Computational Investigation of Strongly Correlated Yttrium, Europium-based Ternary Hydrides

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Eu-based binary hydrides have been found to exhibit strong magnetic properties due to the complex interaction of localized 4-*f* electrons in Eu-atoms. Motivated from the recent trend of discovery and synthesis of ternary hydrides from the admixture of two binary phases [1-3], using the evolutionary algorithm, we have theoretically investigated the existence of ternary phases $YEuH_x$ (x = 8, 10, 12, 14, 16, 18, 20) formed from YH_x and EuH_y binaries. Our ternary-hull analysis revealed novel ternary hydrides namely *Pm*-$YEuH_{18}$, *P*1-$YEuH_{12}$, *Cmmm*-$YEuH_8$ at 200GPa and *Pm*-$YEuH_8$ at 100GPa, for which we confirmed their thermodynamic stability. These compounds exhibit cage-like clathrate H-sublattice structure even for very low symmetry phases such as *P*1 and *Pm* without H_2 molecular units. Electron-phonon interaction is found to be weak, nevertheless, our magnetic ordering calculation reveals that *P*1-$YEuH_{12}$ and *Pm*-$YEuH_{18}$ show antiferromagnetic ordering, whereas *Cmmm*-$YEuH_8$ and *Pm*-$YEuH_8$ possess ferromagnetic ordering having absolute magnetic moment as high as 6.3 μ_B/Eu-atom (see Figure 1).

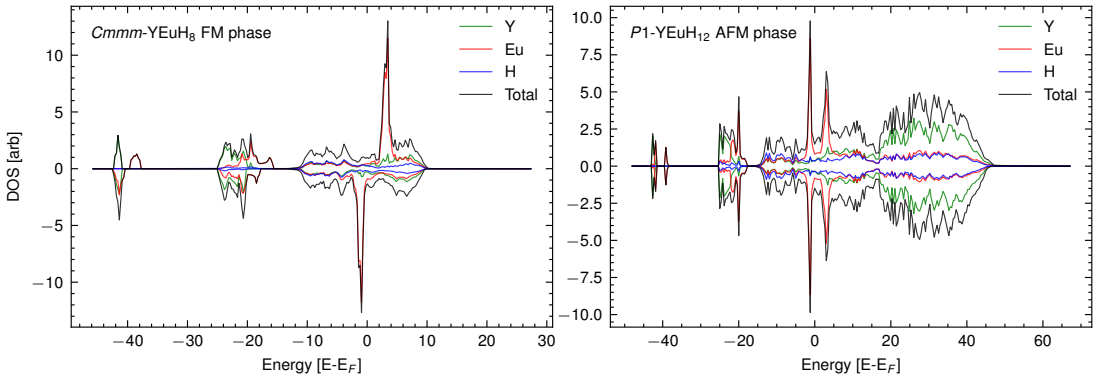

Figure 1: Spin-polarized DOS of FM *Cmmm*-$YEuH_8$ and AFM *P*1-$YEuH_{12}$ configurations.

References

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