Structures and electronic structures of $K_3C_{60}$ monolayers

Hyoung Joon Choi$^1$, Steven G. Louie$^2$, and Marvin L. Cohen$^2$

$^1$School of Computational Sciences, Korea Institute for Advanced Study, Seoul 130-722, Korea.
$^2$Department of Physics, University of California, Berkeley, CA 94720, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

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.
