Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project - DTU Orbit (16/12/2018)

Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project

We present a computational screening study of ternary metal borohydrides for reversible hydrogen storage based on density functional theory. We investigate the stability and decomposition of alloys containing 1 alkali metal atom, Li, Na, or K (M1); and 1 alkali, alkaline earth or 3d/4d transition metal atom (M2) plus two to five (BH4)− groups, i.e., M1M2(BH4)2–5, using a number of model structures with trigonal, tetrahedral, octahedral, and free coordination of the metal borohydride complexes. Of the over 700 investigated structures, about 20 were predicted to form potentially stable alloys with promising decomposition energies. The M1(Al/Mn/Fe)(BH4)4, (Li/Na)Zn(BH4)3, and (Na/K)(Ni/Co)(BH4)3 alloys are found to be the most promising, followed by selected M1(Nb/Rh)(BH4)4 alloys.

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