Density Functional Studies of C_{60}-Pd Nanostructure

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Conductivity and hybridization of C_{60}-Pd nanostructure have been investigated using density functional calculations. From analysis of geometry, energetics and electronic structures, the interaction of C_{60} mono-layer and Pd clusters gives rise to electronic charge transfer at the interface and facilitates the dissociation and uptake of hydrogen, which lead to hydrogen storage. The first-principles studies are carried out by self-consistent plane-wave method. The interaction between ions and electrons is described by projector-augmented wave (PAW) approach. In our calculations, the C_{60} monolayer is doped by the Pd_n atoms on *h*-BN with $n = 1\text{-}4$ and 15, but it also forms a metal-C_{60} nano-array with the Pd clusters.

Charge transfer occurs at the interface, from the Pd atoms towards the C_{60} monolayer. This electronic property strongly depends on the nature and number of metal atoms, but also the type and strength of the interaction. A large amount of charge transfer between the Pd atoms and the C_{60} monolayer indicates a strong interaction under the ionic effect, in contrast with the interaction of the C_{60} monolayer and a metallic surface [1, 2]. The *h*-BN surface merely gains very few electrons (~ 0.1 electron/molecule) via C_{60}, proving that *h*-BN is an insulating material.

Pd is a good catalyst for dissociation and storage of hydrogen on the C_{60} molecules. Hydrogen is sufficiently dissociated in the presence of the Pd atoms/clusters, which assists in bonding of the individual H atoms to C_{60}. Dehydrogenation of $C_{60}H_x$ is also discussed in energetics.

[1] L-L Wang and H-P Cheng, Phys. Rev. B **69**, 045404 (2004).
[2] L-L Wang and H-P Cheng, Phys. Rev. B **69**, 165417 (2004).