Electronic Structure and Charge Distribution in the C_{60}-FET

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We study the charge profile of a C_{60}-FET (field effect transistor) as used in the experiments of Schön, Kloc and Batlogg. Using a tight-binding model, we calculate the charge profile treating the Coulomb interaction in a mean-field approximation [1]. At low doping, the charge profile behaves similarly to the case of a continuous space-charge layer and becomes confined to a single interface layer for doping higher than ~ 0.3 electron (or hole) per C_{60} molecule. The morahedral disorder of the C_{60} molecules smoothens the structure in the density of states. In the case of high doping, a similar approach was used on the molecular level in order to study the charge distribution in the interface layer. In this regime, the C_{60} molecules behave like metallic spheres and screen efficiently the electric field of the FET. As a consequence, the molecular Stark effect due to the electric field is substantially reduced and the nature of the LUMO and HOMO orbitals is not significantly changed.

We also considered the effect of a planar step in the interface layer. Such a step causes a potential drop which in turn is screened by the doped carriers. We find the transmission coefficient through the step is strongly density dependent. At larger dopings the step acts as a weak link and generates a Josephson junction when the system goes superconducting.

[1] S. Wehrli, D. Poilblanc and T. M. Rice, Eur. Phys. J. B **23**, 345 (2001)