Contribution ID: **7** Type: **not specified**

Prediction of pressure-induced superconductivity in ternary systems YScH2n(n=3-6)

Monday, 25 September 2023 10:35 (15 minutes)

Hydrogen-rich ternary compounds are promising candidates for realizing of room-temperature superconductivity due to the synergistic effects of crystal structure and electronic properties under high-pressure conditions. Here, the high-pressure structures, electronic properties, and superconductivity of the ternary YScH2n (n=3-6) system are investigated by using the prediction method of particle swarm optimization structure combined with first-principles calculations. We find four stable structures, each with different hydrogen sublattices:YScH6, YScH8, YScH10, and YScH12, all of them are potential high-temperature superconductors. The electron local function (ELF) results indicate a lack of interaction between hydrogen atoms in YScH6, while the weak H-H covalent interactions are observed in the other stoichiometric ratios. Strikingly, YScH6 maintains dynamic stability down to ambient pressure and keeps a high superconducting critical temperature (Tc) of 66 K. At 140 GPa, the pressure-stabilized YScH8 and YScH10 structures exhibit high Tc of 110 and 116 K, respectively. Upon further increasing the content of hydrogen, the lowest dynamically stable pressure of YScH12 is increased to 200 GPa, and the calculated Tc is up to 179 K. In all YScH2n structures, YScH6 (stabled at 1 atm to 100 GPa), YScH8 and YScH10 (stabled at 140 to 250 GPa), YScH12 (stabled at 200 to 300 GPa), strong electron-phonon coupling and large electronic density of states of hydrogen at the Fermi level play important roles in their high-temperature superconductivity. It is discussed that that phonon softening in the mid-frequency region induced mainly by Fermi surface nesting effectively enhances the electron-phonon coupling. Our work prospectively discovered high-temperature superconducting hydrides that can be stable at atmospheric pressure, taking an important step towards understanding the superconductivity and structural stability of ternary hydrides.

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Session Classification: 多学科组