

Spin split molecular orbital induced by interface with a magnetic surface measured by spin polarized STM

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Abstract Molecular spintronics is based on the exploitation of spin transport properties of organic materials connected to magnetic electrodes. In such devices, the interface between molecules and magnetic electrodes plays a major role. Therefore, the interfacial hybridization and spin polarization between the organic layer and the ferromagnetic electrodes has to be understood at the molecular scale. When an organic molecule is brought into contact with a metallic electrode, its molecular levels are generally broadened and shifted depending on the geometrical and electronic details of the contact. In the case of a magnetic electrode, these broadening and shifting are in principle spin dependent leading finally to a spin-polarized density of states of the molecule itself.

Using spin polarized scanning tunneling microscopy (SP-STM) we have studied the spin polarization of single C₆₀ molecules adsorbed on a Cr(001) substrate [1]. The Cr(001) surface exhibits an antiferromagnetic coupling between adjacent terraces that can be revealed in the dI/dV spectroscopic signal using a tungsten tip coated by an iron layer [2,3]. Comparing the dI/dV spectra of molecules adsorbed on adjacent terraces allows therefore to access to the spin dependant electronic transport of C₆₀ when the tip and the sample are in the parallel or antiparallel magnetic configurations. Figure 1 shows a composite SP-STM image where the 3D topography is color coded by the spin resolved differential conductance levels, revealing the two in-plane opposite magnetization of adjacent chromium terraces. A sparse distribution of single molecules all adsorbed on pentagonal rings allows simultaneous individual and statistical investigation of the spin-dependent transport through the fullerene molecules. We performed a spectroscopic study of the spin resolved electronic density of states of the adsorbed molecules allowing us to obtain information on the spin dependent transport in the tunnel regime through single C₆₀ molecules. We found TMR values up to 100% that reverses its sign between -0.5V and 0V. A spatial mapping of the spin resolved local density of states allowed to visualize the spin polarization of the molecular orbitals that appear at these energies. Using ab initio calculations all the molecular orbitals observed by STM were identified. The hybridization with the substrate was shown to lead to a spin split of the LUMO state with a large energy separation of 0.5 eV for the spin up and spin down channels. This hybridized molecular state is responsible for an inversion of sign of the tunneling magnetoresistance depending on energy.

These results show the strong spin polarization of a non magnetic molecule contacting a magnetic electrode opening new routes for the engineering of molecular spintronic devices.

References

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Figures

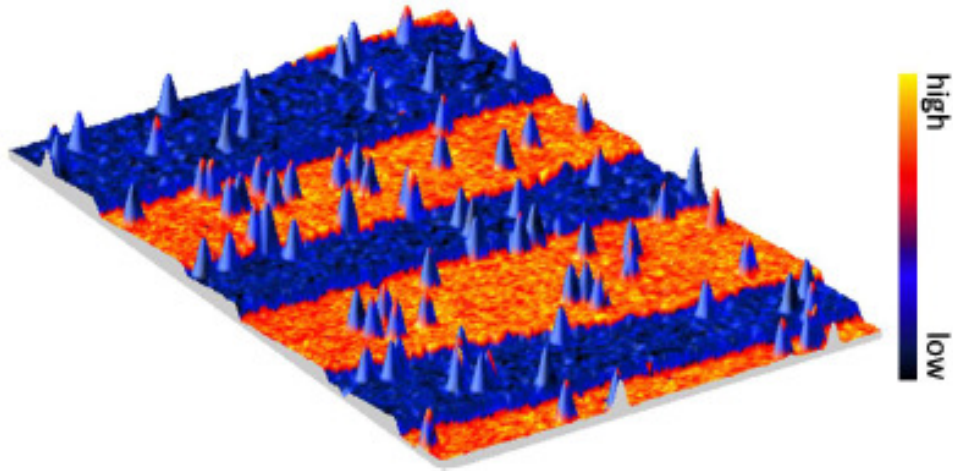


Fig. 1. Constant current STM image ($100 \times 65 \text{ nm}^2$) of the C₆₀/Cr(001) system mapped with the color coded dI/dU values.