First-Principles Investigation of $C_{60}$-Pd Interface

LAN LI, HAI-PING CHENG — Conductivity and hybridization of $C_{60}$-Pd nano-system 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 $n = 1$-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. 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. The $h$-BN surface merely gains 0.1 electrons via $C_{60}$, proving that $h$-BN is an insulating material. We also find that 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.