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IAPME Seminar

Intercalation in 2D materials and in-situ studies

4 December 2025

Prof. Zhiyuan ZENG
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Venue: N23-4016
Time: 15:00 - 16:00
Hosted by: Prof. Guichuan XING

Abstract

Intercalation of atoms, ions, and molecules is an effective means of tuning the properties of two-dimensional materials, while in situ imaging and spectroscopy provide powerful tools for deciphering intercalation dynamics and mechanisms. Firstly, we developed a lithium ion battery intercalation & exfoliation method with detailed experimental procedures for the mass production of 11 2D transition metal dichalcogenides (TMDs) and inorganic nanosheets, such as MoS_2, WS_2, TiS_2, TaS_2, ZrS_2, graphene, h-BN, $NbSe_2$, WSe_2, Sb_2Se_3 and Bi_2Te_3, among them 3 TMDs achi eved mono- or double layer yield > 90%. The Li insertion can be monitored and finely controlled in the battery testing system, so that the galvanostatic discharge process is stopped at a proper Li content to avoid decomposition of the intercalated compounds. Secondly, we discovered that small current and high cut-off voltage (0.005 A g^{-1}, 0.9 V) produces pure 2H WS_2 bilayers. while large current and low cut-off voltage (0.02 A g^{-1}, 0.7 V) leads to 1T’ WS_2 monolayers. For lithium intercalation mechanism, the state-of-the-art In-Situ Liquid Phase TEM is an ideal technique for identifying the phase changes during intercalation process. Combining with in-situ XAS, XRD and Raman, etc, the underlying lithium intercalation mechanism in TMDs were elucidated to achieve scalable production. For water decontamination, our metallic 1T/1T′ phase 2D TMDs (MoS_2, WS_2, TaS_2, TiS_2) nanosheets exhibited exceptional Pb^{2+} removal capacity (up to 758 mg·g^{-1}) with treatment capacity of 55 L-water/g-adsorbent for feeding Pb^{2+} concentration of 1 mg·L^{-1}, which is 1-3 orders of magnitude higher than other 2D materials and commercial activated carbon, holding great potential as Point-of-use (POU) devices. Then, a one-step covalent functionalization of MoS_2 nanosheets was used for membrane fabrication, which exhibits rejection rates of >90% and >80% for various dyes and NaCl in reverse osmosis (RO). After that, we found that 1T′-MoS_2 electrode demonstrates exceptional volumetric desalination capacity of 65.1 mgNaCl cm^{-3} in capacitive deionization.

Biography

Prof. Zhiyuan ZENG received his BSc, Mphil and PhD degrees all in MSE from Central South University, Zhejiang University and Nanyang Technological University in 2006, 2008 and 2013, respectively. After 4 years postdoc at Lawrence Berkeley National Laboratory (LBNL) and 2 years Engineer working in Applied Materials Inc. (Silicon Valley), he joined the Department of Materials Science and Engineering, City University of Hong Kong in 2019, and was promoted as Associate Professor in 2024. His research interests are using lithium intercalation strategy, in-situ liquid phase TEM technique to investigate Transition-metal dichalcogenides (TMDs), which can be used for energy and environmental applications.

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