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On the inhomogeneous structure and charge transfer of C_{60} monolayer on Ag(001) XIEQIU ZHANG, AIDI ZHAO, XUDONG XIAO, Department of Physics and Institute of Nano Science and Technology, Hong Kong University of Science & Technology, Hong Kong, China, WEI HE, JINLONG YANG, Heifei National Laboratory for Physical at Microscales, University of Science and Technology of China, Heifei, Anhui 230026, China — We have studied the morphological and electronic structure of C_{60} ML/Ag(001) by STM/STS and first principles calculation. The bright-dim contrast of adsorbed C_{60} molecules is identified as originating from geometric effects. Among the dim C_{60} molecules, there consist of dim monomers (DM) and dim dimers (DD), which display distinguished STS. The dI/dV spectra give the energy locations of HOMO, LUMO and LUMO+1-derivated energy bands and the different STS spectra for B, DM, and DD C_{60} molecules indicate that the charge transfer from the substrate is strongly inhomogeneous. The charge transfer has been estimated as $\sim$0, $\sim$1, $\sim$2 electrons/molecule for B, DM and DD from the shift of their corresponding LUMO+1 energy bands, respectively. The DFT calculations give the consistent spectra for B, DM and DD C_{60} molecules with experimental STS data, but with smaller charge transfer.

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