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First principles investigation of one monolayer of C60 on h-BN/Ni(111)[1] JINGGUANG CHE[2], Department of Physics and Quantum Theory Project, University of Florida, Gainesville, USA, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, USA
— The geometric and electronic structures of a monolayer of C60 on a monolayer h-BN on Ni(111) surface are studied by first principles calculations. The interaction between ions and electrons is described by the projector-argumented wave method. The most stable structure is found to be N on the top and B on the fcc site of Ni(111). The structure in which a hexagon of the C60 molecular is parallel to the substrate is 0.1eV in energy more favorable than that of a pentagon parallel to the substrate. For the most stable adsorption sites of C60 on h-BN/Ni (111), the distance between the bottom hexagon of C60 and the h- BN/Ni substrate is 3.6A. The calculated results show that the energy differences for different orientations are all smaller than 0.2eV. No magnetic moment is found for C60 monolayer. The calculated electronic structures confirm that the h-BN/Ni(111) may be a good insulator platform to study the electronic structures of C60 ultrathin films, since only a weak interaction and a few charge transfer exist between C60 and h-BN/Ni(111).

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