化生研 講演会/ CLS Seminar

Institute of SCIENCE TOKYO

Integrating Multi-Scale Simulations and Machine-Learning Interatomic Potentials to Explore Surface and Interface Behaviors in Energy Materials

Lecturer: Prof. Hong-Kang Tian
Department of Chemical Engineering,
National Cheng Kung University (NCKU), Taiwan

Time & Date: 15:30-17:00, Thursday 17 October 2024

Place: The 1st Seminar Room,R1 bldg. Suzukakedai campus
(R1棟2F 第一会議室)

Abstract: With the advancements in computational power, simulations, and machine learning techniques, exploring complex behaviors in materials has become increasingly feasible. In this talk, I will present several of our recent works, highlighting how we integrate first-principles calculations, numerical simulations, and machine-learning interatomic potentials to investigate surface and interface behaviors in energy materials, including batteries and catalysts. The topics covered will include interfacial contact, internal stress, and ion/electron transfer in all-solid-state batteries; the impact of the solid electrolyte interphase (SEI) on Li/Mg dendrite formation mechanisms; the influence of defects and dopants on photo- and electro-catalytic oxygen and hydrogen evolution reactions (OER and HER); and the electron transfer mechanisms at the interfaces of upconversion nanoparticles.

Contact: Prof. Yoshitaka Tateyama (045-924-5277) @ Tateyama-Ando Group