香港大學 機械工程系
Department of Mechanical Engineering
THE UNIVERSITY OF HONG KONG

SEMINAR

Title **Thermodynamics of Solvation Process in Liquid Electrolytes**

Date: **April 17, 2026 (Friday)**
Time: **3:00 – 4:30pm**
Venue: **Tam Wing Fan Innovation Wing Two**
G/F, Run Run Shaw Building, HKU

Speaker: **Prof. Feifei Shi**
Assistant Professor of Energy Engineering
John and Willie Leone Family
Department of Energy and Mineral Engineering
University Park, USA

Abstract:

Corelating solvation structure and thermodynamic properties with transport properties serve as the foundation for electrolyte design. While various physicochemical properties, such as relative solvating power, solvation energy and spectroscopies have been used to study Li+ solvation, fundamental investigations in thermodynamic properties of solvation equilibrium across broad temperature ranges are still lacking.

In this work, we combined temperature-resolved Infrared and Raman spectroscopies to systematically pinpoint the dynamic evolution of Li+-solvent and Li+-anion local coordination in typical ether and carbonate electrolytes. We identified a trend of temperature-driven equilibrium among electrolyte components. By quantifying the temperature-responsive mean coordination number and ionic species concentrations, we reveal a preferential CIP association in carbonates compared to ethers. Gibbs free energy changes in diverse electrolytes exhibit a strong correlation with their respective Li^+ transference number. The thermodynamic properties of solvation equilibrium can serve as new descriptors for quantifying dynamic solvation structure and facilitate the precise extraction of transport properties across a broad spectrum of battery electrolytes.

Biography:

Bio: Dr. Feifei Shi currently serves as assistant professor of energy engineering in the John and Willie Leone Family Department of Energy and Mineral Engineering. Shi holds a B.S. degree in chemistry from Fudan University, China in 2010, and a Ph.D. degree in mechanical engineering from the University of California, Berkeley in 2015. Before joining Penn State in August 2019, Shi was a postdoctoral researcher in the material science and engineering department at Stanford University. Shi received awards including 2023 NSF CAREER Award, 2022 J&J WiSTEM2D Scholar by Johnson & Johnson, and 2019 Virginia S. and Philip L. Walker Faculty Fellow at Penn State University. The author of more than 60 articles (h-index 46) and one book chapter, she serves as the guest editor for Frontiers in Energy Research, Energy & Environmental Materials (EEM) and the editorial board of Energy Materials. Shi's research interest lies at the intersection of surface chemistry, material science, and mechanical engineering, with an emphasis on integrated energy systems.

ALL INTERESTED ARE WELCOME
For further information, please contact Prof. Chunyi Zhi