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A First-principles Investigation of Superionic Behavior: α-AgI as a Case Study BRANDON WOOD, NICOLA MARZARI, Department of Materials Science and Engineering, MIT — First-principles molecular dynamics simulations are well suited to the study of conductivity in superionic solids, thanks to the relatively high frequency of observable diffusion events. AgI offers a paradigmatic example of superionic behavior and as such presents itself as an excellent candidate for our investigation. We combine results from Car-Parrinello simulations of α-AgI with static and linear-response calculations in order to characterize various structural, dielectric, and vibrational properties of the system. The dynamics simulations offer a unique and unbiased characterization of the atomistic mechanisms involved in fast-ion diffusion, including a statistical analysis of most-frequented conduction pathways and sublattice ordering; and direct examination of the maximally localized electronic orbitals offers insight into chemical interactions present between ionic sublattices. We are further able to extract information on the nature of the superionic phase transition, including an investigation of possible thermodynamic and structural motivations for superionic behavior.

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