First Principles Investigation of the Stability and the Chemical Behavior of Hydrogen in ThCoH₄

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We address the changes in the electronic structure brought by the insertion of hydrogen into ThCo leading to the experimentally observed ThCoH₄. Full geometry optimization positions the hydrogen in three sites stabilized in the expanded intermetallic matrix. From a Bader charge analysis, hydrogen is found to be in a narrow ionic-covalent (\(\sim -0.6\)) to covalent (\(\sim -0.3\)) bonding which should enable site-selective desorption. The overall chemical picture shows a positively charged Th\(\delta^+\) with the negative charge redistributed over a complex anion \(\{\text{CoH}_4\}\delta^-\) with \(\delta \sim 1.8\). Nevertheless this charge transfer remains far from the one in the more ionic hydridocobaltate anion CoH₅\(^4-\) in Mg₂CoH₅, due to the largely electropositive character of Mg.

Key words: ThCo Intermetallic, DFT, CrB Type, Hydrides, Bader Charge, Chemical Bonding