Hierarchical screening for Li-based solid electrolytes using fast, interpretable machine-learned potentials

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Li-based solid-state electrolyte materials enable safer, all-solid-state batteries but the computational search for candidates with favorable stability and Li-ion conductivity is challenging due to the size of the search space and the cost of evaluating transport properties with ab initio methods [1]. The prohibitive cost of high-throughput screening with DFT has lead to the development of surrogate models using geometric analysis, empirical potentials, and descriptors for ionic transport [2]. Here, I will discuss a hierarchical screening approach for identifying promising materials using a combination of density functional theory, bond-valence methods, and machine learning potentials generated with the Ultra-Fast Force Fields (UF3) framework [3]. We show how the inexpensive bond-valence method can be used to guide the generation of training samples for machine learning, in addition to filtering candidates. Finally, we apply the hierarchical workflow to screen for stability and ionic conductivity across a database of Li-containing compounds.

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