MECHANICAL & MATERIAL COLLOQUIUM

Organic Electrode Materials for Affordable and Sustainable Na-ion Batteries

by Chao Luo (Department of Chemical, Environmental, and Materials Engineering University of Miami)

Na-ion batteries (NIBs) are promising alternatives to Li-ion batteries (LIBs) due to the low cost, abundance, and high sustainability of sodium resources. However, the high performance of inorganic electrode materials in LIBs does not extend to NIBs because of larger ion size of Na^+ than Li^+ and more complicated electrochemistry. Therefore, it is vital to search for high performance electrode materials for NIBs. To this end, organic electrode materials (OEMs) with the advantages of high structural tunability and abundant structural diversity show great promise in developing high-performance NIBs. To achieve advanced OEMs, a fundamental understanding of the structure–performance correlation is desired for rational structure design and performance optimization. Tailoring molecular structures of OEMs can enhance their performance in NIBs, however, the substitution rules and the consequent effect on the specific capacity and working potential remain elusive.

Herein, we investigated the electrochemical performances and reaction mechanisms of organic anode materials and polymer cathode materials based on azo, amine, imine, and carbonyl groups for NIBs. The influence of structural isomerism, halogenation, conjugation structures, and spatial effects on the electrochemical performance of carboxylate anode materials was studied. Our findings demonstrate that the position of carboxylate groups, fluorine atoms, extended conjugation structure, and planar structure are crucial for optimizing the performance of carboxylate anode materials in NIBs. Furthermore, we discovered that the electrochemical performance of one-dimensional polymer cathode materials with an extended conjugated structure such as a naphthalene backbone structure is better than that with benzene and biphenyl structures due to faster kinetics and lower solubility in the electrolyte. It unravels the rational design principle of extended π-conjugation aromatic structures in redox-active polymers to enhance the electrochemical performance. In addition to the one-dimensional polymers, two-dimensional and three-dimensional polymers were also investigated to gain a deeper understanding of the effects of porosity and crosslinked structure on the electrochemical performances. Our results provide a valuable guideline for the design principle of high-capacity and stable OEMs for sustainable energy storage.

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Dr. Chao Luo is an Associate Professor in the Department of Chemical, Environmental, and Materials Engineering at the University of Miami. His research focuses on developing organic materials, polymers, carbon materials, carbon/sulfur composites, and electrolytes for high-energy and sustainable batteries. He obtained B.S. degree from Wuhan University and Ph.D. degree at the University of Maryland, College Park. Before moving to the University of Miami in 2024, he was an Assistant Professor and Associate Professor at the George Mason University. He has published more than 80 peer-reviewed articles with total citation over 13,000 and h-index of 53. He is also the recipient of NSF CAREER award, an Emerging Investigator 2021 by *Journal of Materials Chemistry A*, and an Emerging Investigator 2023 by *Chemical Communications*.

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