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High Temperature Superconductivity at High Pressures for $\text{H}_3\text{SixP}(1-x)$, $\text{H}_3\text{PxS}(1-x)$ and $\text{H}_3\text{ClxS}(1-x)$ ¹ DIMITRIOS PAPACONSTANTOPOULOS, FUDONG FAN, George Mason Univ, MICHAEL MEHL, Naval Research Lab — Recent experimental and computational works have established the occurrence of superconducting temperatures, T_c , around 200K at corresponding 200GPa pressures in hydrogen-based sulfur compounds. In this work we have investigated the effects of phosphorus and chlorine substitutions of sulfur on T_c , as well as the effect of hydrogen vacancies. In addition, we have explored the superconductivity-relevant parameters in the $\text{H}_3\text{SixP}(1-x)$ system. In executing this work we have used the virtual-crystal-approximation and performed a systematic set of LAPW calculations for many different concentrations of the sulfur component. From the densities of states and the scattering phase-shifts at the Fermi level, we calculated electron-ion matrix elements and estimated the electron-phonon coupling constants for different concentrations as well as T_c . We find that the high values of T_c correlate with the position of the Fermi level with respect to peaks (van Hove singularities) in the density of electronic states of these materials.

¹US Department of Energy

Dimitrios Papaconstantopoulos
George Mason Univ

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