

**PHTHTALOCYANINE DERIVATIVES ON (111) NOBLE METAL SURFACES –
MULTIPHASE BEHAVIOR AND CAPABILITY OF HOSTING OTHER
MOLECULES**

Tomas Samuely (a), Shi-Xia Liu (b), Nikolai Wintjes (a), Mihaela Enache (a), Marco Haas (b), Silvio Decurtins (b), Thomas A. Jung (c), Meike Stöhr (a)

(a) Institute of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

(b) Department of Chemistry and Biochemistry, Freiestrasse 3, University of Bern, 3012-Bern, Switzerland

(c) Laboratory for Micro- and Nanostructures, Paul-Scherrer-Institute, 5232 Villigen, Switzerland

tomas.samuelyt@unibas.ch

Symmetrically substituted phthalocyanines (Pcs) with eight peripheral di-(tert-butyl)phenoxy (DTPO) groups¹ self-organize on (111) noble metal surfaces into various assembly structures (Fig. 1a). The rotational degrees of freedom allow all the DTPO substituents to be arranged above the plane of the Pc core, forming a bowl-like structure, which in turn enables the interaction of the Pc core with the metal substrate. The structural phases can coexist due to a significant retardation of the thermodynamic optimization of the conformations, caused by the proximity of the Pc core to the metal substrate together with the steric entanglement between neighbouring DTPO substituents.² Moreover, a substitution of a dipyrido[3,2-f:2',3'-h]quinoxaline (DPQ) in place of two adjacent DTPO groups results in an asymmetric structure of the Pc derivative.¹ Such a variation induces even more assembly structures by further expanding the plethora of conformational possibilities. (Fig. 1b)

The specific conformation with the DTPO groups arranged above the plane of the Pc core predetermines such assemblies to serve as hosts accommodating other guest molecules. This can be of great importance for the construction of possible future applications by the bottom-up approach. As an example, C₆₀ molecules, upon deposition on the densest ordered layer of the symmetric Pc derivatives, bind to two clearly distinguishable sites (Fig. 2), exhibiting different morphologic and electronic properties. The electronic structure of the adsorbed C₆₀ molecules, revealed by tunnelling spectroscopy investigations, are in good agreement with the proposed model of the adsorption and with the expected charge transfer in the Pc- C₆₀ complex.

All measurements were carried out at various temperatures, with a scanning tunneling microscope housed in an ultra high vacuum system, consisting of different chambers for sample preparation and characterization.

References:

[1] Haas, M.; Liu, S. X.; Kahnt, A.; Leiggenger, C.; Guldi, D. M.; Hauser, A.; Decurtins, S., **20** (2007) 7533.

[2] Samuely, T.; Liu, S. X.; Wintjes, N.; Haas, M.; Decurtins, S.; Jung, T. A.; Stohr, M., *Journal of Physical Chemistry C*, **15** (2008) 6139.

Figures:

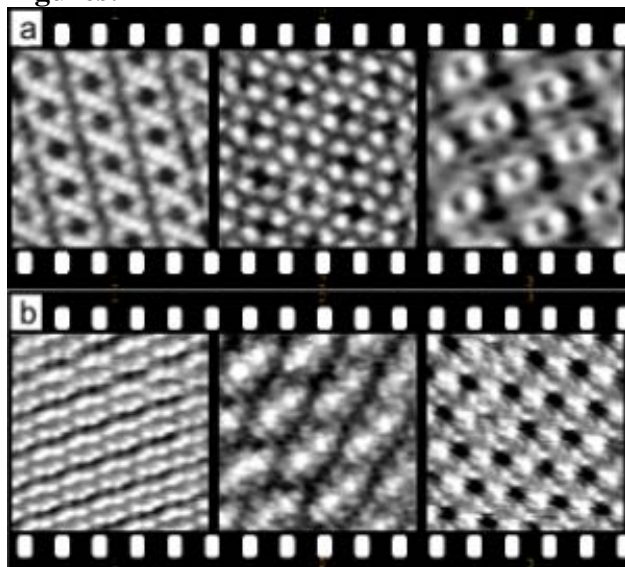


Figure 1. STM images ($10 \times 10 \text{ nm}^2$) of Pc derivatives self-organized on (111) noble metal surfaces. a) Various assemblies of the symmetric DTPO-Pc b) Various assemblies of the asymmetric DTPO-DPQ-Pc

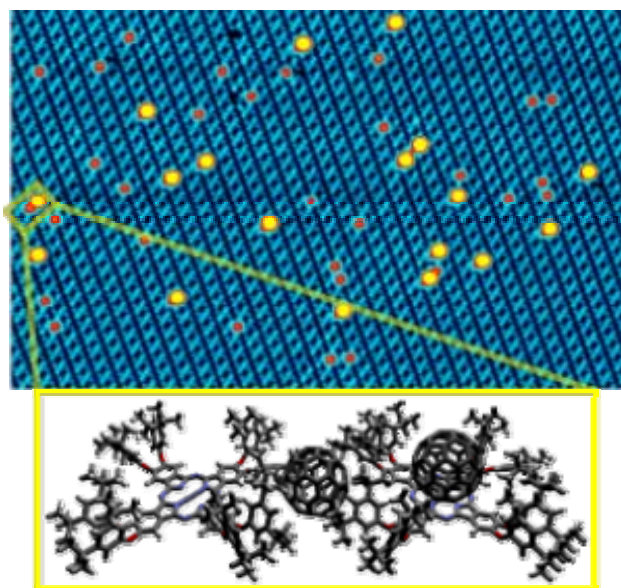


Figure 2. Top: STM image ($80 \times 50 \text{ nm}^2$) of C_{60} molecules adsorbed onto the densest ordered layer of the symmetric Pc derivatives. Bottom: 3D model of the molecules marked by the yellow rectangle in the STM image.