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Simulation of Fe_n-doped C_{60} Monolayer on *h*-BN/Ni (111)[1] LAN LI, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — We have performed first-principles calculations based on density functional theory to investigate the structure, electronic structure and magnetic properties of Fe_n-C_{60} complexes. Interfaces that consist of a C_{60} monolayer, a supporting h-BN/Ni (111) layers, and the transition metal Fe_n (n = 1-4 & 15) have been thoroughly characterized. Electron transfer has been observed from the Fe ions to the C_{60} molecules, which leads to the domination of ionic character on the Fe-C_{60} bonding. Furthermore, the Fe_n-doped C_{60} systems show strong hybridizations between s-, d- orbitals of Fe atoms and p-orbital (π-like) of C atoms. The spin of the net transferred electrons from Fe_n to C_{60} is spin minority, which leads to a magnetic moment in C_{60} opposite to the total magnetic moment of the system. All of the electronic structure calculations have been performed in generalized gradient approximation (GGA) and local density approximation (LDA). In Fe_4C_{60} and $Fe_{15}C_{60}$ systems, we have also performed GGA+U and LDA+U calculations for comparison.

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