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Hydrogen Absorption/Desorption in Palladium and Metal Hydrides

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Abstract: Electrical generation from hydrogen, the element with higher energy density per unit mass, requires appropriated materials that can be used in its storage [1]. Palladium, with a high capacity to dissociate, absorb and desorb gaseous hydrogen, has been widely used for hydrogen storage [2], in separation membranes [3] and catalytic hydrogenation [4]. The present DFT calculations on clusters models reveal interesting details of the hydrogen absorption/desorption process in palladium and metal hydrides. The results point to the existence of a pre-absorption state of the hydrogen atom on palladium and indicate that occupation of the tetrahedral site is preferred at low hydrogen concentrations (α-phase), whereas in β-phase the octahedral site is the most stable. Taking the absorption and desorption energies of palladium as reference, we analyzed the properties of the metal hydrides AlH_3, MgH_2, $Mg(BH_4)_2$, $Mg(BH_4)(NH_2)$ and Li_2NH for hydrogen storage. Among these compounds, MgH_2 most closely resembles the properties of palladium, but the complex hydrides in borohydrides (BH_4^-) and amide (NH_2^-) show better properties both in absorption and desorption. Furthermore we found that Cu and Pd doping of MgH_2 can reduce the desorption energy, improving the hydrogen release.

Keywords: Palladium storage hydrogen; metal hydrides storage hydrogen; DFT calculations;

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