The 132nd GREEN Seminar

Exploration of Solid-State Battery Materials through Virtual Screening and a Combinatorial Approach

Chair: Dr. Kei Kubota (GREEN)

Prof. Naoki Matsui

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We present a combinatorial approach through virtual screening and laboratory experiments to accelerate solid-state battery material discovery. A specialized machine learning potential (F-MACE) was developed for fluoride-ion conductors, enabling systematic screening of 72,325 structures with improved accuracy over general-purpose models. Promising candidates balancing high ionic conductivity and electrochemical stability were identified and experimentally validated. A high-throughput platform coupling combinatorial thin-film synthesis, automated electrochemical characterization, and machine-learning analysis was applied to the CeF_3–LaF_3–SrF_2 system, identifying $Ce_{0.93}La_{0.04}Sr_{0.03}F_{2.97}$ as the optimal composition (2.3×10^{-4} S cm^{-1}). This approach was further extended to the optimization of the anode of an all-solid-lithium battery. This unified strategy enables efficient exploration of vast compositional spaces for next-generation energy storage.

Venue: Auditorium, 1F, NanoGREEN/WPI-MANA Bldg., Namiki-site

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