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Computational Design of Solid Electrolytes: Combining Multi-Scale Modeling and Machine Learning

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Optimizing ion flow in solid electrolytes is critical for future battery technologies. This talk will cover two powerful computational strategies we use to design better materials. First, we'll dive deep into the classic NaSiCON conductor, showing how our detailed multi-scale simulations pinpointed an exact chemical composition with optimal performance, a prediction we then verified in the lab. Next, we'll shift to a broader challenge: discovering entirely new materials in complex, multi-element systems. We'll introduce our use of cutting-edge Machine Learning Interatomic Potentials (MLIPs) to rapidly screen a novel family of halide electrolytes. This data-driven approach successfully identified a new, highly promising material and taught us how ions move within it. Together, these examples illustrate a powerful workflow that combines rigorous physical modeling with machine learning to dramatically accelerate the discovery of next-generation solid-state electrolytes.

References:

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