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Analyzing lithium ion conductivity in thiophosphate glassy electrolytes via machine learning

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Glasses such as lithium thiophosphates ($\text{Li}_2\text{S-P}_2\text{S}_5$) show promise as solid electrolytes in lithium-ion batteries, but a poor understanding of the mechanism by which the disordered structure affects lithium transport properties limits the development of glassy electrolytes. To address this, we here simulate glassy $\text{Li}_2\text{S-P}_2\text{S}_5$ electrolytes with varying fractions of polyatomic anion clusters using classical molecular dynamics. Based on the determined variation in ionic conductivity, we use a classification-based machine learning metric termed “softness” – a structural fingerprint that is correlated to the atomic rearrangement probability – to unveil the structural origin of lithium-ion mobility. To derive a real-space origin of the machine-learned softness metric, we analyze the energy barrier of softness-coded lithium ions migrating between two sites, showing that soft lithium-ion migration requires a smaller energy barrier to be overcome relative to that observed for hard lithium-ion migration.