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Structure, lattice dynamics, and high-Tc superconductivity in hydrogen sulfide under high pressure LINDA HUNG, TANER YILDIRIM, NIST Center for Neutron Research — The recent discovery of superconductivity near 200 K in hydrogen sulfide under pressures 200 GPa has sparked interest in the search for hydrogen-rich superconducting materials. The observed large isotope effect and earlier first-principles calculations convincingly suggest that the high Tc is due to strong electron-phonon coupling, i.e., that hydrogen sulfide is a conventional superconductor. Hence, first-principles predictions of phonon properties can be used in the search for new phases that can superconduct at even higher temperatures and lower pressures. In this talk, we present structural and lattice dynamics calculations of various phases of H_2S/H_3S, examining the electron-phonon coupling and superconductivity in each phase using the finite-displacement and frozen-phonon approaches. The effect of anharmonicity on electron-phonon coupling, isotope effect, and superconducting temperature is discussed. Finally, we explore the properties of potential new hydrogen-sulfide-based materials.

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