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Nanostructured catalyzing agents for hydrogen desorption from light metal hydrides

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Hydrogen, as an energy carrier, is nowadays considered as one of the best alternatives for mobile and stationary power sources for both propulsion and fuel cells. However, one of the major drawbacks of this technology is the problem of storing hydrogen safely, since in liquid and gas form, this demands high pressure or cryogenic reservoirs. An alternative is the use of solid state hydrogen storage, wherein the light metal hydrides represent a promising solution. However, since these are usually highly stable compounds, where the hydrogen atoms are held by strong covalent bonds, high temperatures are required for the hydrogen desorption. In order to surpass this difficulty the addition of catalysts has been considered, such as transition metals and nanostructured agents. In this study first, principle calculations based on density functional theory are performed to investigate the role of catalysts in dehydrogenation from clusters of light metal hydrides. It is shown that the addition of titanium and nanostructured carbonaceous catalysts contributes for a significant gain in the energy cost for hydrogen desorption from the metal hydrides. The combined addition of titanium with carbon fullerenes is even more beneficial for decreasing the energy cost of dehydrogenation. This effect is confirmed for different metal hydrides like alanates and boranates. For example, the calculated energy cost for H-removal from the magnesium boro-hydride is 4.18 eV, which decreases to 4.08 eV upon the addition of the fullerene C60, and to 3.32 eV in the presence of C67. The combined addition of Ti and these fullerenes lead to a decrease of energy cost for the H-removal to 4.04 eV and 2.78 eV, respectively. The energetics of dehydrogenation is also investigated in super-halogen clusters of light metal hydrides, and the results show that the hydrogen release is substantially less energy demanding in these highly reactive moieties. Results of van der waals-corrected DFT calculations show a rather significant gain in the energy cost for H desorption with the addition boron-doped fullerene catalysts. In the source of this effect is the disturbance introduced in the distribution of bonding charge upon the hybridization of states in the interplay between the hydride cluster and the fullerene with a consequent weakening of the hydrogen bonds, leading therein to an enhanced kinetics for the hydrogen release.

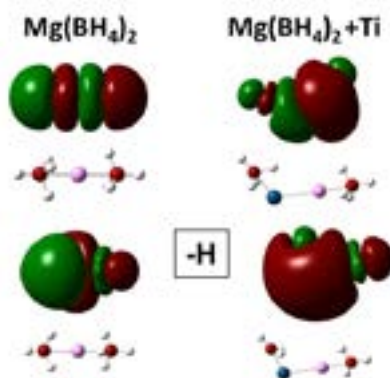


Fig. 1: HOMO plots of $Mg(BH_4)_2$ with the addition of titanium and upon H-removal.

Biography

Clederson Paduani is currently working as an Associate Professor at Universidade Federal de Santa Catarina in Florianópolis, SC, Brazil. He has been working with DFT calculations in clusters, solids and nanostructures, after completing his Post-doctoral degree at CNRS, Grenoble, UCSC, CA, VCU, VA, and UPenn, PA.

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