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The structural and electronic properties of a K-doped C60 monolayer of on h-BN/Ni(111)[1] HAI-PING CHENG, JINGGUANG CHE[2], Department of Physics and Quantum Theory Project, University of Florida, Gainesville, USA — The structural and electronic properties of a K-doped C60 monolayer are investigated using first principles calculations based on density functional theory. The K-doped C60 monolayer is deposited on an insulator h-BN monolayer on a Ni(111) surface. The interaction between ions and electrons is described by the projector-argumented wave method (PAW). It is found that K atoms are incorporated into the interstitial sites of the C60 monolayer with a distance of 2.9∼3.0A to the h-BN/Ni substrate, while the distance of a hexagon face of C60 to the substrate is 3.6A. The calculated results indicate that with K doping the electron occupation on bands that are derived from the C60 lowest unoccupied molecular orbital (LUMO) is enhanced. For doping of four K atoms per C60 molecule, the LUMO is almost half- filled. Detailed analysis and comparison with an un-doped C60 monolayer on the same substrate and with pure metal surfaces will be presented.

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