北海道大学
大学院総合化学院
GRADUATE SCHOOL OF CHEMICAL SCIENCES AND ENGINEERING
HOKKAIDO UNIVERSITY

北海道大学 理学部
School of Science,
Hokkaido University

化学部門特別講演会

Designing Novel Nano Structures, Polymer Electrolytes, and Biomacromolecules with Predictive Molecular Simulations

【ABSTRACT】

Electrostatic interactions plays a dominant role in charged materials systems. Understanding the complex correlation between macroscopic properties with microscopic structures is of critical importance to develop rational design strategies for advanced materials. But the complexity of this challenging task is augmented by interfaces present in the charged materials systems, such as electrode-electrolyte interfaces or biological membranes.

In this talk, I'll present our ongoing efforts to enable predictive molecular simulations of these highly charged systems. A key advancement has been made with the development of predictive multi-scale force field for ionic liquids (ILs) and polymers based entirely on first-principle calculations, and the development of simulation algorithms to treat surface polarization and proper thermal equilibrium in polarizable MD simulations. New physical insights gained from the new simulation model and simulation algorithms will be discussed, which includes deducing the mechanism of dielectric reduction of highly confined water, as well as sophisticated design of nanoparticles and polymer electrolytes for next generation energy storage material with tailored structural and dynamic properties Another important study investigates utilizing lipid membranes and biological complexes for controlling molecular transport across the complex interface abundant in biology. Our critical analysis brings two prominent field of energy materials and biological science under common perspective, to stimulate crossover in both research field that have been largely separated.

※本講演はHIS2025「世界を先導する分子化学ⅡB(物質情報化学の最前線)」の一部として開催します

日時：2025年6月17日（火）16:30～18:00

会場：北海道大学 理学部 本館 N-308室

講師：Chang Yun SON 教授

Seoul National University

ソウル国立大学



主催：総合化学院

共催：「物質科学フロンティアを開拓する
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連絡先：世話人　北海道大学理学研究院化学部門
村越 敬（TEL:011-706-2704）