化生研 講演会/ CLS Seminar

Institute of SCIENCE TOKYO

Ion dynamics study at bulk and grain boundaries of Li-ion conductors by molecular dynamics simulations with machine learning potentials

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Time & Date: 10:30-12:00, Thursday 22 Jan 2026
Place: The 2nd Seminar Room, R1 bldg. Suzukakedai campus
(R1棟2F 第二会議室)

Abstract: Recently, computational modeling based on machine learning interatomic potentials (MLIPs) that are trained on high-accuracy density functional theory (DFT) datasets (energies, forces, stresses) have been employed extensively in understanding material properties. In this presentation, I will discuss our recent works related to the ion dynamics study at the bulk and grain boundaries of Li ionic conductors (e.g., N-doped $Li_6Zr_2O_7$, Li_3PS_4) which are crucial materials to realize high-performance all-solid-state Li rechargeable batteries, using MLIPs that are trained by passive and active learning approaches. Detailed analyses on the structural and Li diffusivity (an)isotropic properties of Li ionic conductors will also be presented.

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