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Short-lived K_2S Molecules in Superionic Potassium Sulfide YUSUKE OKEYA, KAZUO TSUMURAYA, Meiji University — The first principles molecular dynamics method allows us to elucidate the formation of short-lived K_2S molecular states in superionic potassium sulfide. The covalent and the Coulomb bonds exist between the ionized mobile potassiums and the ionized immobile sulfurs. Both the bonds induces indirect covalent and indirect Coulomb attractions between the di-interstitial potassiums on the mid-sulfurs, which forms the short-lived K_2S molecular states. The covalent electron density also exists between short-lived potassium dimers. The three attractions reduce Haven's ratios of the potassiums in the conductor. The molecule formation indicates the electronic state of the conductor is intermediate between the ionic and covalent crystals. The absence of the long-lived potassium dimers implies a failure of the caterpillar diffusion model or the Frenkel-Kontorova chain model for the superionic diffusion of the potassiums in the sulfide. The incompletely ionized cations and anions reduce the Coulomb attractions between them which induces the sublattice melting of smaller size of the potassiums than the sulfurs.

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