Advancements in Ternary Hydrides: Predictive Modeling of Y-Th-H System for High-Tc Superconductivity

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Recent discoveries of compressed ternary hydrides [1, 2, 3] exhibiting high-T_c superconducting temperatures have sparked renewed interest in the field and opened new avenues for research. These ternary hydrides demonstrate remarkable synergistic properties, manifesting higher T_c values at lower pressures compared to their binary counterparts. In line with this, we have explored the phase space of Y-Th-H hydrides, motivated by the earlier reports on superconducting binary hydrides of Yttrium (YH_3, YH_6, YH_9) and Thorium (ThH_4, ThH_6, ThH_{10}), their high-T_c superconducting properties, and most importantly their similar atomic radii, which ensures the stability of lattice formed from the admixture of Y, and Th-based ternary hydrides. In this study, employing an evolutionary algorithm, we have successfully predicted stable hydrides based on the Y-Th-H system: *I4/mmm*-Y_2ThH_{12}, *P4/mmm*-$YThH_8$, and *P6m2*-$YThH_{18}$. To ensure their dynamic stability, phonon calculations were performed, followed by the application of the Allen-Dynes modified McMillan formula to predict their superconductivity. Our calculation reveals that under a pressure of 200 GPa, *P6m2*-$YThH_{18}$ exhibits a remarkable superconducting transition temperature of up to 130 K. These discoveries highlight the potential of ternary hydrides as promising candidates for achieving high-T_c superconductivity and offer valuable insights into their stability, superconducting properties, and potential applications in advanced superconducting systems.

References

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