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Structure dependence of fracture toughness and ionic conductivity in glassy electrolytes for solid-state batteries

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Abstract

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, their ionic conductivity and mechanical properties need to be improved, which is a complicated task due to the disordered structure and non-equilibrium nature of glasses. Here, we focus on two series of glassy electrolytes, namely lithium borophosphate and lithium thiophosphate glasses. Based on combined experimental and simulation studies, we investigate the structural origin of the variation in fracture toughness and ionic conductivity in the glassy electrolytes with varying compositions. We analyze the changes in glass structure using topological data analysis and classification-based machine learning in order to establish composition-structure-property relations, with important implications for the design of future glassy electrolytes.

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