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High T_c phase of $(H_2S)_2H_2$ at high pressures

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Hydrogen was predicted to metalize at high pressures and believed to be a room-temperature superconductor. However, metallization of hydrogen is still under debates. As an alternative, hydrogen dominated materials were extensively explored because of their lower metallization pressure. Here I present the high-pressure studies on structures, metallization, and superconductivity of $(H_2S)_2H_2$ from *ab initio* calculations [1]. At lower pressures, two phases containing H_2 units are stable with $P1$ (<37 GPa) and $Cccm$ (37-111 GPa) symmetries, which are still insulators. Upon further compression, H_2 units disappear and two intriguing metallic structures with $R3$m and Im-$3m$ symmetries are reconstructive above 111 GPa and 180 GPa, respectively. Remarkably, the estimated T_c of Im-$3m$ phase at 200 GPa achieves a very high value of 191 $\sim$ 204 K. Moreover, T_c decreases with pressure at an approximate rate (dT_c/dP) of -0.12 K/GPa. Our predicted high T_c and its pressure dependence in Im-$3m$ phase are subsequently verified by recent experiments [2]. Our findings support the conjecture that hydrogen-rich materials are a way to achieve a metallic phase with high T_c at accessibly experimental pressures and represent a significant step toward the understanding of high-pressure behavior of metallic hydrogen.

[1] D. Duan, Y. Liu, T. Cui, et al. Sci. Rep., 4, 6968 (2014)
[2] A. P. Drozdov, M. I. Eremets, and I. A. Troyan, arXiv:1412.0460, (2014)