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Superconductivity in compressed sulfur hydride: Dependences on pressure, composition, and crystal structure from first principles

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The recent discovery of high-temperature superconductivity in sulfur hydride under extreme pressure has broken the long-standing record of superconducting transition temperature (Tc) in the Hg-cuprate. According to the isotope effect measurement and theoretical calculations, the superconducting transition is mainly ascribed to the conventional phonon-mediated pairing interaction. It is, however, not enough for understanding the high-Tc superconductivity in the sulfur hydride. To elucidate various possible effects on Tc with accuracy, we have analyzed Tc with first-principles methods without any empirical parameters. First, for various pressures and theoretically proposed crystal structures, we calculated Tc with the density functional theory for superconductors (SCDFT) to examine which structure(s) can explain experimentally measured Tc data [Akashi et al., PRB 91, 224513(2015)]. We next solved the Eliashberg equations without introducing the renormalized Coulomb parameter mu*, which is the Green-function-based counterpart of the SCDFT, and evaluated the effects of rapidly varying electron density of states, atomic zero-point motion, and phonon anharmonic corrections on Tc [Sano et al, in preparation]. In the talk, we review these results and discuss the dominant factors for the Tc and their relation to the experimental results. We also report some crystal structures that we recently found with first-principles calculations, which could have a key role for the pressure-induced transformation to the high-Tc phase.