

Investigation of electric properties of single organic molecules deposited on surfaces

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Abstract

In this dissertation a model system is presented for investigation of properties of single organic molecules connected to a metal electrode. The system is prepared by deposition of gold atoms on InSb(001) $c(8 \times 2)$ surface to form metal electrodes, growing a film of KBr for electric insulation and finally by adsorbing small amount of PTCDA molecules on top. After each step, the system is investigated using scanning tunnelling microscopy and tunnelling spectroscopy. PTCDA molecule's properties are investigated in the following systems: PTCDA on InSb(001) $c(8 \times 2)$, PTCDA on thin layer of KBr/InSb and PTCDA on thin layer of KBr/InSb, and contacted to metallic nanoisland.

It is found that a negative charge is accumulated on PTCDA molecule adsorbed on clean InSb(001) $c(8 \times 2)$ surface and orbital, corresponding to LUMO of free molecule, is observed as occupied. Analysis of the experimental data compared to theoretical results obtained by DFT calculation enabled exact determination of positioning of adsorbed PTCDA molecule on InSb(001) surface.

There are not experimental indications for electrical charging of PTCDA molecule adsorbed on thin layer of KBr/InSb. Corresponding to HOMO of free PTCDA orbital is occupied and corresponding to LUMO of free PTCDA molecule orbital is empty. Difference between energy of HOMO and LUMO of PTCDA adsorbed on KBr layer is not less than 3eV, and HOMO orbital is positioned 0.9eV below substrate's Fermi level.

Bias dependence of STM images and dI/dV curves for molecules on thin layer of KBr/InSb and connected to the metallic nanoisland showed, that an interaction with metallic island modify electronic state of the PTCDA molecule. The molecule at the island has lowered (along energy axis) unoccupied orbitals levels: the relative shift (compared to the molecule on KBr layer) is about 1eV.