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Full Phonon Softening and Fast Ag Diffusive Dynamics in Liquid-like Argyrodites Ag8GeSe6

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Argyrodites exhibit weak temperature dependence and low magnitude lattice thermal conductivity (κL) along with decent electrical performances at the high-temperature cubic superionic phase in the virtue of the partially occupied mobile Ag-sublattice interpenetrating a rigid network of (Si, Ge, Sn)X4 tetrahedra. However, the fundamental understanding of the interesting κL in terms of temporal-spatial lattice dynamics and atomic diffusion in the superionic phase of Argyrodites remains unexplored. Herein, we report the inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS) investigations of the lattice dynamics and atomic diffusion on Ag8GeSe6 complemented by synchrotron x-ray diffraction (SYXRD) and Ab initio molecular dynamics simulation (AIMD). We observe a full phonon softening and increasing QENS signal across the superionic phase transition temperature Tc ~ 350 K. We identify a fast Ag diffusion process with a short residence time (τ) of ~ 0.68 ps and reveal the Ag diffusion mechanism. The results emanated from this study will provide a coherent multi-scale understanding of the lattice dynamics and atomic diffusion mechanism, and enrich our knowledge of the heat conduction of Argyrodites.

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