**First-Principles Investigation of C\textsubscript{60}-Pd Interface**

LAN LI, HAI-PING CHENG — Conductivity and hybridization of C\textsubscript{60}-Pd nano-system have been investigated using density functional calculations. From analysis of geometry, energetics and electronic structures, the interaction of C\textsubscript{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\textsubscript{60} monolayer is doped by the Pd\textsubscript{n} atoms on h-BN with n = 1-4 and 15, but it also forms a metal-C\textsubscript{60} nano-array with the Pd clusters. Charge transfer occurs at the interface, from the Pd atoms towards the C\textsubscript{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\textsubscript{60} monolayer indicates a strong interaction under the ionic effect, in contrast with the interaction of the C\textsubscript{60} monolayer and a metallic surface. The h-BN surface merely gains 0.1 electrons via C\textsubscript{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\textsubscript{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\textsubscript{60}. Dehydrogenation of C\textsubscript{60}H\textsubscript{x} is also discussed in energetics.

Lan Li

Date submitted: 26 Nov 2007  
Electronic form version 1.4