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IAPME Seminar

Design of High-Energy Density Lithium-Sulfur Batteries

27 September 2024

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Venue: E11-G012
Time: 10:30 - 11:30
Hosted by: Prof. Kwun Nam HUI

Abstract

Lithium-sulfur (Li-S) batteries are among the most promising next-generation high-energy density secondary batteries. However, their practical application is hindered by issues such as the shuttle effect, slow reaction kinetics, and lithium dendrite growth on the anode during cycling. This report focuses on the key materials and device designs necessary for high-energy density Li-S batteries. It proposes a rational design for cathode catalysts by examining the electronic structure at the catalyst surface. Specifically, it introduces the concept of hybridization between the d-orbitals of transition metal catalysts and the p-orbitals of lithium polysulfides, which can serve as a descriptor for screening single-atom catalysts in Li-S batteries. Machine learning is employed to develop a binary descriptor that can efficiently screen transition metal compound catalysts, elucidating the electronic and structural effects in Li-S catalysis. A universal strategy is proposed for tuning the spin and orbital topology of the catalysts. The report also explores the transition between different orbital hybridizations over time in Li-S battery catalysts. To address the uncontrolled growth of lithium dendrites and the associated safety risks, the coupling mechanism between the Li-S cathode and anode under co-regulated mass and charge transport is unveiled, guiding the rational design of electrode structures. An artificial solid electrolyte interphase (SEI) layer based on a layered structure is proposed to stabilize the lithium metal anode and prevent dendrite formation. Additionally, by adjusting the solvation structure of the electrolyte, molecular-level control of the SEI layer is achieved, resulting in stable cycling of the lithium metal anode. Building on this foundation, a systematic strategy for preparing high-sulfur-loading electrodes has been developed. The report investigates the construction of Li-S full cells, analyzing how key technologies and process parameters affect the charge-discharge and cycling performance of Li-S pouch cells. After optimizing these parameters, the pouch cells achieved an energy density exceeding 400 Wh kg^{-1}.

Biography

Prof. Guangmin ZHOU is an Associate Professor in Tsinghua Shenzhen International Graduate School, Tsinghua University. He received his Ph.D. degree from Institute of Metal Research, Chinese Academy of Sciences in 2014, and then worked as a postdoc in UT Austin during 2014-2015. After that, he was a postdoc fellow at Stanford University from 2015 to 2019. His research mainly focuses on the development of advanced energy-storage materials and devices, and battery recycling. He has published more than 290 articles in peer-reviewed scientific journals, and first/corresponding-authored papers published in Nature Catalysis, Nature Nanotechnology, Nature Energy, Nature Sustainability, Nature Communications, PNAS, Advanced Materials, National Science Review, etc. These publications have been cited more than 44300 times with an H-index of 92. Prof. Zhou was honored “Highly Cited Researcher” in Materials Science field by Clarivate Analytics for consecutive 6 years (2018-2023), EcoMat Young Researcher Award (2023), Young Scientist Award of Hou Debang Chemical Science and Technology (2021), Young Scientist Award of Guangdong Materials Research Association (2020), etc. Prof. Zhou served as Associate Editor/Scientific Managing Editor of Energy Storage Materials.