Accelerating Materials Design via Computation and Machine Learning Combined Approaches

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ABSTRACT

A long-standing challenge for materials design is to clarify materials microscopic features, and discover their linkage to macroscopic properties and processing parameters. With the recent development of computing equipment and algorithms, modeling and simulations, assisted by artificial intelligence techniques, have become a promising means to tackle the above problem. In this presentation, computation-based strategies for accelerating materials design will be discussed, through the demonstration of three examples from different aspects on combining modeling and machine learning. In the first example, an effective ensemble learning framework was proposed, for automated identification on complex atomic crystal structures from molecular dynamics trajectories, as a generalizable tool to extract materials descriptors. In the second example, Bayesian optimization guided coarse-grained molecular dynamics simulations were performed, to systematically investigate the effects of molecular level material properties on lithium-ion transport in polymeric material systems, for promoting an efficient screening of solid polymer electrolytes. In the last example, a three-dimensional generative-adversarial-networks-based model was established, as an attempt toward inverse design of composite materials with complex structures and multiple optimization objectives.