# Y-Mg 系三元水素化物高温超伝導体の構造安定性に関する系統的研究

## The systematic study on the stability and superconductivity of Y-Mg-H compounds under high pressure

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Recently, with the experimental verification of room temperature superconductivity in C-S-H compounds ($T_c$ ~ 288K at ~ 267GPa), [1] ternary hydrides have been playing an increasingly important role in the search for novel high-temperature superconductors. [2] Here we have investigated structural stabilities of high-pressure $YMgH_x$ phases ($x$ = 2 ~ 10, 12, 14, and 16) and their superconductivities by employing evolutionary-algorithm-based crystal search combined with first-principles calculations. For predicted candidate structures of $YMgH_x$, our convex hull and phonon analyses revealed seven stable and two metastable phases. For all the predicted phases, we also predicted superconducting transition temperatures ($T_c$) by using the McMillun formula. We found $P4/mmm$-$YMgH_6$ having $T_c$= 76 K at 300 GPa comparable to the boiling temperature of liquid nitrogen, and high-$T_c$ (≥ 77 K) being predicted for the H-richer phases, $P4/mmm$-$YMgH_8$ (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), which possess clathrate structures composed of $H_{14}$, $H_{18}$, $H_{24}$, and $H_{24}$ cages, respectively. To elucidate why the H-rich phases attain high-$T_c$, we analyzed electronic and phonon band structures as well as electron-phonon coupling strength based on Eliashberg spectral functions. The clathrate structures exhibit both a larger H-driven electronic density of states at the Fermi level and a denser H-driven phonon density of states, correlating with larger EPC constants. Our structural and chemical bonding analyses has revealed that the highest-$T_c$ phase $Fd\bar{3}m$-$YMgH_{12}$ has $H_4$ units formed in the sodalite cage (Fig. 1).

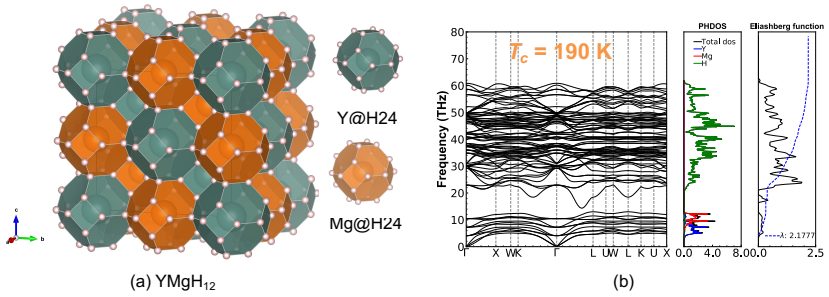


図 1: (a) Clathrate structure and (b) Phonon dispersions, projected phonon densities of states, and Eliashberg spectral function of $Fd\bar{3}m$-$YMgH_{12}$.

## 参考文献

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