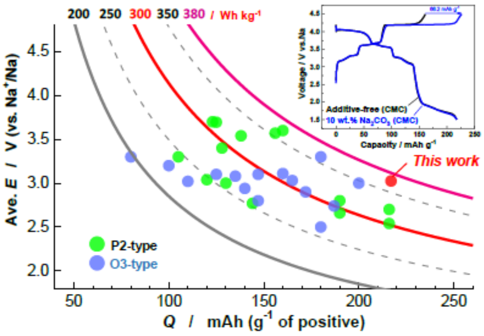


Figure 1 Capacity per weight of positive active materials and their theoretical energy density based on electrode weight (Inset: Initial charge/discharge curves of P2-NiMn positive electrodes with/without Na_2CO_3 sacrificial salt).

Reference:

(1) M. Matsuzaki, R. Tatara, *et.al.*, and S. Komaba, *Batter. Supercaps* **7**, e202400009 (2024).

(2) C. Lee, M. Shimizu, *et al.*, and S. Komaba, *ACS Appl. Energy Mater.* **8**, 5867 (2025).

Biography:

Changhee Lee is an Assistant Professor at the Tokyo University of Science. He received a Ph.D. degree in Engineering with honors from Kyoto University, Japan, in 2021, supported by a government-funded (MEXT) scholarship. Following his doctoral studies, he served as an Assistant Professor at Kyoto University and as an Adjunct Professor at Sungkyunkwan University (SKKU). His research focuses on next-generation rechargeable battery systems, particularly with a focus on the electrode/electrolyte interfacial reactions in Li, Na, K, and F-ion batteries.

#33

High-Yield Synthesis of Lignin-Derived Hard Carbons for Sodium-Ion Batteries

Aoto Koizumi,[1] Yuki Fujii,[1] Changhee Lee,[1] Zachary T. Gossage,[1] and Shinichi Komaba*[1]

[1] Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan

E-mail: komaba@rs.tus.ac.jp

Keywords: Negative electrode • Hard carbon • Lignin • High initial coulombic efficiency • High-rate

Abstract:

Hard carbon (HC) is a promising negative electrode material for sodium-ion batteries. To improve the cost performance and production efficiency, researchers are exploring optimized synthesis conditions for HC using biomass-derived raw materials.[1] In our previous study, HC synthesized via carbonization of lignin showed high yields with a notable impact of the pre-heating temperature on the pore structure and sodiation potential (i.e. the plateau potential).[2] However, the initial coulombic efficiency (ICE) of approximately 80% was relatively low among other HC materials. In this study, we synthesized HC samples combining careful adjustment of the synthesis temperature with the use of a graphite crucible. Finally, a higher ICE, over 90 %, and a superior rate-capability were achieved in the Na-cell. To prepare HC, commercial reagent-grade lignin (Kanto Chemical Co.) was first pre-heated at 250 or 600 °C for 10 hours under an Ar atmosphere. The pre-heated lignin samples were sequentially sonicated in hydrochloric acid and deionized water. The dried powders were then heated at 1400 °C for 1 hour under an Ar atmosphere. Either a graphite crucible or alumina boat were used as the synthesis container. The samples are labelled based on the synthesis container, "G" or "A", and temperature, e.g., "250G−1400G" was synthesized in a graphite crucible using 250 °C and 1400 °C for pre- and post-heating, respectively. **Figure 1** shows galvanostatic charge-discharge curves of HCs in the initial cycle. All HCs show slope (> 0.15 V) and plateau (< 0.15 V) capacities attributed to Na adsorption/intercalation in interlayers and filling of nanopores, respectively. 250G−1400G HC delivered the best performance showing 343 mAh g^{-1} and a high ICE of 91.8 %. Furthermore, dQ/dV curves of the second cycle, as shown in **Figure 2** enlarging the plateau region, indicate the cathodic-peak potential was shifted up to ~70 mV, similar to Li intercalation into graphite. We will discuss about the improved mechanism through detailed characterizations including pore structure and elemental analysis.

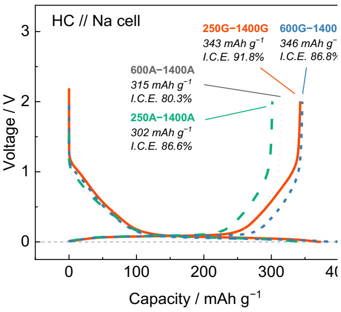


Figure 1. Galvanostatic charge-discharge curves of lignin-derived HCs in Na-cell.

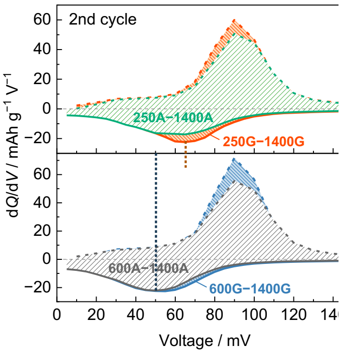


Figure 2. dQ/dV curves of (de)sodiation process of HC electrodes in 2nd cycle.

References

1. C. Vaalma, S. Passerini et al., *Nat. Rev. Mater.*, **3**, 18013 (2018).
2. Y. Fujii, A. Koizumi, S. Komaba et al., *ACS Appl. Energy Mater.*, **8**, 6577 (2025).

Acknowledgement

This study was partially supported by JST-GteX, grant No. JPMJGX23S4.

Biography:

Aoto Koizumi is a first-year master's student in the Department of Applied Chemistry at the Tokyo University of Science, Japan. He is currently conducting research on anode materials for sodium-ion batteries.

#34

“Post-treatments on carbon xerogels to improve their performance as negative electrodes of Na-ion batteries”

Berke Karaman*[1], Hélène Tonnoir[1,2], Da Huo[2], Jimena Castro Gutiérrez[3], Bryan Carré[1], Alexandre F. Léonard[4], Marion Bermont[2], Zoé Deckers[1], Alain Celzard[3,5], Vanessa Fierro[3], Carine Davoisne[2], Raphaël Janot[2], Nathalie Job[1]

[1]Department of Chemical Engineering - NCE (Nanomaterials, Catalysis, Electrochemistry), University of Liège, 4000 Liège, Belgium

[2]Laboratoire de Réactivité et Chimie des Solides - LRCS, UMR7314 CNRS, Université de Picardie Jules Verne, Amiens, France

[3]Université de Lorraine, CNRS, Institut Jean Lamour - IJL, 88000 Épinal, France

[4]Department of Chemical Engineering - CARPOR, University of Liège, 4000 Liège, Belgium

[5]Institut Universitaire de France - IUF, 75231 Paris, France

(Corresponding author :berke.karaman@uliege.be)

Keywords: Na-ion battery, carbon xerogels, CVD coating

Abstract:

Energy storage using batteries plays a key role for a more sustainable future. However, the demand increase requires better concepts in terms of critical material use and manufacturing processes. Those new concepts should help solving issues of material availability (in particular Li) and of toxic or difficult-to-recycle materials use in electrode manufacturing (e.g. NMP as solvent and PVDF as binder). This published [1] study focuses on developing carbon materials for negative electrodes of Na-ion batteries; electrodes are further manufactured from carbon powders with a water-based process using a biosourced binder, xanthan gum.

A series of nanostructured hard carbons (carbon xerogels - CXs) were synthesized by pyrolysis of phenolic resins at 800°C [1]. Those hard carbons are made of interconnected microporous nodules of various sizes (i.e. 50 nm, 1 µm, 1.3 µm and 2 µm). As such, it is foreseen that they cannot perform properly as Na-ion insertion materials due to their high specific surface area (> 600 m^2/g for all samples), leading to high irreversibility at the first electrochemical cycle. In order to overcome those shortcomings, a few methods to improve carbon xerogels have been discussed [3]. Chemical vapor deposition of carbon is one of those methods that allows blocking the micropores, which leads to reducing the surface area accessible to the electrolyte [3], and thus could improve the Initial Coulombic Efficiency (ICE). Therefore, the selected CXs were coated by a secondary carbon layer by cracking of ethylene at 675°C.

Firstly, the effect of the CX nodule size to performance of the electrodes has been observed and it has been concluded that, with increasing the nodule size, both the capacity and ICE increase. While ICE could be as low as 29% for the 50 nm nodule size CX, it can go up to 80% ICE for the 2 µm nodule sized CX. Changes in ICE is a result of SEI formation on the surface of the electrode: in literature, that phenomenon is generally correlated with the BET surface area (i.e. measured under gas phase) of the material. However, in this study it was concluded that ICE is highly related with the area accessible to the electrolyte since all four powders had almost the same BET surface areas but different ICE values. Additionally, around 250 mAh/g reversible capacity with 80% ICE could be obtained with the CX with 2 µm nodules: to our knowledge, this is the highest value obtained at such a low pyrolysis temperature.

Secondly, the effect of the CVD coating has been studied. The secondary carbon layer has a very significant impact on the pore texture. The BET surface area of the powders drops from ~600 m^2/g to 131 m^2/g for the CX with the smallest nodule size (50 nm) and to 2 m^2/g for the CX with the largest nodule size (2 µm). In the meantime, the performance of the corresponding electrodes also changes massively as both capacity and ICE improve. The capacity goes up to 300 mAh/g and 84% ICE in the case of 2 µm CVD coated sample.

Reference:

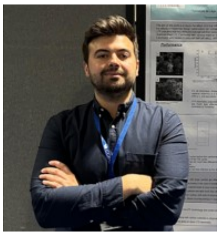
[1] B. Karaman, H. Tonnoir, D. Huo, B. Carré, A.F. Léonard, J.C. Gutiérrez, M.L. Piedboeuf, A. Celzard, V. Fierro, C. Davoisne, R. Janot, N. Job, CVD-coated carbon xerogels for negative electrodes of Na-ion batteries, Carbon 2024, 225, 119077. (doi:10.1016/j.carbon.2024.119077)

[2] N. Job, R. Pirard, J. Marien, and J. P. Pirard, Porous carbon xerogels with texture tailored by pH control during sol-gel process. Carbon 42 (2004) 619–628, (doi: 10.1016/j.carbon.2003.12.072.)

[3] C. del Mar Saavedra Rios, A. Beda, L. Simonin, and C. M. Ghimbeu, Hard Carbon for Na-ion Batteries: From Synthesis to Performance and Storage Mechanism, in Na-ion Batteries (2021), L. Monconduit and L. Croguennec (Eds.), Wiley, ISBN: 9781789450132, pp. 101-146. (doi: 10.1002/9781119818069.ch3).

[4] M. L. C. Piedboeuf, A. F. Léonard, F. L. Deschamps, and N. Job, Carbon xerogels as model materials: toward a relationship between pore texture and electrochemical behavior as anodes for lithium-ion batteries. J Mater Sci 51 (2016) 4358–4370 (doi: 10.1007/s10853-016-9748-3).

Biography:



Berke Karaman completed his PhD in 2024 in University of Liége, on the subject of low environmental impact battery materials. During the thesis, he worked extensively on carbon materials for Na-ion batteries and obtained encouraging results that are published in CARBON. Now he continues as a post-doc in the same department trying to move the encouraging results even further.

#35

DFT-MD study on Na cluster formation process and fast Na-ion diffusion in hard carbon pores

Che-an Lin[1*], Huu Duc Luong[1], Yoshitaka Tateyama[1*]

[1] Laboratory for Chemistry and Life Science, Institute of Integrated Research, Institute of Science Tokyo, R1-25, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8501, Japan

E-mail: lin.c.ag@m.titech.ac.jp (C. -a. L.) tateyama@cls.iir.isct.ac.jp (Y. T.)

Keywords: DFT-MD • hard carbon pore • Na cluster • Na-ion diffusion

Abstract:

Na-ion batteries (NIBs) have been a promising alternative for Li-ion batteries (LIBs) with a similar working principle, a lower cost, and more abundant raw materials. To achieve commercialization of NIBs, anode materials with low cost and high capacity are essential. While graphite being a suitable commercial anode material for LIBs, it is not compatible with NIBs due to unfavorable Na-ion intercalation. In search of other suitable carbonaceous materials, hard carbon (HC) appears to be a suitable anode material for NIBs because of its low cost, good stability, and high energy density. The galvanostatic charge/discharge curves of a HC anode can be separated into two parts, the slope region (> 0.1 V vs Na/Na^+) and the plateau region (< 0.1 V vs Na/Na^+). Researchers have been trying to pursue high plateau capacity which is not only reversible but also works at low potential. The pore filling by Na cluster formation has been reported to dominate the contribution of plateau capacity in HC anodes.[1,2] However, there is a lack of thorough insight into the process and the mechanism of Na cluster formation in pores. Furthermore, how Na ions diffuse and the influence of defects and graphene distortion on the diffusion in pores are also unclear.

In this work, density-functional-theory (DFT) based first-principles molecular dynamics (DFT-MD) simulations were carried out to analyze Na cluster formation and Na-ion diffusion in HC pores. The results show that pore filling in HC begins with Na-ion adsorption at the defect sites. Then, the defect-adsorbed Na ions were found to repel with other Na ions at the early stage of pore filling, and the gathering of the repelled Na ions is the beginning of quasi-metallic Na cluster formation. Instead of acting as nucleation sites for Na cluster formation, the defect-adsorbed Na ions are included into the quasi-metallic Na cluster at the end of pore filling when there are sufficient Na ions to contribute electron donation to carbon. In addition, various Na cluster structures and pore sizes were tested for better Na cluster formation, and 1.5 nm was found to be the most suitable pore size for Na cluster formation with a close-packed arrangement. Furthermore, Na ions were found to have high self-diffusivity in the model HC pores even with the presence of defects at 300K ($\sim 10^{-5}$ cm^2 s^{-1}), and the drastic change in Na-ion charge from large interlayer distance (pores) to small interlayer distance (tunnels and graphite regions) could be the reason of impeded long-distance Na-ion diffusion in HC. The resultant mechanism for Na cluster formation and the suggested pore size for Na cluster formation could be helpful in HC anode design for pursuing high reversible capacity. Besides, the obtained Na-ion diffusivity in pores helps to clarify the rate limiting step for sluggish Na-ion diffusion in HC anodes.

Reference:

[1] A. Kamiyama, K. Kubota, D. Igarashi, Y. Youn, Y. Tateyama, H. Ando, K. Gotoh, S. Komaba, Angew. Chem. Int. Ed. **60**, 5114-5120 (2021).

[2] Y. Youn, B. Gao, A. Kamiyama, K. Kubota, S. Komaba, Y. Tateyama, *npj* Comput. Mater. **7**, 48 (2021).

Biography:

#36

Deciphering the Effect of Surface Oxygen Functionalities on Hard Carbon

Felix Bauer, 1 Marius Ast1 and Dr. Frieder Scheiba* 2

1 Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344, Germany

E-mail: felix.bauer@kit.edu

E-mail: marius.ast@kit.edu

2 Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344, Germany

E-mail: frieder.scheiba@kit.edu

Keywords: Anode • Hard Carbon • Oxygen Functional Groups • Surface Analysis • X-ray Photoelectron Spectroscopy

Abstract:

Hard carbon is one of the most promising anode materials for sodium-ion batteries due to its ability to reversibly store sodium ions at low potentials. The material is predominantly composed of carbon, yet a significant amount of oxygen-containing surface groups remains after pyrolysis due to the composition of the precursor material. The chemical nature and distribution of these oxygen functionalities are diverse and still not fully understood. Understanding the reactivity of oxygen surface groups is crucial, as they significantly influence solid electrolyte interphase (SEI) formation, initial Coulombic efficiency (ICE), and long-term cycling stability in sodium-ion batteries. While X-ray photoelectron spectroscopy (XPS) can distinguish between different oxidation states of carbon and oxygen, it cannot directly reveal the reactivity of these groups. This reactivity becomes relevant under battery cycling conditions, where surface functionalities can strongly interact with SEI formation and contribute to irreversible losses.

In this study, a derivatization approach is employed to selectively label oxygen surface functionalities using fluorinated reagents. Trifluoroacetic anhydride targets hydroxyl groups, trifluoroethanol reacts with carboxylic acids, and trifluoroethylhydrazine is used to derivatize carbonyl functionalities. The measured fluorine content serves as an indicator of the type and concentration of respective oxygen groups on the hard carbon surface. To validate the selectivity and efficiency of the derivatization reactions, functionalized polymers incorporating the respective oxygen groups are used as reference materials.

Derivatization techniques using fluorinated reagents have been applied to various carbon-based materials, but their systematic use on hard carbon has not yet been explored. Beyond characterization, this approach could pave the way for rational surface design by enabling targeted introduction and control of specific oxygen functionalities. This opens new opportunities for tailoring interfacial properties and optimizing the electrochemical performance of hard carbon anodes in sodium-ion batteries.

Biography:

Felix Bauer holds a Master's degree in Chemistry with a focus on electrochemical energy storage. He began his research career working on redox-flow batteries as a student assistant and later completed his Master's thesis on sodium-metal anodes. Currently, he is pursuing a PhD focused on hard carbon anode materials for sodium-ion batteries. His research centers on surface chemistry and the controlled functionalization of carbon surfaces to elucidate the impact of oxygen-containing groups on electrochemical behavior.

#37

Improving Lignin-Derived Hard Carbon Microstructure for Sodium-Ion Battery Anode Application

Nethmi Kulanika Dayarathne[1], Eric Campbell[2], Mansi Goyal[1], Xueping Song[3], Cheng Yan[4], Hongxia Wang[5], Dawei Wang[6], Yulin Zhong[2], Zhanying Zhang* [1]

[1]School of Mechanical, Medical and Process Engineering, Centre for Agriculture and the Bioeconomy, Queensland University of Technology, Brisbane, QLD 4000, Australia

[2]Queensland Micro- and Nanotechnology Centre, School of Environment and Science, Griffith University Nathan, Brisbane, QLD 4111, Australia

[3]Guangxi Key Laboratory of Clean Pulp & Papermaking and Pollution Control, College of Light Industry and Food Engineering, Guangxi University, Nanning 530004, China.

[4]School of Mechanical, Medical and Process Engineering, Centre for Material Science, Queensland University of Technology, Brisbane, QLD 4000, Australia

[5]School of Chemistry and Physics, Centre for Material Science, Queensland University of Technology, Brisbane, QLD 4000, Australia

[6]Faculty of Materials Science and Engineering, Shenzhen University of Advanced Technology, Shenzhen 518000, Guangdong, China

*Corresponding author: Zhanying Zhang: jan.zhang@qut.edu.au

Keywords: Lignin • hard carbon • sodium-ion battery • reversible capacity • initial coulombic efficiency.

Abstract:

Sodium-ion batteries (SIBs) show significant commercial potential as an alternative energy storage solution to lithium-ion batteries (LIBs), which depend on more costly lithium resources. Nevertheless, the advancement of SIBs faced challenges due to their lower ion storage capacities, initial coulombic efficiency (ICE) and rate capabilities, resulting in reduced energy densities compared to the LIBs. Hard carbon (HC) has emerged as a promising high-performance anode material for SIB applications. Another major obstacle to SIB commercialization is the cost of anode materials. Although sodium resources are cheaper than lithium resources, the anode materials for SIBs tend to be considerably more expensive. Thus, utilizing bio-based precursors such as lignin for HC production can help reduce these costs, as it is an economical substrate with a relatively high carbon content. Lignin is a key by-product of lignocellulosic biomass processing that shows great potential as a sustainable precursor for HC anodes in SIBs. This study utilizes common alkaline lignin, which typically contains polysaccharides derived from hemicellulose. Hence, this study focuses on the removal of hemicellulose from alkaline lignin to improve the microstructure of HC and its performance. The findings indicate that removing hemicellulose improves electrochemical performance significantly, achieving a maximum reversible capacity of 277.5 mAh g^{-1} and an ICE of 76.1%. This performance surpasses that of crude alkaline lignin which contains hemicellulose. This improvement is attributed to the carbonization of hemicellulose-free alkaline lignin because hemicellulose tends to produce HC with an increased number of surface functional groups and higher structural defects, all of which negatively impact having the Na^+ ion storage with higher reversible capacity and ICE. Therefore, this work emphasizes the critical role of hemicellulose removal in boosting the performance of alkaline lignin-derived HC and offers a scalable approach for producing a high-performance anode for sustainable energy storage.

Biography:

Nethmi Kulanika Dayarathne completed her bachelor's degree (hons) in Chemistry in 2021 from the University of Colombo, Sri Lanka. After completing her bachelor's degree, she worked as a Teaching Assistant in the Department of Chemistry at the University of Colombo, Sri Lanka. In 2022, she joined the Centre for Agriculture and the Bioeconomy at Queensland University of Technology, Australia, to pursue her PhD studies. She is currently working on the development of high-performance anode materials from agricultural waste for alternative sodium-ion battery applications.

#38

Tailoring Derived Carbon Microstructures for High-Performance Sodium-Ion Battery Anodes

Pinky Saharan [a b c 1], Md. Robiul Alam[c], Dr. Sanjay R. Dhakate [a b*], Dr. Nasir Mahmood [c*]

[a] Advanced Carbon Products and Metrology Department, CSIR-National Physical Laboratory (CSIR-NPL), New Delhi 110012, India

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

[c] School of Science, RMIT University, Melbourne, VIC 3001, Australia

E-mail: nasir.mahmood@rmit.edu.au, dhakate@nplindia.org

Keywords: Sodium-ion batteries (SIBs), lithium-ion batteries (LIBs), Anode, Petroleum coke, graphitization

Abstract:

Sodium-ion batteries (SIBs) are emerging as a promising alternative to lithium-ion batteries for grid-scale and stationary energy storage, owing to the earth-abundance, low cost, and environmental sustainability of sodium resources. However, the commercialization of SIBs remains challenged by the absence of high-performance anode materials capable of accommodating the larger ionic radius and slower kinetics of Na^+ ions compared to Li^+. In this study, we investigate carbon materials derived from petroleum coke- a low-cost and industrially abundant carbon source, as potential anodes for SIBs. By subjecting the precursor to a range of heat treatment temperatures we systematically engineer the carbon microstructure to enhance its sodium storage properties. Detailed characterization using X-ray diffraction (XRD), Raman spectroscopy, and electron microscopy (SEM/TEM) reveals critical changes in interlayer spacing, degree of graphitization, defect density, and porosity. These structural features play a pivotal role in determining Na^+ ion accessibility and storage capacity. Electrochemical testing in half-cell configurations demonstrates that carbon treated at an optimal temperature delivers a high reversible capacity, excellent cycling stability, and favourable rate capability. The enhanced performance is attributed to the balanced combination of disordered domains for sodium adsorption and short-range graphitic regions facilitating Na^+ diffusion. Our findings highlight the importance of heat-treatment-induced microstructural control in tuning the electrochemical behaviour of carbon anodes. This work not only establishes a structure-property correlation but also presents a scalable and sustainable route to engineer efficient carbon materials for next-generation sodium-ion batteries.

Biography:

I am a PhD student at RMIT University, Melbourne, Victoria. My research focus on the development of low cost carbon based Anode materials for Sodium Ion batteries.

#39

High-Capacity Bimetallic Transition Metal Sulfide Anode for Sodium-Ion Batteries

Md. Robiul Alam[1], Pinky Saharan [1], Mahdokht Shaibani[1*] Nasir Mahmood[1*]

[1]School of Science, RMIT University, Melbourne, VIC 3001, Australia.

E-mail: nasir.mahmood@rmit.edu.au, mahdokht.shaibani@rmit.edu.au

Keywords: Sodium-Ion • Anode • Bimettallic• Capacity • Stability

Abstract:

Sodium-ion batteries are gaining attention as a viable alternative to lithium-ion systems due to their abundant sodium resources and cost-effectiveness. Despite these advantages, the widespread implementation of sodium-ion technology is hindered by challenges such as low energy density, limited cycle life, and the need for stable and efficient anode materials. The development of advanced anodes is crucial to overcoming these obstacles and enhancing battery performance. This study presents a novel bimetallic transition metal sulfide anode, designed to address the specific challenges associated with sodium-ion battery anodes, such as capacity fading and structural degradation. Achieving an impressive charge capacity between 500 and 550 mAh g^{-1}, the anode demonstrates enhanced electrochemical stability and efficiency. These exceptional performance characteristics are attributed to the innovative synergistic effects of the bimetallic composition, which optimises ion diffusion and structural integrity during cycling. The study highlights how targeted material design and synthesis techniques can substantially improve capacity and longevity, thus advancing the field of sodium-ion batteries. The results underscore the potential for this anode to contribute significantly to the development of sustainable and high-performance energy storage systems. This research provides valuable insights into addressing current limitations and establishes a foundation for future advancements in sodium-ion battery technology.

Biography:

I am a PhD student at RMIT University, Melbourne, Victoria 3001. My research area is developing high-capacity and stable conversion-type anodes for metal-ion batteries.

#40

Exploring MXene-Based Anode Materials for Sodium-Ion Batteries

Sahithi Thatipamula, Sharafadeen Gbadamasi, Dr. Nasir Mahmood*

School of Science, RMIT University, Melbourne, VIC 3001, Australia

E-mail: nasir.mahmood@rmit.edu.au

Keywords: Sodium-ion batteries (SIBs), MXene, anode materials, electrochemical analysis, charge-discharge curves, cyclic voltammetry.

Abstract:

Sodium-ion batteries (SIBs) are gaining attention as promising alternatives to lithium-ion batteries due to the natural abundance, wide availability, and low cost of sodium resources. However, the search for efficient and stable anode materials remains a key challenge to achieving practical SIB applications. MXenes, a family of two-dimensional transition metals of carbides and nitrides, have emerged as attractive candidates owing to their layered structures, excellent electrical conductivity, and tunable surface chemistries, which facilitate sodium-ion intercalation. This study presents an electrochemical analysis of MXene and metal-doped MXene for their suitability in SIB. Using Na metal as the cathode in 1.0 M NaPF6 as the electrolyte, we performed cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) experiments to evaluate the sodium storage behaviour and electrochemical performance of these materials. Among the tested materials, compositional and structural differences significantly influenced the observed electrochemical characteristics, highlighting the importance of MXene structures to enhance capacity and cyclic stability. The findings from this study contribute to a deeper understanding of MXene-based materials as high-potential anodes for sodium-ion batteries.

Biography:

I am a PhD student at RMIT University, Melbourne, Victoria. My research focuses on the development of Anode materials for sodium, Aluminium, and Lithium batteries.

#41

Tantalum-Based Sodium-Ion Conducting Chlorides

Kota Motohashi*, Atsushi Sakuda, and Akitoshi Hayashi

Department of Applied Chemistry, Graduate School of Engineering, Osaka Metropolitan University,
1-1 Gakuen-cho, Naka-ku, Sakai, Osaka, 599-8531, Japan

E-mail: kota.motohashi@omu.ac.jp

Keywords: Solid electrolytes • Amorphous • Chloride • Fluoride • Mechanochemical

Abstract:

Developing materials with high sodium-ion conductivities is crucial for improving the electrochemical performance of all-solid-state batteries. Chlorides are candidates as promising solid electrolytes for all-solid-state batteries due to their high ionic conductivity, oxidation stability, and formability. Compared to lithium-ion conducting materials, fewer sodium-ion conducting chlorides have been found. In this study, we have developed $NaTaCl_6$ as an end-member of sodium-ion conductors [1]. $NaTaCl_6$ was synthesized via the mechanochemical method and exhibited an ionic conductivity of 6.2×10^{-5} S cm^{-1} at 25 °C. All-solid-state sodium cells ($Na_{15}Sn_4/Na_3V_2(PO_4)_3$) with $NaTaCl_6$ as the solid electrolytes showed good cyclability. We reported that the addition of Ta_2O_5 to $NaTaCl_6$ increased conducitivty and the obtained amorphous oxychloride containing nanoparticles exhibited an ionic conductivity of 2.5×10^{-3} S cm^{-1} [2]. The sodium-ion conducting fluorides with Central tantalum cation ($NaTaF_6$, Na_2TaF_7, and Na_3TaF_8) were also synthesized via the mechanochemical method [3]. Among the prepared three fluoride samples, Na_2TaF_7 showed the maximum conductivity of 1.1×10^{-6} S cm^{-1} at 100 °C. The electrochemical stability window of Na_2TaF_7 is between 1.6 and 4.2 V versus Na_2Sn at 100 °C. The oxidation and reduction stabilities of the Na_2TaF_7 sample were wider compared with those of the $NaTaCl_6$ chloride.

Acknowledgement: This work was partly supported by JSPS KAKENHI (Grant Numbers: JP24H02204 and 25H00904), MEXT Program: Data Creation and Utilization-Type Material Research and Development Project Grant Number JPMXP1122712807, and JST Adopting Sustainable Partnerships for Innovative Research Ecosystem Grant Number JPMJAP2313.

References

[1] K. Motohashi *et al.*, *ACS Mater. Lett.*, 6 (2024) 1178. [2] K. Motohashi *et al.*, *Chem. Mater.,* 36 (2024) 9914. [3] K. Motohashi *et al.*, *J. Ceram. Soc. Jpn.*, 132 (2024) 619.

Biography:

Kota Motohashi receved his Ph.D. from Tohoku University, Japan. He is currently an assistant professor in Professor Akitoshi Hayashi's research group in Osaka Metroplotan Univsersity, Japan. His research interests include solid state ionics, inorganic materials chemistry for rechargeable batteries.

#42

Effect of $BaTiO_3$ Addition on the Structural and Electrochemical Properties of $NaTaCl_6$ Chloride Electrolyte

Takuto Magome, [1] Takehiro Nakao, [1] Kota Motohashi, [1] Atsushi Sakuda, [1] and Akitoshi Hayashi * [1]

[1]Department of Applied Chemistry, Graduate School of Engineering, Osaka Metropolitan University, 1–1 Gakuen-cho, Naka-ku, Sakai, Osaka 599–8531, Japan

E-mail: akitoshihayashi@omu.ac.jp

Keywords: Chloride solid electrolyte • Filler • Amorphous • Ionic conductivity • Electrochemical stability

Abstract:

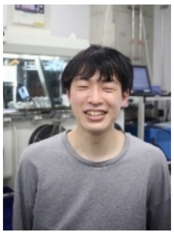
For a sustainable future, the practical use of all-solid-state sodium batteries attracts attention, given by their abundant raw materials, high safety, and energy density[1, 2]. Solid electrolytes, typically categorized into sulfides, oxides, and halides, play a crucial role in the batteries. Among them, chloride electrolytes offer high ionic conductivity, good processability at room temperature, and excellent compatibility with high-voltage positive electrode materials[3, 4]. For instance, our research group has reported that $NaTaCl_6$ synthesized via the mechanochemical method exhibits an ionic conductivity of 6.2×10^{-5} S cm^{-1} at 25°C[5]. The incorporation of oxide into chloride solid electrolytes has the potential to enhance ionic conductivity. Previous studies have demonstrated that the addition of Ta_2O_5 to $NaTaCl_6$ led to improved the ionic conductivity[6]. In this work, $BaTiO_3$ was added to $NaTaCl_6$ as a filler to improve the ionic conductivity, and $x BaTiO_3 \cdot NaTaCl_6$ chloride electrolytes ($x = 0.1$–1, molar ratio) were prepared.

The $x BaTiO_3 \cdot NaTaCl_6$ samples were prepared through the mechanochemical method using a planetary ball mill apparatus. As the amount of $BaTiO_3$ increased, the XRD peaks corresponding to $NaTaCl_6$ gradually weakened, while those of $BaTiO_3$ became more intense. These results indicated that the addition of $BaTiO_3$ promotes the amorphization of $NaTaCl_6$. Among all compositions, the sample with $x = 0.3$ exhibited the highest ionic conductivity, reaching 2.7×10^{-3} S cm^{-1} at 25°C. To evaluate the electrochemical stability, cyclic voltammetry (CV) measurements were performed. In the CV tests of the stainless steel (SS)/Na/$0.3BaTiO_3 \cdot NaTaCl_6$/SS cell, reduction reaction started around 1 V vs. Na^+/Na, indicating the electrolyte decomposed below this voltage. Because $NaTaCl_6$ without additives ($x = 0$) decomposed at 2 V[5], the addition of $BaTiO_3$ improved the ionic conductivity and the reduction stability.

Reference:

[1] C. Zhao *et al*., *Adv. Energy Mater*., **8** (2018) 1703012.
[2] J. -J. Kim *et al*., *Small Methods*, **1** (2017) 1700219.
[3] H. Kwak *et al*., *Energy Storage Mater*., **37** (2021) 47.
[4] E. A. Wu *et al*., *Nat. Commun*., **12**, (2021) 1256.
[5] K. Motohashi *et al*., *ACS Mater. Lett*., **6** (2024) 1178.
[6] K. Motohashi *et al*., *Chem. Mater.,* **36** (2024) 9914.

Biography:



Takuto Magome received his B.S. degree in Applied Chemistry from Osaka Prefecture University in 2025. He is currently a master's student at Osaka Metropolitan University, engaged in research on the structural analysis and ionic conduction properties of solid-state electrolyte materials.

#43

Enhancing Reduction Tolerance of Na_3PS_4 Solid Electrolyte by Sodium Oxysalts Addition for All-Solid-State Na Metal Batteries

T. Asakura, Y. Fujita, R. Yamanaka, D. Suehiro, K. Imai, K. Koga, K. Motohashi, A. Sakuda, and A. Hayashi *

Department of Applied Chemistry, Graduate School of Engineering, Osaka Metropolitan University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka, 599-8531, Japan

E-mail: akitoshihayashi@omu.ac.jp

Keywords: All-solid-state Na batteries • Sulfide electrolyte • Na metal • Amorphous • Interface

Abstract:

Na batteries are a promising energy-storage option due to the abundance and low cost of sodium materials. Na metal is an attractive negative electrode due to the lowest redox potential (−2.71 V vs. the standard hydrogen electrode) and high capacity (1165 mAh g^{-1}). All-solid-state Na batteries, in which flammable organic liquid electrolytes are replaced by flame-retardant inorganic solid electrolytes, are expected to increase the battery safety. As solid electrolyte candidates, sulfide solid electrolytes, such as Na_3PS_4, are attractive because of their high ionic conductivity and formability. However, cell failure due to the formation of reductive decomposition layers at the Na/Na_3PS_4 interface hinders their practical application[1]. Therefore, sulfide electrolytes with high reduction tolerance are required. In this study, to improve the reduction tolerance of the Na_3PS_4 electrolyte and the Na stripping/plating performance in all-solid-state Na metal cells, a series of Na_3PS_4 electrolytes doped with sodium oxysalts (e.g., Na_3PO_4, Na_2SO_4, and Na_2SO_3) were prepared by the mechanochemical process.

The addition of a small amount of each sodium oxysalt led to the amorphization of Na_3PS_4. The doping of a sodium oxysalt decreased the ionic conductivity of crystalline Na_3PS_4 to approximately 1×10^{-5} S cm^{-1} at 25 °C. The formability of the sodium oxysalt added Na_3PS_4 was enhanced, and the relative density of the powder compacts prepared by cold pressing at 360 MPa increased to ~90%. The Na plating/stripping behaviours were investigated using cyclic voltammetry and galvanostatic cycling tests. By adding Na_3PO_4 into Na_3PS_4, relatively reversible Na plating/stripping was realized, and the increase in cell overpotential during Na plating/stripping cycling was considerably suppressed. These results indicated that the addition of the sodium oxysalts enhanced the reduction tolerance. Additionally, the improved formability resulting from the amorphization of Na_3PS_4 is considered to suppress short-circuiting caused by local current concentration. In conclusion, the amorphization and high reduction tolerance achieved by adding the sodium oxysalts to Na_3PS_4 enabled stable cycling of the all-solid-state Na metal batteries.

Reference:

[1] A. Nasu *et al.*, *ACS Appl. Mater. Interfaces*, 14 (2022) 24480.

Biography:

Taichi Asakura is a Ph.D. student in the Department of Applied Chemistry at Osaka Metropolitan University (OMU), Japan. He received his bachelor’s and master’s degrees in engineering from OMU. His research focuses on the development of interfacial materials for sulfide-based all-solid-state lithium or sodium batteries.

#44

Molecular engineering in quasi-solid polymer electrolyte enabling a stable electrode-electrolyte interface for high-performance sodium metal battery

Vineeth Sasikumar Kala,[1,2] Minsu Han,[2] Yusuke Yamauchi,[2] and Vipin Kumar*[1,2,3]

[1] 1 University of Queensland- IIT Delhi Academy of Research (UQIDAR), Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India 110016

[2] Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Brisbane, QLD 4072, Australia

[3] Department of Energy Science and Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India 110016

E-mail: vkumar@dese.iitd.ac.in, minsu.han@uq.edu.au

Keywords: Quasi-solid Polymer Electrolytes • Electrode- Electrolyte Interface • High Energy Density Battery• Polymer Engineering• Sodium Metal battery

Abstract:

The quest for quasi-solid polymer electrolytes (QSPEs) for high-performance sodium metal batteries is considered promising. However, poor electrode-electrolyte interface with low ionic conductivity and transference number limits its employment in sodium metal batteries. To overcome this limitation, poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) based QSPE is developed. Molecular engineering is enabled by introducing electron-withdrawing groups in the system. This directly enhanced the room-temperature ionic conductivity (~1.01 mS cm^{-1}), and transference number (0.78), and widened the electrochemical stability window to ~5 V. Furthermore, the developed system favoured aggregate ion pairs, which are decisive for the formation of inorganic-rich interphase. Symmetric cells based on sodium stably functioned over 200 hrs at a high current density of 1 mA cm^{-2}. Moreover, the SMB based on an in-house fabricated Prussian blue cathode displayed performance over 500 cycles with a high initial capacity of 159 mAh g^{-1} at 0.5 C and exhibited an average Coulombic efficiency of ~98%. Overall, the concept of molecular engineering strategy was shown to be an effective solution to catalyse the growth of various QSPE-based high-performance SMB systems.

Biography:

Mr. Vineeth Sasikumar Kala is a Ph.D. research scholar focused on designing and developing advanced polymer electrolytes for room-temperature sodium-sulfur/ sodium metal batteries. He is a joint Ph.D. scholar in the prestigious University of Queensland - IIT Delhi joint research academy (UQIDAR). As a published scholar with experience in polymer engineering and technology, he is passionate about energy storage technology. His research interests include various aspects of polymers, nanotechnology, and energy storage devices, with a specific focus on developing materials for next-generation batteries.

#45

Solid-state borate-based polymer electrolytes for sodium batteries.

Margaux Guiraud, 1 Mega Kar1, Maria Forsyth1 and Faezeh Makhlooghi Azad*1
1 IFM Electromaterials, Deakin university, 221 Burwood highway, 3125, Australia
f.makhlooghiazad@deakin.edu.au

Keywords: Solid-state • Borate • Sodium batteries • Polymerized ionic liquid • Weakly coordinated

Abstract:

Solid-state sodium batteries (SSSBs) are emerging as next-generation energy storage devices due to their low-cost, high safety and high-energy density. Nevertheless, one of the main challenges in developing SSSBs stems from choosing an ideal solid electrolyte that can offer low-flammability, high conductivity, high chemical stability, good mechanical integrity, and superior cycling performance. This study focuses on developing electrolytes comprised of a polymerized ionic liquid, poly(diallyldimethylammonium) bis(fluorosulfonyl)imide, ([PDADMA][FSI]) mixed with weakly coordinating borate-based sodium salt for SSSBs. This choice of borate-based anions aims to enhance ion dissociation, consequently increasing ionic conductivity. Previous research has also demonstrated their efficiency in enhancing the stability of the Solid Electrolyte Interphase (SEI) in lithium batteries1. However, the effect of incorporating borate-based anions in polymerized ionic liquid electrolytes for SSSBs remains in its early stages.

This study focuses specifically on the [PDADMA][FSI] – Na[DFOB], (sodium difluoro(oxalate)borate), mixed system, investigating its thermal-phase behavior, ionic conductivity, and morphology as a function of sodium salt concentration. The results reveal that salt content has a key role in the crystallinity and ionic conductivity of the membranes. Furthermore, compared to liquid systems containing Na[DFOB], the addition of a small amount of borate salt (2 wt%) is sufficient to enhance ionic properties and stabilize the SEI2. Building on these findings, Na[DFOB] was also used as an additive in [PDADMA][FSI]–Na[FSI] (sodium bis(fluorosulfonyl)imide) based electrolytes, demonstrating further improvements in electrolyte performance.

References:

1. B. Roy et al., “Lithium Borate Ester Salts for Electrolyte Application in Next-Generation High Voltage Lithium Batteries,” *Adv Energy Mater*, **2021**, *11*, no. 36, 1-12.
2. L. Gao, J. Chen, Q. Chen, and X. Kong, “The chemical evolution of solid electrolyte interface in sodium metal batteries,” **2022**.

Biography:

Margaux Guiraud is a third year PhD student in Institute for Frontier Materials (IFM) Electromaterials at Deakin University in Melbourne, Australia. Her research focuses on polymer solid electrolytes for sodium batteries, using weakly coordinated borate-based cations. She holds an engineering degree (equivalent to a Master’s) majored in Industrial Ceramics at ENCIL-ENSCI in Limoges, France.

#46

Development and Evaluation of PVDF-HFP/Ionic Liquid Gel Polymer Electrolytes for Na-ion Batteries

Shun Sugayama,1 Changhee Lee,1 Fumi Ariura,2 Gérôme Godillot,3 Shinichi Komaba1

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

E-mail: komaba@rs.tus.ac.jp

2 Kyoto research park, Arkema, 93, Chudojiawata, Shimogyo, Kyoto 600-8815, Japan

3 Arkema GRL, BP34, Lacq 64170, France

Keywords: gel polymer electrolyte • polymer electrolyte • ionic liquid • positive electrode

Abstract:

Solid polymer electrolytes, which are nonflammable and highly flexible, are being studied as promising candidates for next-generation electrolytes. However, they generally face issues such as low ionic conductivity and poor interface contact with electrode surfaces. From this perspective, gel polymer electrolytes (GPEs), which combine solid polymers and liquid solvents, have been proposed as a solution. Particularly, poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP), known for its excellent mechanical properties, high chemical stability, and ease of processing, is an attractive base polymer material for GPEs. Furthermore, ionic liquids can offer advantages such as nonvolatility, thermal stability, and adjustable ionic conductivity and viscosity in GPEs, which are key factors for enhancing their performance in rechargeable battery systems.

In this study, we developed GPEs by blending PVDF-HFP (supplied by Arkema) with ionic liquids (supplied by Proionic), specifically pyrrolidinium-based ionic liquid (PYR14-FSA) and imidazolium-based ionic liquid (EMIM-FSA), for next-generation Na-ion batteries. Figures 1a and 1b show the results of plating/stripping tests of GPEs using different ionic liquids with a Na symmetric cell, confirming their stability with Na metal. The EMIM-based GPE showed an increase in polarization after 300 cycles (Figure 1a), whereas the PYR14-based GPE maintained low polarization and stable cycling characteristics. Additionally, Figure 1c presents the first cycle results of the charge-discharge test in Na/GPE/P2-Na2/3Ni1/3Mn2/3O2 (P2-NiMn) cells. In the PYR14-based cell, a relatively high Coulomb efficiency and a stable potential plateau, which is related to the phase transition of the cathode material, were clearly observed. These results suggest that the reduction stability of GPE at the Na metal anode are crucial for maintaining the performance of Na-ion cells. In the presentation, we will also discuss the system with diglyme as a co-solvent and the evaluation of charge/discharge characteristics using Na3V2(PO4)3 as a cathode material, as well as the physical/structural properties of GPEs.

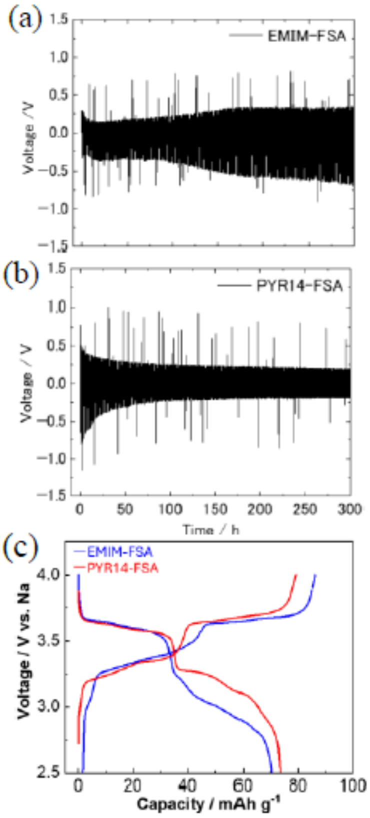


Figure 1 Na stripping/plating tests with (a) EMIM and (b) PYR14-based GPEs. (c) Charge/discharge curves of Na/GPE/P2-NiMn cells with EMIM and PYR14-based GPEs.

Reference:

1. F. Baskoro, H. Yen et al., *ACS Appl. Energy Mater.*, **2**, 3937-3971 (2019)
2. A. Manuel Stephan, J. *Wilson., Eur. Polym. J.*, **42**, 1728-1734 (2006)
3. C. Ding, R. Hagiwara, *J. Power. Sources*, **238**, 296-300 (2013)

Biography:

#47

Ionic liquid electrolytes for anode-free sodium batteries

Ajit Kumar*, [1] and Robert Kerr* [1]

[1] Institute for Frontier Materials(IFM), Deakin University, Burwood, VIC 3125, Australia

E-mail: ajit.kumar@deakin.edu.au, robert.kerr@deakin.edu.au

Keywords: Ionic liquid 1 • electrolyte 2 • anode-free 3 • sodium-batteries 4 • sustainable 5

Abstract:

Anode-free sodium batteries (AFSBs) offer an exciting path toward safer, more affordable, and higher-energy storage systems by removing the need for handling reactive sodium metal anodes. In this study, we focus on designing ionic liquid (IL)-based electrolytes and modifying the surface of current collectors to overcome key challenges in sodium plating and stripping. By carefully selecting and optimizing ILs with phosphonium, ammonium, pyrrolidinium, and imidazolium cations paired with FSI anions, we were able to form stable and durable solid electrolyte interphases (SEIs) that help suppress the growth of sodium dendrites.

Electrochemical testing showed strong performance, with Coulombic efficiencies above 99% and stable cycling at various current densities. These results highlight how thoughtful electrolyte formulation and interface design can enable practical, scalable AFSBs. Overall, this work offers a promising step forward in the development of safer and more efficient sodium-based batteries for both grid-level and portable energy storage.

Biography:

Dr. Ajit Kumar is a Research Fellow at Deakin University's Institute for Frontier Materials (IFM), Australia. He specialises in next-generation energy storage systems, with a focus on lithium and sodium-based batteries. His research integrates electrolyte design, electrode–electrolyte interface engineering, and advanced characterization techniques to enhance the performance and scalability of high-energy battery technologies. Dr. Kumar completed his PhD jointly at Monash University (Australia) and IIT Bombay (India), earning the Best Thesis Award for his pioneering work on room-temperature sodium-sulfur batteries. He has authored more than 26 peer-reviewed publications, contributed to several patents, and collaborates with leading academic and industry partners on battery innovation and sustainability.

#48

Electrochemical and interfacial analysis of EMC based non-aqueous electrolytes in high mass loaded Prussian White and hard carbon systems.

Dumindu P. Siriwardena,*[1] Jan Felix Schuster,[1] Lasse Dettmann,[1] Wessel W.A. van Ekeren,[1] Andrew J. Naylor[1] and Reza Younesi[1]

[1] Department of Chemistry, Ångström Laboratory-Structural Chemistry, Uppsala University, 75237, Sweden

E-mail: dumindu.thanaweera-achchige@kemi.uu.se

Keywords: Prussian White • Full-cells • Commercial mass loadings • EMC • Interfacial analysis

Abstract:

Sodium-ion batteries (SIBs) are being largely considered as a complementary technique for lithium-ion batteries (LIBs). However, several drawbacks should be addressed to realise the true potential of SIBs. The issues related to lower energy densities, cycling stability and poor rate capability of SIBS can be minimised by effective electrolyte and interfacial engineering.[1] Ethylene carbonate (EC) serves as the primary non-aqueous organic solvent in LIB electrolyte systems. Ethyl methyl carbonate (EMC), which is another organic solvent, is also widely used as a co-solvent in LIBs along with EC due to its favourable physical properties.[2] However, the utilisation of EC and EMC containing electrolyte systems in SIBs, especially in Prussian White (PW) and hard carbon (HC) full-cells, has been scarce. Thus, in this work, the effect of several EC-EMC compositions [xEC: (1-x)EMC] towards the electrochemical and interfacial properties of high-mass loaded PW and HC full-cell systems (mass loading up to 23 mg/cm^2 for PW) was systematically analysed. Furthermore, the impact of several additives on the observed electrochemical properties was also analysed. Differential capacity analysis (dQ/dV), real-time resistance evolution, as well as operando pressure evolution and interfacial analysis using synchrotron-based hard X-ray photoelectron spectroscopy (HAXPES), were utilised to obtain an in-depth understanding of the effects of EC to EMC ratio and the additives towards PW|HC electrochemical behaviour. The results displayed the inability of EMC to form stable interfaces on PW and HC electrodes and demonstrated the beneficial effect of small quantities of EC (Figure 1), as well as additives, towards stable electrochemical properties.

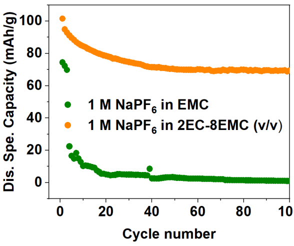


Figure 1. A comparison of long-term discharge capacities of EC and 2EC: 8EMC systems.

References

1. Zhao, L. et al. Engineering of Sodium-Ion Batteries: Opportunities and Challenges. Engineering 24, 172–183 (2023).
2. Jung, T., Wang, A. A. & Monroe, C. W. Overpotential from Cosolvent Imbalance in Battery Electrolytes: LiPF6 in EMC:EC. ACS Omega 8, 21133–21144 (2023).

Biography:

Dumindu P. Siriwardena obtained his Ph.D. from Queensland University of Technology (QUT-Australia) in 2022 and currently works as a postdoctoral researcher at the Ångström Advanced Battery Centre, Uppsala University, Sweden. His primary focus areas are electrolytes, interphases and materials for sustainable sodium-ion batteries.

#49

Constructing Robust Cathode-Electrolyte Interphase on Prussian Blue Analogues Via Interfacial Orbital Hybridisation

Cheng-Lin Ko [1], Qingbing Xia[1], Ruth Knibbe[1]

[1] School of Mechanical and Mining Engineering, Faculty of Engineering, Architecture and Information Technology, The University of Queensland Brisbane QLD 4072 Australia

E-mail: chenglincolin.ko@uq.edu.au and ruth.knibbe@uq.edu.au

Keywords: Prussian blue analogues • cathode-electrolyte interphase • interfacial orbital hybridisation • sodium-ion batteries

Abstract:

Sodium-ion batteries (SIBs) have attracted considerable attention in grid energy storage and electric vehicles, making them a promising advancement in the post-lithium-ion battery (LIB) era.[1] Current SIBs still face challenges in achieving high energy density, long cycling stability and fast charge/discharge capacity. These limitations are due to the larger ionic radius and higher redox potential of Na^+ ions when compared to Li^+ ion, which significantly affects the design and development of electrode materials.[2]

Prussian blue analogues (PBAs) are considered a promising cathode material for SIBs as they have a high theoretical capacity and are suitable for large-scale production.[3] However, the presence of structural defects and water molecules in the PBA structure induce irreversible structural change during cycling, which eventually leads to poor cycling stability and rate performance.[4] Therefore, optimising synthetic method and constructing robust cathode-electrolyte interphase (CEI) are promising strategies to stabilise the PBA structure during cycling.[4, 5]

In this work, we introduce a robust CEI by using 1-Propene 1,3-Sultone as an electrolyte additive. The CEI demonstrates strong coordination to the PBA cathode via interfacial orbital hybridisation, which enhances both structural integrity and Na^+ diffusion kinetics in the cathode materials. As a result, the CEI-modified PBA cathode exhibits excellent capacity retention over 1500 cycles at 1 C (80.3%) and rate capability at ultrahigh current rate (90 C), demonstrating a strong potential for high-performance SIBs.

References

[1] F. Duffner, N. Kronemeyer, J. Tübke, J. Leker, M. Winter, R. Schmuch, *Nat. Energy.* **2021**, *6*, 123.
[2] J. Y. Hwang, S. T. Myung, Y. K. Sun, *Chem. Soc. Rev.* **2017**, *46*, 3529-3614.
[3] Q. Liu, Z. Hu, M. Chen, C. Zou, H. Jin, S. Wang, S.-L. Chou, Y. Liu, S.-X. Dou, *Adv. Funct. Mater.* **2020**, *30*, 1909530.
[4] W. Wang, Y. Gang, J. Peng, Z. Hu, Z. Yan, W. Lai, Y. Zhu, D. Appadoo, M. Ye, Y. Cao, Q.-F. Gu, H.-K. Liu, S.-X. Dou, S.-L. Chou, *Adv. Funct. Mater.* **2022**, *32*, 2111727.
[5] N. Zhang, B. Wang, F. Jin, Y. Chen, Y. Jiang, C. Bao, J. Tian, J. Wang, R. Xu, Y. Li, Q. Lv, H. Ren, D. Wang, H. Liu, S. Dou, X. Hong, *Cell Reports Physical Science* **2022**, *3*, 101197.

Biography:

My name is Cheng-Lin Ko, and I am a first-year PhD student in Associate Professor Ruth Knibbe's group at The University of Queensland. I completed my Bachelor of Science (Honours) degree in 2024, where I built a strong foundation in sodium-ion battery research. My current research focuses on optimising separator and current collector in anode-free sodium metal batteries with the goal of developing safer and higher-performing energy solutions.

#50

Synthesis of oxalate-structured anions and their application as additives for sodium-ion batteries

Kentaro Kamada,* Shaoning Zhang, Duanfei Han, Kohei Nishimoto, Jinkwang Hwang,
Kazuhiko Matsumoto

Graduate School of Energy Science, Kyoto University, Yoshida, Sakyo-ku, Kyoto 606-8501, Japan
E-mail: kamada.kentarou.27a@st.kyoto-u.ac.jp

Keywords: sodium ion battery • electrolyte additive • oxalate

Abstract:

Sodium-ion batteries (SIBs) are gaining attention due to the abundance and low cost of sodium resources. In SIBs, electrolytes play a critical role not only in ion transport but also in forming solid electrolyte interphase (SEI) and cathode electrolyte interphase (CEI) on electrode surfaces. Recent studies have shown that adding functional additives can extend the electrochemical window and promote the formation of stable SEI and CEI layers.

Among such additives, oxalate-structured anions such as sodium difluoro(oxalate)borate (Na[BF_2(ox)], Na[DFOB]), which contains both fluorine and oxalate group, have demonstrated a potential to suppress transition metal dissolution, inhibit sodium metal deposits on hard carbon, and reduce electrolyte decomposition [1]. However, while these types of additives have been extensively explored in lithium-ion systems, systematic studies in sodium-ion batteries remain limited.

In this study, we synthesized a series of phosphate- and borate-based anions with controlled numbers of fluorine and oxalate groups and evaluated their electrochemical properties as electrolyte additives. Their performance was compared with conventional additives such as fluoroethylene carbonate (FEC), vinylene carbonate (VC), and sodium difluorophosphate (Na[PO_2F_2], Na[DFP]). Full-cell tests were conducted using $NaFe_{0.4}Ni_{0.3}Mn_{0.3}O_2$, $Na_3V_2(PO_3)_4$, and hard carbon electrodes, which revealed distinct interfacial behaviors and provided new insights into the role of these additives in enhancing the performance and stability of sodium-ion batteries.

References

[1] X. Liu, J. Zhao, H. Dong, L. Zhang, H. Zhang, Y. Gao, X. Zhou, L. Zhang, L. Li, Y. Liu, S. Chou, W. Lai, C. Zhang, S. Chou, *Adv. Funct. Mater.* **34** (2024) 2402310.

Biography:

Kentaro KAMADA received his Ms degree in Graduate School of Engineering, Tottori University in 2023 and is currently a third-year PhD student in Graduate School of Energy Science, Kyoto University under the supervision of Prof. Kazuhiko Matsumoto. His research focuses on fluorine chemistry and the development of electrolyte additives for sodium-ion batteries. He was honored to receive the Outstanding Student Presentation Award at the 91st Annual Meeting of the Electrochemical Society of Japan.

#51

Deciphering and Enhancing Rate-Determining Step of Sodium Deposition towards Ultralow-Temperature Sodium Metal Batteries

Yuxiang Niu[1], Jinlin Yang*[1], Fanbin Meng[2,3], Zejun Sun[1], Chonglai Jiang[1,2], Yuan Liu[1], Hongfei Xu[1,4], Meng Wang[1], Haotian Yang[1,2], Yupeng Zhu[1], Gang Wu*[5], Wei Chen*[1,2,3]

[1] Department of Chemistry, National University of Singapore, 3 Science Drive 3, 117543, Singapore

E-mail: yangjinlin@u.nus.edu, phycw@nus.edu.sg

[2] Joint School of National University of Singapore and Tianjin University, International Campus of Tianjin University, Binhai New City, Fuzhou, 350207, P. R. China

[3] Department of Physics, National University of Singapore, 2 Science Drive 3, 117542, Singapore

[4] School of Materials Science & Engineering, Beihang University, Beijing, 100191, China

[5] Institute of High-Performance Computing, Agency for Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, 138632, Singapore

E-mail: wug@ihpc.a-star.edu.sg

Keywords: low temperature • sodium metal batteries • high voltage • solvation structure • ion transportation in electrolyte

Abstract:

Achieving high ionic conductivity and stable performance at low temperatures remains a significant challenge in sodium-metal batteries (SMBs). In this study, we propose a novel electrolyte design strategy that elucidates the solvation structure-function relationship within mixed solvent systems. A mixture of diglyme and 1,3-dioxolane was developed to optimize the solvation structure towards superior low-temperature electrolyte. Molecular dynamics simulations and Raman spectra results reveal the solvent-separated ion pairs and contact ion pairs dominated solvation structure in the designed electrolyte, displaying a superior ionic conductivity of 1.78×10^{-3} S cm^{-1} at -40 °C. Besides, comprehensive kinetic analysis shows Na^+ transportation in the electrolyte shows a greater impact on sodium plating than Na^+ transport through the solid electrolyte interphase or charge transfer. As a result, the electrolyte enables stable operation for over 12,000 hours in Na||Na cells at -40 °C. In Na||$Na_{2/3}Ni_{1/4}Cu_{1/12}Mn_{2/3}O_2$ full cells, it maintains a high capacity retention of 92.4% over 600 cycles with an initial specific capacity of 89.4 mAh g^{-1} at -40 °C, and achieves 81.7% capacity retention after 50 cycles with an initial specific capacity of 75.3 mAh g^{-1} at -78 °C. These results pave the way for the development of high-performance SMBs capable of operating under ultralow temperatures.

Biography:

Yuxiang Niu received his Bachelor's degree from Tianjin University in 2021 and his Master's degree from the National University of Singapore in 2022. He is currently pursuing a Ph.D. in Professor Wei Chen's group at the National University of Singapore. His primary research focus is the modification of electrolytes for sodium metal batteries.

#52

Low temperature electrolytes for commercial sodium ion batteries

Jan Felix Schuster*1, Charles Aram Hall1, Reza Younesi1

1Department of Chemistry - Ångström Laboratory, Structural Chemisty, Lägerhyddsvägen 1, 75237 Uppsala

*Email: jan-felix.schuster@kemi.uu.se

Keywords: sodium ion battery • low temperature electrolyte • non aqueous electrolyte • manganese iron nickel oxide • electrochemical impedance spectroscopy

Abstract:

Sodium-ion batteries are emerging as a strong contender in the renewable energy sector. They provide competitive energy density and performance while being produced from cost-effective and abundant materials. Due to their lower Stokes radius and higher ionic conductivity relative to lithium ions, sodium ions have the potential to deliver superior power output and enhanced low-temperature performance. Furthermore, the compatibility of hard carbon anodes with solvents unsuitable for graphite opens opportunities for novel electrolyte systems. Solvents such as propylene carbonate and ethyl acetate have demonstrated improvements in both rate capability and low-temperature stability. 1,2 However, these systems still suffer from limited capacity and poor rate performance under cold conditions compared to traditional carbonate-based electrolytes.3 Ethyl acetate, with its low solvation energy, enhances performance, while fluoroethylene carbonate (FEC) used alone remains insufficient for achieving long-term and low-temperature stability.

This research focusses on ethyl acetate as a base solvent, asking the questions: (i) what are it's major decomposition routes, and (ii) and how can we alleviate them without significantly affecting the properties of ethyl acetate that make it promising for low temperature performance? Experiments were conducted in commercial dry cells from LiFun using a nickel manganese iron oxide (Nax[Mn0.34Fe0.31Ni0.24Zn0.09]O2) and hard carbon electrodes. Commercial cells were used to showcase the industrial applicability (or lack thereof) of the developed electrolytes, as issues like excessive gas formation or electrolyte decomposition are effectively masked in low-mass-loading, excess-electrolyte cell formats typically used in research. Various ratios of ethyl acetates were tested in combination with ethylene carbonate, propylene carbonate, and diethyl carbonate. Addtives such as FEC and succinonitrile were investigated. Our results indicate the use of the platizier succinonitrile lowers the internal resistance of the cell and changes the impedance of full cells. Using carbonates in combinations with ethyl acetates and additves significantly lowers the impedance as well as increases the performance at low temperature. Work is ongoing to more thoroughly understand the role that these additives and cosolvents play in improving the stability of the ethyl acetate-based electrolyte, however we can report that significant capacity can be retained cycling at 0.33 C at -20 degrees Celsius.

References:

(1) Desai, P.; Abou-Rjeily, J.; Tarascon, J.-M.; Mariyappan, S. Practicality of Methyl Acetate as a Co-Solvent for Fast Charging Na-Ion Battery Electrolytes. *Electrochimica Acta* **2022**, *416*, 140217. https://doi.org/10.1016/j.electacta.2022.140217.

(2) Jayakumar, R.; Pollard, T. P.; Borodin, O.; Shipitsyn, V.; Chak, C. (Michael); Pastel, G.; Zheng, A.; Johnson, M.; Hasan, F.; Bejger, C. M.; Schroeder, M. A.; Greenbaum, S. G.; Zuo, W.; Ma, L. Weakly Solvating Ester Electrolyte for High Voltage Sodium-Ion Batteries. *Nano Energy* **2024**, *128*, 109969. https://doi.org/10.1016/j.nanoen.2024.109969.

(3) Bai, Z.; Yao, Q.; Wang, M.; Meng, W.; Dou, S.; Liu, H. kun; Wang, N. Low-Temperature Sodium-Ion Batteries: Challenges and Progress. *Adv. Energy Mater.* **2024**, *14* (17), 2303788. https://doi.org/10.1002/aenm.202303788.

Biography:

Jan Felix Schuster is a second year PhD student at the Ångström advanced battery center in Sweden working on non-aqeous electrolytes and their effect on the ageing of alkali ion batteries. He holds a M.Sc. in Chemistry for Uppsala University and B.Sc. in Chemistry with minor in industrial engineering from Constructor University Bremen, Germany. His work focuses on testing electrolytes in model systems and large scale batteries. He has presented work on solid electrolyte interphase dissolution in sodium and potassium ion batteries.

#53

Commercial sodium-ion batteries: Operando neutron diffraction, X-ray tomography studies

B. D. K. K., Thilakarathna*[1], Daniel Brocklebank[1], Patrick Kin Man Tung[2], Vanessa Peterson[3], N. Sharma[1]

[1] School of Chemistry, UNSW, Sydney, NSW, 2052, Australia.

E-mail: neeraj.sharma@unsw.edu.au

[2]Research Technology Services, UNSW, Sydney, NSW, 2052, Australia.

[3]Australian Nuclear Science and Technology Organisation, New Illawarra Rd, Lucas Heights NSW, 2234, Australia.

Keywords: • Degradation • structural evolution • multiscale analysis • $NaNi_{1/3}Mn_{1/3}Fe_{1/3}O_2$

Abstract:

Sodium-ion batteries (SIBs) have gained significant attention as complimentary systems to lithium-ion batteries (LIBs), primarily due to the abundant availability and cost-effectiveness of sodium resources. This study investigates the performance and structural evolution of commercially available 18650 SIB using advanced characterization techniques. X-ray diffraction (XRD) and energy-dispersive X-ray spectroscopy (EDS) identified O3-structured $Na_xNi_{1/3}Mn_{1/3}Fe_{1/3}O_2$ as the active cathode material and $CaCO_3$-templated hard carbon as the anode material in the discharged 18650 cell. Electrochemical testing demonstrated a capacity retention of 89% after 100 cycles at a current density of 100 mA. However, at higher current densities (1 A), capacity retention declined to 73% after 100 cycles, with significant degradation observed after approximately 70 cycles. All cells cycled at 1 A produced minimal capacity after 300 cycles. In operando neutron diffraction provided critical insights into the structural changes during cycling, revealing reversible phase transitions between the O3 and P3 phases within the voltage range of 1.5–4.0 V. The P3 phase, characterized by comparatively larger unit cell volume changes, was present for approximately 74% of the charge-discharge cycle at 0.30 A cycling. At higher applied current, the O3-P3 phase transitions spanned broader voltage windows, highlighting the impact of current density on structural changes. Additionally, computed tomography (CT) offered a detailed evaluation of the battery's internal architecture and structural features that could influence performance and long-term stability. These findings provide valuable insights into the structural evolution and stability of commercially available sodium-ion batteries. They emphasize the behavior of constituent materials and highlight key structural and mechanistic factors that can be optimized to improve the commercial viability of this energy storage system.

Biography:

B. Dilan K. K. Thilakarathna is a fourth-year PhD candidate at the University of New South Wales (UNSW), Australia, supported by the University International Postgraduate Award (UIPA). His research focuses on the electrochemical and thermal evolution of sodium-ion battery cathode materials, with a particular emphasis on layered transition metal oxides. His work integrates structural characterization techniques, including X-ray diffraction (XRD) and neutron diffraction, to investigate phase evolution under various electrochemical and thermal conditions.

#54

INVESTIGATING THE ORIGIN OF HIGH SODIUM STORAGE CAPACITY IN HARD CARBON VIA X-RAY ABSORPTION SPECTROSCOPY

Syuaibatul Islamiyah, 1, 2 and Kei Kubota* 1, 2

1 Graduate School of Chemical Sciences and Engineering, Hokkaido University, Hokkaido, Sapporo, 060-0810, Japan
2Research Center for Energy and Environmental Materials (GREEN), National Institute for Materials Science (NIMS), Ibaraki, Tsukuba, 305-0044, Japan

E-mail: kubota.kei@nims.go.jp

Keywords: hard carbon • sodium storage mechanism • sodium-ion batteries • X-ray absorption

Abstract:

Hard carbon is a promising negative electrode material for Na-ion batteries due to its abundant resources, high capacity, low operating potential, and good cycling stability. Some hard carbons have discharge voltage curves very close to 0 V vs. Na+/Na, with the risk of metallic Na deposition. To avoid such metallic Na deposition, it is essential to understand the microstructure of hard carbon and the sodium storage mechanism. In this study, we utilize X-ray absorption spectroscopy (XAS) technique to investigate the electrical states of sodium in the two types of hard carbon: commercial hard carbon with a reversible capacity of 309.4 mAh g-1 and ZnO-templated hard carbon with 413.8 mAh g-1. Hard carbon electrodes in fully sodiated and desodiated were electrochemically prepared with Na metal as the counter electrode, and their Na K-edge XAS data were collected in partial fluorescence yield mode and compared with those of Na metal, NaF, and Na2CO3 as standard reference materials. Na K-edge absorption energies of X-ray absorption fine structure (XANES) spectra are intermediate between Na metal and ionic Na compounds for both hard carbon electrodes in the fully sodiated state. However, ZnO-templated hard carbon has absorption energy closer to that of Na metal reference than the commercial hard carbon. This result implies that the Na stored in the ZnO-templated hard carbon have less ionic character, possibly due to the formation of quasi-metallic Na clusters within its micropores. Small-angle X-ray scattering analysis revealed that the ZnO-templated hard carbon has larger micropore size of 1.44 nm compared to 1.03 nm of the commercial one. The enhanced capacity of ZnO-templated hard carbon can therefore be attributed to its ability to accommodate bigger Na metallic clusters inside its larger pores.

Biography:

Syuaibatul Islamiyah is a first-year doctoral student in the Graduate School of Chemical Sciences and Engineering, NIMS-Hokkaido University Joint Graduate School Program. She received her B.Sc in Chemistry from Institut Teknologi Sepuluh Nopember (ITS) in Indonesia, and her master’s degree from Kyushu University, Japan. Her current research focuses on elucidating the sodium storage mechanism in hard carbon using advanced characterization techniques, such as X-ray Absorption Spectroscopy, under the supervision of Associate Professor Kei Kubota in Battery Materials Analysis Group.

#55

Overcoming hard carbon’s irreversible losses using an ionic liquid-mediated pre-sodiation technique

Sruthi Kancharla1, Urbi Pal1, Maria Forsyth1,Ajit Kumar1 , Robert Kerr1,*

Institute for Frontier Materials, Deakin University, Burwood, Victoria 3125, Australia

*Email: s223705052@deakin.edu.au

Keywords: Pre-sodiation, solid-electrolyte interphase, initial Coulombic efficiency, hard carbon

Abstract:

Hard carbons (HC) are the most used anode materials for sodium-ion batteries, but they suffer from significant irreversible losses during the initial cycles. This is primarily due to sodium-ion consumption in forming the solid-electrolyte interphase (SEI) and trapping within the hard carbon structure, leading to reduced capacity and performance. Although various presodiation techniques have been developed to address this, many have limitations.

In this study, we demonstrate a simple direct-contact presodiation method to mitigate irreversible losses in HC. The HC was placed in direct contact with sodium metal in a high salt concentration ionic liquid electrolyte (50 mol% NaFSI in C3mpyrFSI) at 50°C for 15 minutes. This approach presodiates the HC without requiring extra cathode mass in full-cell configurations.

The presodiated HC was paired with sodium vanadium phosphate (NVP) in full cells (N/P ratio = 1.2, same electrolyte), delivering an initial discharge capacity of 96 mAh/g (NVP) at C/10 (1C = 117.6 mA/g) and an initial coulombic efficiency (ICE) of 97%. The cell maintained 88% of its capacity (83 mAh/g) after 1000 cycles at C/2 and 50 °C. Post-cycling analysis using solid-state MAS NMR and XPS confirmed SEI formation on the presodiated HC anode, contributing to improved stability and reduced irreversible losses. To enhance its practical applicability, hard carbon is presodiated using the same ionic liquid electrolyte, washed with dimethyl carbonate (DMC), and assembled into the full cell with 1 M $NaPF_6$ in EC/DEC. This full cell delivered excellent results, with a 96% ICE and 92% capacity retention (82.5 mAh/g(NVP)) after 500 cycles, demonstrating the potential of this methodology for a broad range of applications.

Biography:

I am Sruthi Kancharla, a second-year Ph.D. student at the Institute for Frontier Materials (IFM) at Deakin University. My research focuses on sodium-ion batteries, with particular interest in presodiating hard carbon anodes to treat irreversible losses at the full cell level. I have experience in electrode coatings, cell fabrication, testing, and surface characterization techniques relevant to advanced energy storage systems.

#56

Effects of Functional Binders on Electrochemical Properties of Hard Carbon Electrodes for Na-ion Batteries

Lu Yin,[1] Changhee Lee,[1] Rena Takaishi,[2] Kimio Misaki,[2] Takashi Matsuyama,[2] and Shinichi Komaba[1]

[1] Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan

E-mail: komaba@rs.tus.ac.jp

[2] NIPPON A&L INC. 3-1-98 Kasugadenaka, Konohanaku, Osaka, 554-8558, Japan

Keywords: Binders • Anode • Hard Carbon • Surface Analysis • Full Cells

Abstract:

Conventionally used poly(vinylidene fluoride) (PVdF) requires the use of flammable and toxic organic solvents, raising safety and environmental concerns. This necessitates the development of alternative binders that are compatible with aqueous processing, among which aqueous latex-based binders such as styrene-butadiene rubber ($\mathrm{SBR_{std}}$) and sodium polyacrylate (PANa) have been widely utilized. In this study, these aqueous binders were applied to hard carbon (HC) electrodes for Na-ion batteries to investigate their impact on electrochemical performance. Additionally, a modified binder ($\mathrm{SBR_{CN}}$) was synthesized by copolymerizing $\mathrm{SBR_{std}}$ with a certain amount of acrylonitrile monomer to enhance electrode properties. The electrodes were prepared using HC, acetylene black, and each binder, and evaluated in Na metal half-cells.

Figure 1a shows the capacity retention of hard carbon electrodes with various $\mathrm{SBR_x}$, PANa, and PVdF binders. As shown in the results, electrodes utilizing SBR_x and PANa binders exhibited superior capacity retention over 50 cycles compared to those using PVdF. Furthermore, **Figure 1b** presents a comparison of the discharge rate capabilities. At a high current density of 1250 mA g^{-1}, electrodes with $\mathrm{SBR_{std}}$ and $\mathrm{SBR_{CN}}$ demonstrated significantly higher discharge capacities than PVdF-based counterparts. These enhancements are attributed to favorable modifications in the surface film composition at the electrode/electrolyte interface.[1, 2] Detailed discussions on the interfacial behavior, binder physical properties, and surface analysis results will also be presented.

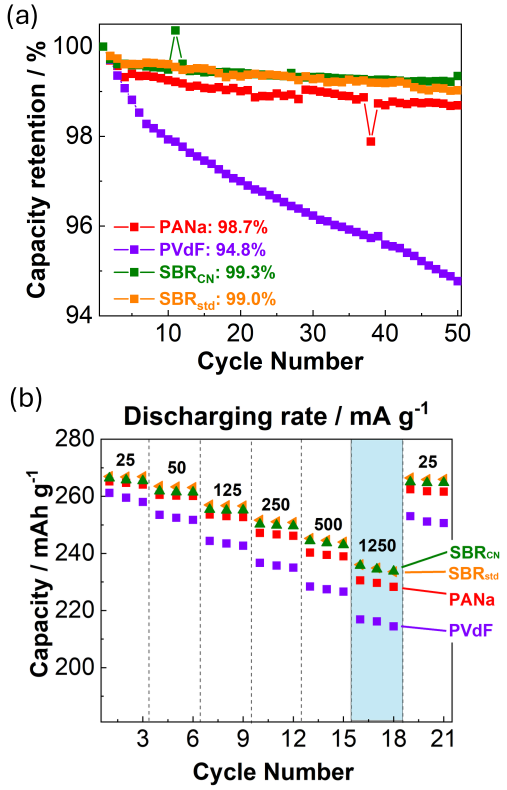


Fig. 1. (a) Cycle performance and (b) rate capability of HC electrodes cycled in 2.0 – 0.002 V with different binders.

Reference:

1. H. Isozumi, S. Komaba *et al.*, *J. Power Sources*, **468**, 228332 (2020).
2. Y. Yoda, S. Komaba *et al.*, *ACS Appl. Mater. Interfaces*, **10**, 10986 (2018).

Biography:

#57

ADVANCING ANODE-FREE SODIUM METAL BATTERIES THROUGH SODIOPHILIC CURRENT COLLECTOR DESIGN

Lakshmy Kadavil Subhash [1], Qingbing Xia* [1] and Ruth Knibbe* [1]

[1] School of Mechanical and Mining Engineering, Faculty of Engineering, Architecture and Information Technology, The University of Queensland, Brisbane, QLD 4072, Australia

E-mail: qingbing.xia@uq.edu.au, ruth.knibbe@uq.edu.au

Keywords: anode-free batteries • sodium metal batteries • self-assembled monolayers • sodiophilic interphase • dendrite suppression

Abstract:

Sodium metal batteries are promising candidates for high energy density and economical energy storage; however, their practical application is hindered by severe dendrite formation. While contemporary approaches such as sodiophilic interphase engineering and seeded nucleation effectively mitigate dendrite growth, they overlook the inevitable depletion of interfacial Na$^+$ ions prior to plating, resulting in increased sodium consumption, lowered cell voltage, and compromised energy density[1].

Achieving robust cycling stability and high-rate performance with minimal or zero excess sodium—i.e., an initially anode-free configuration—is highly sought after for maximizing the energy density of sodium metal batteries. Yet, this remains a significant challenge[2]. The absence of a pre-existing sodium anode imposes a restricted sodium inventory, intensifying irreversible sodium loss, continuous solid electrolyte interphase (SEI) formation, and dendritic growth, which collectively limit capacity retention and cycling stability. Conventional anode-free sodium metal batteries (AFSMBs) with unmodified current collectors exhibit poor sodium nucleation and heterogeneous deposition, accelerating parasitic reactions. In contrast, current collector engineering—such as sodiophilic surface modification—enables uniform sodium plating, suppresses dendrite formation, and stabilizes the SEI, thereby markedly improving coulombic efficiency and cycle life[3,4].

In this work, hexadecylamine (HDA) is employed to functionalize the anode current collector, thereby enhancing interfacial sodiophilicity and directing uniform sodium nucleation and growth for better performance. Self-assembled monolayers (SAMs)—ordered molecular films that spontaneously form on surfaces—enable precise tuning of interfacial properties and have been previously utilized in metal battery systems[5]. However, the application of HDA-based SAMs on copper for sodiophilic modification in AFSMBs represents a novel strategy, leveraging the unique amine-copper interaction and molecular architecture of HDA to promote homogeneous sodium deposition and suppress dendrite formation.

References

1. Zhuang R, Zhang X, Qu C, et al. Fluorinated porous frameworks enable robust anodeless sodium metal batteries. *Sci Adv*. 2023;9(39):1-15. doi:10.1126/sciadv.adh8060
2. Tang F, Yang Y, Liu C, et al. Initially anode-free sodium metal battery enabled by strain-engineered single-crystal aluminum substrate with (100)-preferred orientation. *Nat Commun* . 2025;16(1):1-11. doi:10.1038/s41467-025-57424-2
3. Cai Z, Tang F, Yang Y, et al. A multifunctional super-sodiophilic coating on aluminum current collector for high-performance anode-free Na-metal batteries. *Nano Energy*. 2023;116(May):108814. doi:10.1016/j.nanoen.2023.108814
4. Hu Z, Liu L, Wang X, Zheng Q, Han C, Li W. Current Progress of Anode-Free Rechargeable Sodium Metal Batteries: Origin, Challenges, Strategies, and Perspectives. *Adv Funct Mater*. 2024;2313823:1-24. doi:10.1002/adfm.202313823
5. Liu Y, Tao X, Wang Y, et al. Self-assembled monolayers direct a LiF-rich interphase toward long-life lithium metal batteries. *Science (80-)*. 2022;375(6582):739-745. doi:10.1126/science.abn1818

Biography:

I am a PhD candidate at the School of Mechanical and Mining Engineering, University of Queensland. With a background in Physics and Materials Science, I engage in seemless interdisciplinary research. My work emphasises using in-situ and ex-situ TEM techniques to investigate how sodium metal nucleates and grows on current collectors in anode-free batteries.

#58

IMPACT OF SYNTHESIS PARAMETERS ON DIRECT RECYCLING AND STRUCTURAL EVOLUTION OF PRUSSIAN WHITE

Subha Samanta, * 1 Bowen Liu, 1 Peter Slater, 2 and Emma Kendrick * 1

1 School of Metallurgy and Materials Science, University of Birmingham, B15 2TT, United Kingdom

E-mail: (s.samanta@bham.ac.uk, e.kendrick@bham.ac.uk)

2 School of Chemistry, University of Birmingham, B15 2TT, United Kingdom

Keywords: Direct Recycling • Sodium-ion Batteries • Resodiation Process • Structural Evolution • Prussian White

Abstract:

Sodium-ion batteries (SIBs) are rapidly emerging as a sustainable alternative to lithium-ion batteries due to their lower cost and abundant raw materials. As their usage grows, efficient recycling becomes crucial to minimize environmental impact and promote sustainability. Current recycling techniques focus on pyro-/hydro-metallurgical processes, which are characterized by high costs and significant energy consumption. This necessitates the development of efficient direct recycling strategies that will be crucial to support the widespread use of SIBs and ensure a circular economy.

In this work, the efficacy of a low energy route for direct recycling is investigated. This involves the critical role of process parameters, including pH value, on the efficiency of direct recycling of Prussian White (PW) from used sodium-ion batteries and improving the structural integrity of recycled materials. The effectiveness of the recycling process is then evaluated through various characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), elemental mapping (EDS), Raman analysis, and electrochemical performance testing. These results demonstrate that under optimised synthesis conditions, the recycled PW retains its structural integrity and electrochemical properties, comparable to those of pristine PW. The recycled material exhibited around 96% of its pristine PW capacity with long-term cycling stability, making it a viable candidate for reuse in new SIBs.

Herein, we propose a low-temperature, solution-based resodiation route which involves dissolving the recovered material and sodium salt in a solution at lower temperatures and adding a reducing agent, which helps control the pH more effectively and minimizes the loss of metal ions. Our investigation reveals that both higher and lower pH values are unsuitable for effective resodiation, leading to undesirable recycling outcomes. Higher pH value increases the solubility of metal ions, leading to their loss from the solid phase and reducing the overall yield of the recycled material. Low pH conditions are corrosive to the materials involved leading to the degradation of the structural framework and the dissolution of essential components and hinder the resodiation process. In contrast, neutral pH conditions provide a balanced environment which favours the formation of well-defined crystalline structures. This enhances the structural integrity and stability of the recycled material.

In conclusion, this research underscores the importance of developing efficient recycling strategies for battery materials to promote the circular economy and reduce the environmental footprint of energy storage technologies. The successful recycling of Prussian white not only enhances the sustainability of sodium-ion batteries but also contributes to the broader goal of achieving a more sustainable and resilient energy infrastructure.

Biography:

Dr Subha Samanta is a Marie-Curie Postdoctoral Research Fellow working with Prof. Emma Kendrick (Energy Material Group) in the School of Metallurgy and Materials, University of Birmingham, United Kingdom. Her research focuses on recycling and reuse of cathode materials for sodium-ion battery using a wide range of experimental approaches to better understand battery technology.

Prior to her current role, Dr. Samanta served as a Postdoctoral Research Associate at RISE-TCG CREST, India, in 2022, where her work was focussed on halide-based solid-state electrolytes. She received her PhD in Physics from Indian Association for the Cultivation of Science, India (2022) and her M.Sc. in Applied Physics from IIT (ISM) Dhanbad (2016).

#59

Crystal chemistry of sulfates for sodium-ion batteries: from mineral-inspired structures to functional electrode materials

Vadim M. Kovrugin [1,2,]* and Valérie Pralong [1,2]

[1] CRISMAT, ENSICAEN, Université de Caen Normandie, CNRS UMR 6508, 14000 Caen, France

* E-mail: vadim.kovrugin@ensicaen.fr

[2] RS2E, FR CNRS 3459, 80039 Amiens Cedex 1, France

Keywords: Na-ion • electrode material • sulfate • crystal structure • mineral

Abstract:

Polyanionic sulfate compounds have emerged as a promising class of electrode materials for sodium-ion batteries (SIBs) primarily due to their high redox potentials induced by the strong inductive effect of the SO_4^{2-} group. In this study, we explore the crystal chemistry of sulfates as Na^+-intercalation hosts through both historical developments and recent advances, with the objective of unveiling key structure-property relationships essential for the rational design of novel electrode materials. A central theme of our work is the intrinsic connection between synthetic sulfate phases and naturally occurring minerals. Minerals have long served as a powerful source of inspiration in materials science, with several commercial electrode materials, such as, *e.g.*, LFP directly derived from mineral structures (*triphylite* $Li(Fe,Mn)PO_4$ of the *olivine* group). Similarly, the most investigated and best-performing sulfate-based electrodes for SIBs are those related to the *alluaudite*,[1] *triplite*,[2] and *eldfellite*[3] mineral families. Hence, adopting this mineral-inspired perspective, we build upon our previous works on sulfates for SIBs[4–6] to conduct a comprehensive analysis of the diversity of reported sulfate electrode materials, highlighting their close crystallographic parallels with naturally occurring minerals. Special attention is given to the geological formation conditions of these minerals, which may offer invaluable guidance for developing new synthetic strategies for battery electrodes based on sulfates. Given that over 650 sulfate mineral species are recognized by the *International Mineralogical Association*, this family of compounds remains vastly underexplored in the context of energy storage. Our findings emphasize the substantial potential of sulfate-based phases as electrode materials to deliver competitive energy densities, while also offering access to previously unexplored structural motifs favourable for Na^+ ionic conduction. This crystal chemical investigation sets the foundation for the rational design of next-generation SIBs electrode materials based on Earth-abundant and structurally versatile sulfate compounds.

Reference:

[1] S. Li, W. Wang, Y. Jia, H. Xu, R. Liu, Z. Wang, Z. Xie, L. Zhang, R. He, L. Wang, *Small Methods* **2025**, 2402110.

[2] M. Kim, D. Kim, W. Lee, H. M. Jang, B. Kang, *Chem. Mater.* **2018**, *30*, 6346–6352.

[3] S. Singh, D. Singh, R. Ahuja, M. Fichtner, P. Barpanda, *J. Mater. Chem. A* **2023**, *11*, 3975–3986.

[4] M. Gnanavel, O. I. Lebedev, P. Bazin, B. Raveau, V. Pralong, *Solid State Ionics* **2015**, *278*, 38–42.

[5] V. M. Kovrugin, D. O. Nekrasova, O. I. Siidra, O. Mentré, C. Masquelier, S. Y. Stefanovich, M. Colmont, *Cryst. Growth Des.* **2019**, *19*, 1233–1244.

[6] S. Singh, A. Neveu, K. Jayanthi, T. Das, S. Chakraborty, A. Navrotsky, V. Pralong, P. Barpanda, *Dalt. Trans.* **2022**, *51*, 11169–11179.

Biography:

V. Kovrugin, Assistant Professor ENSICAEN

V. Pralong, Senior CNRS Researcher CRISMAT

#60

Photogenerated Holes Induced Deep Sodium Storage of TiO_2/CdSe/NFPP Cathode for High-Efficiency Photo-Rechargeable Sodium Batteries

Mingrui Yang, [1] and Weihua Chen* [1]

[1] College of Chemistry, Zhengzhou University, Zhengzhou, 450001, Henan, China

E-mail: chenweih@zzu.edu.cn

Keywords: photo-rechargeable battery • optical field • holes • interface • high capacity

Abstract:

Resource-friendly photo-rechargeable sodium batteries (PRSBs) integrate energy storage devices with solar cells offering a promising path for sustainable energy. Herein, a novel TiO_2/CdSe/$Na_3Fe_2(PO_4)P_2O_7$ (NFPP) cathode was prepared layer-by-layer utilizing resource-abundant commercialized NFPP and photoactive CdSe. The aligned energy levels with type II band structure ensures effective transfer of photo-generated holes from CdSe (-5.71 eV) to higher valence band of NFPP (-5.10 eV). Experimental results reveal that, during charging, the induced holes in NFPP accelerate the transition of Fe^{2+} to Fe^{3+} with a change of O-Fe hybrid orbitals. The calculations of bond valence sum and energy distribution reveal that NFPP-holes possesses broad Na^+ transport path with reduced transport barrier (from 0.512 to 0.428 eV), improving Na^+ extraction efficiency. Additionally, photo-generated holes could regulate surface charge distribution on NFPP and thus form a film-forming agent fluoroethylene carbonate (FEC)-dominated electric double layer. Finally, it converting to a thinner (9.75 nm-illumination) NaF-rich cathode interphase layer, avoiding subsequent excessive electrolyte decomposition. As a result, the NFPP under illumination delivers high capacity of 119.1 mAh g^{-1} at 1 C, showing 41.11% improvement comparing to dark conditions.

Biography:

Mingrui Yang, Associate Researcher at the School of Chemistry, Zhengzhou University. She focuses on photo-rechargeable sodium-ion batteries, combining green clean solar energy with abundant sodium resources to create low-cost, high-safety portable photo-energy storage systems. These integrated devices simultaneously achieve the absorption, conversion, and storage of solar energy, making them an ideal technology for next-generation power sources. She has published multiple papers in journals including *J. Am. Chem. Soc., Angew. Chem. Int. Ed., Adv. Funct. Mater., ACS Photonics, Batteries,* and *J. Phys. Chem. C.*

#61

Zero-Strain Electrode Materials for Sodium-Ion Batteries

Qingbing Xia*
Mechanical and Mining Engineering, The University of Queensland, Australia
E-mail: qingbing.xia@uq.edu.au

Keywords: Sodium ion batteries • zero-strain • hard carbon • Prussian blue analogues• titanium oxides

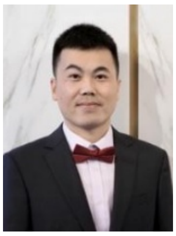
Abstract:

Sodium-ion batteries (SIBs) are considered a complementary or even an alternative energy storage technology to lithium-ion batteries (LIBs). Fundamental challenges, such as sluggish charge transport kinetics, short cycling lifespan, and low energy density, hinder the current technological development of SIBs. Electrode materials hold the key to any success in commercialising SIBs. The past decade has witnessed rapid advances in the design and synthesis of high theoretical capacity anode materials, such as metal/alloys, metal oxides/dichalcogenides, phosphorous/phosphides, etc., for SIBs. These candidates, however, face challenges such as significant volume expansion upon Na ion insertion, limiting their electrochemical reversibility and cycling stability, and sluggish sodiation kinetics, resulting in inferior rate capability. Electrode materials with high specific capacity and zero-stain properties have shown the potential to improve the electrochemical performance of SIBs, but suffer from sluggish kinetics and unstable cycling, especially under extreme temperature environments. This abstract will present our recent research results on developing zero-stain electrode materials, including anodes of hard carbon and titanium oxides and cathodes of Prussian blue analogue, for SIBs with fast charge/discharge capability and long-term cycling performance. It will describe rational structural design and synthesis routes that mitigate volume expansion and optimised electrolytes that enhance interfacial stability, as well as in situ characterisation techniques that elucidate Na ion storage mechanisms and phase evolution with these materials.

References

1. Q. Xia, C.-L. Ko, E. Cooper, Q.F. Gu, E. Knibbe, J. R. Harmer, Adv. Funct. Mater. 2025, 2421976.
2. J. Zhang, Y. Wang, Q. Xia,* X. Li, B. Liu, T. Hu, M. Tebyetekerwa, S. Hu, R. Knibbe, S. Chou, Angew. Chem. Int. Ed. 2024, 63, e202318822.
3. E. R. Cooper, M. Li, I. Gentle, Q. Xia,* R. Knibbe,* Angew. Chem. Int. Ed. 2023, 62, e202309247.
4. Q. B. Xia, Y. R. Liang, E. R Cooper, C. -L. Ko, Z. Hu, W. J. Li, S. L. Chou, R. Knibbe, Adv. Energy Mater., 2024, 2400929.
5. Q. B. Xia, Y. R. Liang, Z. H. Lin, S. W. Wang, W. H. Lai, D. Yuan, Y. H. Dou, Q. F. Gu, J. Z. Wang, H. K. Liu, S. X. Dou, S. M. Fang and S. L. Chou, Adv. Energy Mater., 2020, 10, 2001033.
6. Q. Xia, Y. Huang, J. Xiao, L. Wang, Z. Lin, W. Li, H. Liu, Q. Gu, H. K. Liu and S. L. Chou, Angew. Chem. Int. Ed., 2019, 58, 4022-4026.
7. Q. Xia, Z. Lin, W. Lai, Y. Wang, C. Ma, Z. Yan, Q. Gu, W. Wei, J. Z. Wang, Z. Zhang, H. K. Liu, S. X. Dou and S. L. Chou, Angew. Chem. Int. Ed., 2019, 58, 14125-14128.

Biography:



Dr Qingbing Xia received his PhD from the University of Wollongong (Australia) and is currently a Postdoctoral Research Fellow in the School of Mechanical and Mining Engineering at the University of Queensland. His research focuses on nanostructured electrode materials for rechargeable batteries, solid-state lithium/sodium batteries, and the development of in situ techniques for investigating the mechanical behavior of battery reactions.

#62

Selective C_2 Electroproduction via Back Bonding in Asymmetric Copper-Copper

Chenchen Fang, and Jingwen Sun*

Key Laboratory for Soft Chemistry and Functional Materials, Ministry of Education School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology

E-mail: Jingwen_Sun@njust.edu.cn

Keywords: Asymmetric copper-copper motifs • CO_2 reduction reaction • Electrochemistry • Energy generation and conversion • π back bonding

Abstract:

CO_2 reduction reaction (CO_2RR) is considered a highly attractive approach to reduce carbon emissions and yet encounters challenges in further converting $*C_1$ intermediates to valuable two-carbon (C_2) products. Although copper-based catalysts exhibit satisfactory adsorption energy for $*C_1$ species, the symmetrical charge distribution at adjacent copper sites leads to a strong repulsive force between adsorbed $*C_1$. Herein, asymmetric copper-copper (Cu_F-Cu_N) motifs with distinct adsorption behaviors have been constructed on the F-Cu_3N substrate using the in situ isostructural substitution method. Compared to the high hybridization of Cu_N 3d and N 2p orbitals, implanted F not only reduces the hybridization strength but also endows the Cu_F with delocalized unpaired electrons. Accordingly, Cu_F, beyond forming an isolated $3d_{z^2}$-$2p_z$ σ bond between Cu and the key $*C_1$ intermediate (*CHO), offers additional $3d_{xz}$-$2p_z$ π back bonding to the *CHO. With dipole interactions in the asymmetric Cu_F-Cu_N motifs, the electrostatic repulsion between adjacent *CHO is diminished, efficiently promoting the C-C coupling in CO_2RR. In situ characterization and computational simulation reveal that the polarized charge distribution of adjacent *CHO adsorbates on Cu_F-Cu_N motifs lowers the energy barrier of C-C coupling, thus enhancing the selectivity for C_2 products and suppressing the pathways to CO and CH_4 formation. Therefore, the asymmetric Cu_F-Cu_N motifs demonstrated an exceptional selectivity of 81.5% with a partial current density of -325.9 mA cm^{-2} and competitive stability in the electrochemical conversion of CO_2 to C_2 products. Our work offers a promising concept for designing asymmetric catalytic sites and paves the way for the development of novel catalysts through atomic-level modulation strategies.

Biography:

#63

Prussian Blue Cathodes for Sodium-ion Batteries

S. Mostafapoor* [1], S. S. Mofarah[1], C.C. Sorrell[1]

[1]School of Materials Science and Engineering, UNSW Sydney, Sydney, NSW, 2052 Australia

s.mostafapoor@unsw.edu.au

Keywords: Prussian blue analogues • Battery • Sodium-ion • cathode • characterisation

Abstract:

In the structure of Prussian blue analogues (PBAs), with the general stoichiometry of M'[M(CN)$_6$], cyanide (CN$^-$) ligand bridges two metal centres (*viz*. M–C≡N–M'), which forms a 3D metalorganic framework capable of reversible intercalating and deintercalation Na$^+$ as charge career. The low-cost precursors, together with the cost-effective synthesis of PBAs, enhances the affordability of Na-ion batteries. In the present work, an Iron-based Prussian blue (Fe[Fe(CN)$_6$]) cathode was fabricated using coprecipitation technique. The effect of fabrication parameter optimisation on the electrochemical performance was evaluated. The optimised cathode delivered a high capacity of 153 mAh·g^{-1} and a retained 81% of its capacity after more than 200 cycles.

Biography:

My name is Saman Mostafapoor, a second-year PhD student at UNSW Sydney; my research focuses on developing advanced battery materials, particularly Prussian blue analogues (PBAs) as a low-cost and promising materials for Na-ion batteries. I work on synthesising the materials and characterisation of their properties using a range of advanced techniques.

#64

Aging and SEI Stability in the Prussian White and Hard Carbon Cell System

Charles Aram Hall[1] and Reza Younesi[1]

[1] Department of Chemistry – Ångström Laboratory, Structural Chemistry, Lägerhyddsvägen 1, 75237 Uppsala

E-mail: charles-aram.hall@kemi.uu.se

Keywords: SEI • electrolyte • aging

Abstract: Though sodium-ion batteries (SIBs) have matured dramatically, there is still progress to be made in extending cycling life. Thus, a key challenge is to understand aging mechanisms in order to minimise their effect. Cells ustilising hard carbon (HC) negative electrodes and Prussian white (PW) positive electrodes have curiously been shown to degrade moreso when cycled only at a low state of charge (SoC; roughly 0 to 50% SoC) than at a high SoC (roughly 50 % to 100% SoC). [1] It is ambiguous whether this dervies from increasing polarisation of the high-spin iron or collapse of the PW structure, increasing resistance in the HC electrode or from an overall loss of sodium inventory, or a combination of all of these mechanisms.

This talk will discuss the observed aging in PW||HC cells cycled in different voltage ranges. [1] Likely aging mechanisms will be discussed, drawing on information *operando* X-ray diffraction (XRD) [2] and operando electrochemical mass spectrometry (OEMS). [3] The results of XRD suggest that though polarisation does increase in the PW positive electrode, it is difficult to link these effects to a structural degredation of the PW. It seems more likely instead that aging is due to a loss of sodium inventory, although it is difficult from XRD to pinpoint where this sodium inventory is lost. From OEMS, it seems possible that one route for sodium inventory loss is via oxidation of the solid electrolyte interphase (SEI) at the end of discharge, requiring a fresh SEI to be formed in the subsequent cycle. Another loss mechanism relates to SEI dissolution, which similarly requires a fresh SEI to be formed in the subsequent cycle. [4] Using this understanding, preliminary results in a model system will seek to test how the electrolyte choice affects the stability of the SEI.

References:

[1] Buckel, Hall, Ma, Colbin, Eriksson, Mogensen and Younesi, Batteries and Supercaps 2023, 7, 2, e202300533

[2] Nielsen, Hall, Mattsso, Younesi, Buckel, Ek and Brant, J. Mater. Chem. A 2024, 12, 17413-17421

[3] Misiewicz, Ulander, Melin, Hall and Berg, Advanced Materials Interfaces 2024, 12, 10, 2400854

[4] Ma, Buckel, Hofmann, Nyholm and Younesi, Advanced Science 2023, 11, 6, 2306771

#65

Optimizing Sc-dopted $Na_3V_2(PO_4)_2F_3$/C as a high-performance cathode material for sodium-ion battery applications

ShaoKang Guo[1], Jian Peng[2], Neeraj Sharma[2], Chunliang Zhou[1], Junnan Liu[1]
[1]Harbin Engineering University [2]School of Chemistry, UNSW Australia

Abstract: A series of Sc-doped carbon coated $Na_3V_{2-x}Sc_{x}(PO_4)_2F_3$/C, were synthesized by the sol-gel method. The optimized NVPF has good electronic conductivity and cycling stability, the NVSPF/C-0.04 electrode exhibits the highest discharge specific capacity (125 mAh g^{-1} at 0.2 C), excellent rate performance (87 mAh g^{-1} at 30 C) and outstanding cycling performance (90% capacity retention after 1000 cycles at 10 C and 94% capacity retention after 100 cycles at 1 C). The NVSPF/C-0.04//HC (hard carbon) full cell performs with a good discharge specific capacity (112 mAh g^{-1} at 1 C).