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Effect of van Hove singularities on high-Tc superconductivity in H3S WATARU SANO, Department of applied physics, University of Tokyo, TAKASHI KORETSUNE, RIKEN Center of Emergent Matter Science, TERUMASA TADANO, Department of applied physics, University of Tokyo, RYOSUKE AKASHI, Department of physics, University of Tokyo, RYOTARO ARITA, RIKEN Center of Emergent Matter Science — One of interesting open questions for the high-Tc superconductivity in sulfur hydrides is why some of the H3S phases under high pressures are so special. Recently, it has been pointed out that the presence of the van Hove singularities (vHs) around the Fermi level is crucial. Interestingly, such vHs are always absent in H2S, for which Tc is estimated to be much lower. Although there have been quantitative calculations of Tc based on the Migdal-Eliashberg theory, the effect of the vHs on the superconductivity is yet to be fully understood. This is because the energy dependence of the density of states (DOS) has been neglected to simplify the Eliashberg equation. In this study, we perform a calculation beyond the constant DOS approximation. In contrast with the conventional calculations, this approach with a sufficiently large number of Matsubara frequencies enables us to calculate Tc self-consistently without introducing the empirical pseudo Coulomb potential. We show that the constant DOS approximation seriously overestimates (underestimates) Tc by ˜60 K (˜10 K) for H3S (H2S). We then consider the effect of the anharmonicity of the phonon and the energy shift due to the zero-point motion. Eventually, Tc is estimated to be 180 K for H3S and 35 K for H2S, which successfully explains the pressure dependence of Tc observed in the experiment.

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