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Transition metal based borohydrides for hydrogen storage CHAKRAM JAYANTHI, University of Louisville, JIANJUN LIU, SUHUAI WEI, YUFENG ZHAO, National Renewable Energy Lab — Using *ab-initio* studies based on the density-functional theory, we have calculated binding energies per hydrogen molecule for decomposition reactions of transition metal borohydrides $MH_xB_{12}H_{12}$ to MB_{12} structures, where M corresponds to Sc*, Ti, or V*. Depending on the valence of the transition metal, x can be $1, 2$, or 3. Crystal structures considered for MB_{12} included both hypothetical and those found in the international crystallographic structural database. On the other hand, the crystal structure considered for $MH_xB_{12}H_{12}$ belongs to C2/c (space group 15) structure as reported in a previous study [V. Ozolins *et al.* JACS, **131,** 230 (2009)]. Among the structures investigated, Titanium-based metal borohydride structure has the lowest binding energy per hydrogen molecule relative to the cubic TiB_{12} structure ($\sim$0.37 eV/H_2). Our finding should be contrasted with the binding energy/H_2 for simple metal based borohydrides (*e.g.*, $CaB_{12}H_{12}$), which has a value of $\sim$ 1.5 eV/H_2, suggesting that transition metals play a significant role in lowering the H_2 binding energy in borohydrides.

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