

conference

Monday August 29th

Facultad de Ciencias
Aula 405, Módulo 13
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10.00h

Structure and stability of a quinquethiophene based self-assembled monolayer

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In organic electronics the use of self-assembly is one promising approach to high yield and reproducibility in device fabrication. Quinquethiophene SAMFETs have been built with a yield of one. Accordingly integrated circuits like bit generators could be realized [1]. Two elements of the molecule are crucial for the monolayer formation and the electronic properties. First the monofunctional anchoring group which avoids uncontrolled polymerization and second the high tendency of quinquethiophene to form nice lateral crystallographic order. This highly ordered system is responsible for the charge transport properties within the self assembled monolayer. Electronic and crystallographic properties have been investigated for the submonolayer state [2]. It is the first system reported with a long range ordered self-assembled monolayer formed on SiO₂.

The formation of monolayers has been followed by atomic force microscopy and x-ray reflectivity. However a slight tendency to form multilayers has been found by AFM. The in-plane order of the monolayer has been investigated by grazing incidence in-plane diffraction which reveals three nicely pronounced Bragg rods already in the submonolayer state. From the in-plane order a herringbone packing of the molecules within a rectangular unit cell is deduced. DFT calculations have been performed to calculate the packing of the molecules within the unit cell determined by the experiments. Two different phases can be seen in the crystal ordering, one consisting of upright standing molecules and another one where the molecules are tilted 13° towards the b-axis of the unit cell. A transition between these phases is forced by temperature treatment of the SAM. In the pristine state right after preparation in the solution the molecules are standing upright. After the first temperature treatment (330K) they are found to be already tilted. At elevated temperatures however the molecules are always standing fully upright. The crystallographic order is lost above 520K, followed by a dramatic decrease in layer thickness at 620K and complete desorption above 880K.

REFERENCES

- [1] E.C.P. Smits et al., "Bottom-up organic integrated circuits", *Nature* **455**, 956-959 (2008)
- [2] S.G.J. Mathijssen et al., "Monolayer coverage and channel length set the mobility in self-assembled monolayer field-effect transistors", *Nature Nanotechnology* **4**, 674 - 680 (2009)

