International Journal of Hydrogen Energy Vol. xx (2013) Page. yy-zz, Article in press,
http://dx.doi.org/10.1016/j.ijhydene.2013.05.035

Hydrogen storage in Laves phases: First principles study of electronic structure and formation energies in HfV_2 hydrides

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We present first principles calculations of the electronic structure, enthalpies of formation and electric field gradients in C15 HfV_2H_x (x = 1, 2, 3, 4). In C15 Laves phases, hydrogen can occupy three possible interstitial positions: 96g, 32e, and 8b. To determine which one of these interstitials is the most favorable for storing hydrogen, enthalpies of formation were calculated for every site, with different concentrations of hydrogen. In order to investigate the change in electronic structure before and after hydrogenation, we calculated the electric field gradients induced by hydrogen on the vanadium, and compared them with the existing nuclear magnetic resonance measurements. This comparison enabled us to study the distribution of hydrogen atoms in the crystal lattice, as well as the occupation of possible interstitials.