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Bayesian-Optimization-Guided Coarse-Grained Molecular Dynamics for Polymer Electrolyte Design

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ABSTRACT

Solid polymer electrolytes (SPEs) are considered as promising components of the next-generation lithium-ion batteries, due to their advantages of high safety, plausible processibility, low cost, and intrinsic flexibility. However, the ionic conductivity of current SPEs has to be significantly improved, to meet the application requirements of batteries under practical working conditions, which demonstrates a pressing need for exploring novel polymer electrolyte materials. To achieve this goal, we developed a SPE material design approach by combining coarse-grained molecular dynamics (CGMD) with Bayesian optimization (BO). The coarse graining of the SPE system not only increased the simulation efficiency with maintaining a reasonable capability of describing polymer conformation; but also helped transform the chemical species design space to a CG space composed of physically interpretable descriptors such as molecular sizes and intermolecular interactions. The BO algorithm was then employed to drive the CGMD simulations, for a global exploration of this CG parameter space. The trained model made predictions on the ion transport properties for several well-known polymer electrolytes, all in good agreements with experimental measurements. In addition, our results successfully revealed the joint effects of molecular-level material intrinsic properties on the Li-ion conductivity of the electrolyte system, based on which improving directions of the anions, secondary sites, and polymer chains were proposed. With moderate modifications, this CGMD-BO approach can be generalized, as a powerful tool, to accelerate the optimization and design process for other complex material systems.