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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.

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