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Soft Phonon Mode Triggering Fast Ag Diffusion in Superionic Argyrodite Ag_8GeSe_6

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The structural coexistence of dual rigid and mobile sublattices in superionic Argyrodites yields ultralow lattice thermal conductivity along with decent electrical and ionic conductivities and therefore attracts intense interest for batteries, fuel cells, and thermoelectric applications. However, a comprehensive understanding of their underlying lattice and diffusive dynamics in terms of the interplay between phonons and mobile ions is missing. Herein, inelastic neutron scattering is employed to unravel that phonon softening on heating to $T_c \approx 350\,\mathrm{K}$ triggers fast Ag diffusion in the canonical superionic Argyrodite Ag_8GeSe_6. *Ab-initio* molecular dynamics simulations reproduce the experimental neutron scattering signals and identify the partially ultrafast Ag diffusion with a large diffusion coefficient of $10^{-4}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$. The study illustrates the microscopic interconnection between soft phonons and mobile ions and provides a paradigm for an intertwined interaction of the lattice and diffusive dynamics in superionic materials.

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