Application of DFT and Machine Learning and Its Challenges for Novel All-Solid-State Battery Electrolyte Search

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Density functional theory (DFT) and machine learning have now become widely adopted in areas of new materials search and material optimization. The field of all-solid-state batteries is one example of this, specifically on the need to find highly (electro)chemically stable and high-conductivity novel solid electrolytes to replace combustion-prone conventional liquid-/organic-based electrolytes. In here, recent efforts of our group about development of smart and data-efficient workflows for finding novel solid electrolytes for all-solid-state batteries will be presented. A real-problem application of the Bayesian optimization scheme for large-scale solid-electrolyte search will be highlighted, with search criteria such as DFT-accurate ion transport properties (e.g., ionic conductivity, ion migration energy) driving the material space exploration. Details on the actual algorithm and material descriptor design will be discussed. Finally, present prevailing issues and challenges to realize an effective search approach for more practical novel solid electrolytes will also be presented.