Abstract Submitted
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First-principles demonstration of superconductivity at 280 K in hydrogen sulfide with low phosphorus substitution YANFENG GE, School of Physics, Beijing Institute of Technology, Beijing 100081, China — Recently BCS superconductivity at 190 K has been discovery in a highly compressed hydrogen sulfide[1,2]. We use first-principles calculations to systematically examine the effects of partially substituting the chalcogenide atoms on the superconductivity of hydrogen chalcogenides under high pressures2. We find detailed trends of how the critical temperature changes with increasing the V-, VI- or VII-substitution rate, which highlight the key roles played by low atomic mass and by strong covalent metallicity. In particular, a possible record high critical temperature of 280 K is predicted in a stable H3S0.925P0.075 with the Im3m structure under 250 GPa[3]. [1] A. P. Drozdov, M. I. Eremets, and I. A. Troyan, Conventional superconductivity at 190 K at high pressures, arXiv:1412.0460 (2014). [2] A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, S. I. Shylin, Conventional superconductivity at 203 K at high pressures in the sulfur hydride system. Nature 525, 73-76 (2015) [3] Y. F. Ge, F. Zhang, and Y. G. Yao, First-principles demonstration of superconductivity at 280 K in hydrogen sulfide with low phosphorus substitution, Phys. Rev. B 93, 224513 (2016).

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