Automated discovery of novel solid-state ionic conductors enabled by large-scale molecular dynamics computations BORIS KOZINSKY, PRATEEK MEHTA, Bosch Research, Cambridge MA — Fast solid-state inorganic Li-ion conductors offer a path toward safer batteries with high energy density, but apart from a few material classes, the inorganic solid-state space remains mostly unexplored. Computational approaches using density functional theory (DFT) have been proven to be successful for the design of electrode materials, but have had few applications for the discovery of electrolytes. This is because the physiochemical factors that regulate ionic conductivity are poorly understood, and conductivity can be very sensitive to small structural and compositional variations. In this work, we present relationships between the ionic conductivity and several potential structural descriptors, like the size and dimensionality of ion-conducting pathways, void fraction, Li-concentration, sensitivity to volume change, etc. We identify these relationships from massive ab-intio molecular dynamics simulations on a comprehensive dataset of approximately 1500 crystalline materials. Our investigation is enabled by computational resources at the Oak Ridge Leadership Computing Facility and the high-throughput automation platform AiiDA.

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