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Progress toward the discovery of a room-temperature superconductor: theoretical studies of the observed superconductivity above 200K in the sulfur hydride system at high pressure

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Abstract content
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It has been long conjectured (1) that metallic hydrogen or hydrogen-containing compounds offer the possibility of extremely high superconducting temperatures, perhaps at room temperature or above, with some explicit electronic structure studies adding further weight to these ideas (2). The discovery of conventional BCS-like superconductivity in a cubic compound of sulfur and hydrogen by Drozdov, et al. (3) has created great excitement in that the holy grail of a room-temperature superconductor may be possible. The highest Tc reported in the H-S system is 203K for a compound likely in the Im-3m structure under high pressure (3). Theoretical studies of this system have been reported by several groups (4,5). Here we present the advances in the understanding of this and similar systems developed by using ab initio electronic structure calculations to determine their electronic and phononic behavior and the electron-phonon coupling strengths that result from these studies. We show that ab initio computer simulations give a very good understanding of the high Tc that is driven by a combination of strong electron-phonon coupling and high frequency hydrogen optic modes. The role of anharmonicity will be put into perspective and we will discuss the underlying chemical bonding in these systems that can provide a guide to discovering materials with even higher values of Tc.

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