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Abstract

Superconducting hydrides have attracted significant attention in recent years due to their potential for achieving high-temperature superconductivity under high-pressure conditions. The discovery of high-temperature superconductivity in hydrogen-rich materials, such as sulfur hydride (H_3S) and phosphine (PH_3), has spurred extensive research efforts to explore novel superconducting hydride materials with the aim of understanding the underlying mechanisms and optimizing their properties for practical applications. Ternary hydrides, comprising multiple metal elements and hydrogen, offer promising candidates for further investigation due to their complex compositions and the possibility of fine-tuning their electronic and structural properties. In this context, this thesis focuses on the investigation of ternary hydrides composed of lanthanum, yttrium, magnesium, scandium, and cerium to uncover new stable phases with enhanced superconducting transition temperatures.

In the La-Y-H system, we investigated their phase and structural stabilities under high pressure using a genetic algorithm and *ab – initio* calculations. Our study revealed that $Pm\bar{3}m$-$LaYH_{12}$ was unstable and identified new stable crystal structures, such as $Cmmm$-$LaYH_{12}$ and $Cmmm$-LaY_3H_{24}. The $Cmmm$ phases exhibited a T_c of approximately 140 K due to their extremely high electron-phonon coupling constant, with an increased T_c in $Cmmm$-LaY_3H_{24} attributed to the chemical pressure of Y.

For the $YMgH_x$ system, the investigation probed the structural stabilities of high-pressure $YMgH_x$ phases and their superconductivities using an evolutionary-algorithm-based crystal search combined with first-principles calculations. The study identified several stable and metastable phases, with high-T_c values ($\geq$ 77 K) predicted for H-richer phases, such as $P4/mmm$-$YMgH_8$ (124 K at 300 GPa), $Cmmm$-$YMgH_{12}$ (152 K at 250 GPa), and $Fd\bar{3}m$-$YMgH_{12}$ (190 K at 200 GPa). These phases feature clathrate structures composed of H_{14}, H_{18}, H_{24}, and H_{24} cages.

The $Mg_xSc_yH_z$ system was examined under high pressure ($100 \leq P \leq 200$ GPa), resulting in the identification of four thermodynamically stable compounds in the hydrogen-middle range, including $R\bar{3}m$-$MgScH_6$, $C2/m$-Mg_2ScH_{10}, $Immm$-$MgSc_2H_9$, and $Pm\bar{3}m$-$Mg(ScH_4)_3$. Among them, $R\bar{3}m$-$MgScH_6$ was predicted to exhibit the highest T_c (i.e., 41 K) at 100 GPa.

In the Y-Ce-H and La-Ce-H systems, the study employed the evolutionary-algorithm-based crystal structure prediction method and first-principles calculations to investigate stability and superconductivity under high pressure. Several stable phases were identified, with T_c values predicted using the Allen-Dynes-modified McMillan formula to be 122 K for $R\bar{3}m$-$YCeH_{20}$ at 300 GPa, 116 K for $R\bar{3}m$-$LaCeH_{20}$ at 250 GPa, and 173 K for $P\bar{6}m2$-$YCeH_{18}$ at 150 GPa. The pressure required to stabilize $P\bar{6}m2$-$YCeH_{18}$ can be reduced to 150 GPa, suggesting an accessible condition for its high-pressure synthesis.

This comprehensive study offers valuable insights into high-temperature superconducting materials and their potential applications. The identification of stable and metastable phases in these

ternary hydride systems and the prediction of their superconducting transition temperatures enhance our understanding of these materials.

Keywords: First-principles calculation, Pressure effects, Structural properties, Hydride ,Superconducting phase transition