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Predicting Fracture and Conduction Propensity in Glassy Electrolytes Using Classification-Based Machine Learning

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Glasses are promising candidates as solid electrolytes for all-solid-state batteries due to their isotropic ionic conduction, formability, as well as high chemical, thermal and electrochemical stability. However, the lack of well-established composition-structure-property relations hinders the design of new glassy electrolytes with tunable functionalities. Here, we combine molecular dynamics simulations with classification-based machine-learning based to clarify the relation between structure and properties in lithium borophosphate glassy electrolytes. Specifically, we focus on the machine learning derived "softness" metric. By isolating the relative effects of Li and B contents on the electrolyte performance, we correlate the fracture behavior and ionic conduction with the bond switching activities of B and the mobility of Li atoms, respectively. Based on the interpretable features of the machine learning model, we identify the most influential structural parameters of the radial order function controlling the atomic behaviors. These results will help to identify new promising compositions of glassy electrolytes with high mechanical stability and ionic conductivity.