



Electrolyte Design for Selective Energy Storage and CO₂ Electrolysis

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Bio: John is a Stanford Energy Postdoctoral Fellow under the supervision of Professors Yi Cui, Zhenan Bao, and Jian Qin. Previously, his PhD was completed at UCSD with Professors Ping Liu and Zheng Chen. His work involves understanding and designing electrolytes and electrochemical devices for energy storage and materials synthesis. This work integrates experimental investigation with atomistic modeling and technoeconomic analysis. So far, this approach has been applied to research in Li-ion and Li metal batteries for electric transport, Zn batteries for grid storage, and CO₂ electrolysis for sustainable chemical production.

Abstract: Electrochemical technologies promise to channel the rapidly falling price of renewable electricity towards the grid, manufacturing, and transportation industries. Among these systems, advanced rechargeable batteries form the foundation of the rapidly expanding EV market and will play a vital role in renewable grid storage. At an industrial level, advanced electrolyzers could be used to produce commodity chemicals from waste CO₂. The advent of these technologies at scale would redefine humanity's relationship with these industries by aligning profit with sustainability. To realize this promise, however, significant improvements in energy efficiency, device lifetime, and high-power performance must be made. Our work involves the design of electrolyte composition and structure to regulate the (electro)chemical processes that define device performance. This is done via a hybrid computational/experimental approach that yields mechanistic insight and informs system design.

In this talk, we will discuss the application of this hybrid methodology to electrolyte design for Zinc batteries. We demonstrate that pairing between Zn²⁺ and halide anions can significantly improve the poor Zn deposition kinetics typically found in organic solvents, while also undercutting the costs of state-of-the-art systems. Deposition from these systems generates polyhedral, textured Zn and exceptional Coulombic efficiencies without any discernable corrosion.

In a separate work, we also demonstrate that electrolyte composition and structure can also be tuned to enhance CO₂ electrolysis. These electrolytes are based on multivalent cations that are stabilized in the bicarbonate buffer solutions common in CO₂ electrolyzers with electrolyte additives. Electrolytes based on these chemistries show increased electrochemical activity for CO₂ reduction relative to hydrogen evolution. Ab-initio molecular dynamics (AIMD) simulations reveal that these additives polarize H₂O away from the cathode and that multivalent cations induce greater activation of *CO₂ than standard monovalent cations.

This talk demonstrates a combined experimental and computational approach to electrolyte design for the advancement of electrochemical energy storage and conversion.