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A First-principles Molecular Dynamics Investigation of Superionic Conductivity BRANDON WOOD, NICOLA MARZARI, Department of Materials Science and Engineering, MIT — Superionic materials—solids with liquid-like transport properties—have found widespread use in a variety of applications in fuel cells, switches, sensors, and batteries. However, reasons for fast-ion conduction in such materials, as well as the specific atomistic mechanisms involved, remain ill understood. Our work uses first-principles molecular dynamics to illuminate the mechanisms, pathways, and motivations for superionic conductivity in two materials representing different classes of ion conductors: α-AgI, an archetypal Type-I superionic; and $CsHSO_4$, an anhydrous solid-state electrolyte candidate for hydrogen fuel cells. For α-AgI, we trace common pathways for silver ion conduction and discuss how a chemical signature in the electronic structure relates to enhanced silver ion mobility. We also characterize the dynamical lattice structure in the superionic phase and present the likely motivations for its existence. For $CsHSO_4$, we isolate the dominant atomistic mechanisms involved in superprotonic conduction and discuss the effect of correlated diffusive events in enhancing proton transport. We also offer a detailed description of the dynamics of the hydrogen bond network topology in the course of proton diffusion and discuss the relevance of atomistic processes with competing timescales in facilitating proton transport.

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