First-principles study of high temperature superconductivity of compressed YKH_{12}

(M2)Peng Song[1,2], Zhufeng Hou[3], Yoshihiko Takano[1,2]

(1. NIMS, 2. Univ. of Tsukuba, 3. CAS)

E-mail: SONG.Peng@nims.go.jp

Recently, with the successful discovery of superconductivity in LaH_{10}(~260 K at ~200 GPa)[1] and H_3S(~200 K at ~ 200 GPa)[2] by experiment, metal hydrides have contributed more and more to the study of high temperature superconductivity (HTSC). The search for superconducting metal-hydride at very high pressures has long been viewed as a key problem in physics. Many researchers have conducted extensive research on binary hydrogen-rich compounds involving the binding of most elements of the periodic table to hydrogen. More than 60% of the binary metal hydrides over the Mendeleev's Periodic Table have been shown superconductivity. The ternary or multi-component hydrides have become the ideal playground to discover HSTC. Recently, the superconductivity in Li_2MgH_{12}[3] was found and shown an ultra-high critical temperature of 473 K (200 GPa) by structure prediction.

In this work, we extensively performed structure search for the high-pressure phase and superconductivity of YKH_{12} using the evolutionary algorithm structure prediction method and first-principles calculations. The results showed that YKH_{12} became stable at 150 GPa and had a C2/m structure. And its stability will increase with the increase of pressure, and the second stable phase $P2_1/m$ appears above 270 GPa. Electron-phonon coupling calculations show that YKH_{12}-C2/m is a potential high-temperature superconductor, with a Tc of 145 K at 200 GPa. YKH_{12} can be regarded as a combination of YH_6 and KH_6, so our current research provides the possibility to find new high temperature superconducting ternary hydrides.

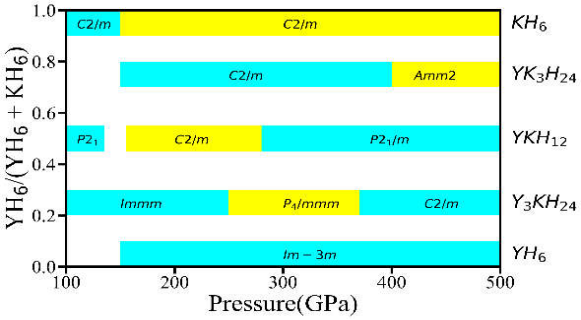

Figure 1. phase diagram of Y-K-H compound

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