Invited Talk Abstract

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Navigating Complex Materials Energy Surfaces: Integrating Optimization and Machine Learning for Large-scale Materials Simulation and Structural Screening

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Time	17:00–17:30
Session	Session 5
Venue	S102, Lecture Hall, Gong-Guan Campus, NTNU

Abstract

Atomic-level understanding of complex material systems, such as defect-rich photocatalysts, solid-state batteries, and dynamic interfaces, is crucial for the development of next-generation energy devices. Traditionally, exploring these systems relies heavily on first-principles methods like density functional theory (DFT) and ab initio molecular dynamics (AIMD). However, these methods suffer from severe computational bottlenecks. They are prohibitively expensive for both the exhaustive screening of vast configurational spaces (such as complex dopant distributions or surface adsorption sites) and the simulation of macroscopic dynamic behaviors over long timescales. While Universal Machine Learning Interatomic Potentials (uMLIPs) offer a promising pathway to achieve near-DFT accuracy at a fraction of the cost, pre-trained models frequently struggle with out-of-distribution (OOD) configurations, often encountering potential energy surface (PES) "softening" when applied to highly reactive or defective environments.

In this talk, we present a robust transfer-learning framework to overcome these limitations by systematically fine-tuning pre-trained MLIPs (e.g., CHGNet, MACE) using targeted DFT and AIMD datasets. This recalibration of the PES enables a two-pronged approach to solving complex materials problems. First, it serves as a highly efficient surrogate model for global optimization, allowing us to rapidly evaluate the objective function (structural energy) across thousands of configurations. We demonstrate this by successfully screening optimal atomic arrangements for vacancy-engineered and doped ZnIn2S4 piezophotocatalysts, as well as identifying the most stable multi-adsorbate geometries on bimetallic surfaces. This high-throughput structural screening bypasses the combinatorial explosion that cripples conventional DFT.

Second, the fine-tuned MLIPs unlock high-fidelity, large-scale molecular dynamics (MLIP-MD) simulations that extend into the nanosecond regime. We apply this to elucidate complex, continuous bond-breaking and reactive events, including the mechanisms of cobalt-induced lithium-ion trapping at solid electrolyte/cathode interfaces and the atomistic environmental degradation pathways of tin-based perovskites and sulfide electrolytes. Ultimately, this work highlights the transformative role of optimized machine learning models in bridging the gap between mathematical optimization algorithms and macroscopic materials engineering, offering a comprehensive paradigm for data-driven materials discovery.

References

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