Structures and electronic structures of K_3C_{60} monolayers

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We present first-principles calculation of structures and electronic structures of K_3C_{60} monolayers on Ag (111) and (001) surfaces. In case of K_3C_{60} monolayers on the Ag (111) surface, we consider C_{60} molecules in a hexagonal lattice with the lattice constant of 10.02 Å, and calculate the total energy and the energy-band dispersion for various molecular orientations. We find a C_{60} molecular orientation whose total energy is very close to the minimum and its LUMO-derived band dispersion has the important features observed by a high-resolution angle-resolve photoelectron spectroscopy (ARPES). The calculated bandwidth, however, is still substantially larger than the measured one, suggesting a renormalization effect in real samples. In case of K_3C_{60} monolayers on the Ag (001) surface, we study c(6*4) structures with different C_{60} orientations, obtaining very different LUMO-derived energy-band dispersions. We interpret the difference of the ARPES energy-band dispersions of K_3C_{60} monolayers on the Ag (111) and (001) surfaces as a result of different molecular orientations of fullerenes in the monolayers.

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