

Interface-driven formation of a two-dimensional dodecagonal fullerene quasi crystal

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Close-packed monolayers of Buckminsterfullerenes (C_{60}) on metallic substrates are very rich systems with respect to their rotational degrees of freedom and possible interactions with different adsorption sites or next neighbors. They have attracted much attention due to their structural and electronic properties. Here, we focus on the ability of C_{60} to form self-assembled monolayers that mirror impressively the electronic properties of the respective substrate. Using low-temperature UHV-STM and STS in combination with DFT calculations the interactions of C_{60} molecules with a metallic surface, an alloy, and a thin titanium oxide film are characterized in detail. The LT-STM images with highly resolved orbital structure allow a detailed assignment of the C_{60} adsorption orientation and geometry with respect to the underlying substrate. Moreover, even second order interface effects, that is, interactions of C_{60} with atoms of the subsurface layer are identified. Most interestingly, in the case of a Pt_3Ti -single crystal alloy used as substrate the influence of subsurface Ti-atoms on the self-assembly behavior of fullerenes is determined. By employing DFT calculations, the preferred adsorption sites of the fullerenes have been identified. Here, third layer Ti-atoms provoke an adsorption energy landscape of the Pt_3Ti -single crystal alloy so that the C_{60} /alloy interfacial interactions result in the formation of a two-dimensional dodecagonal fullerene quasicrystal, which can be described in terms of a square-triangle tiling.

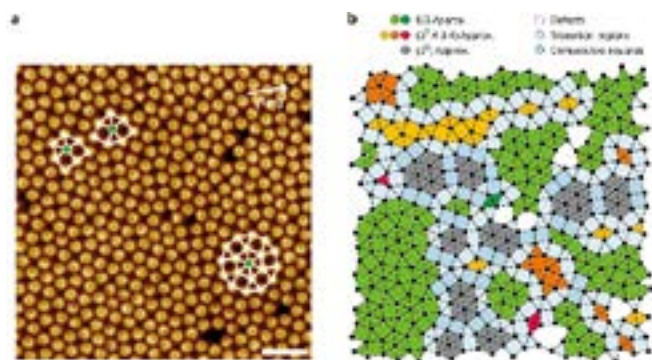


Figure 1: Dodecagonal square-triangle tiling, as measured by STM. (a) High-resolution UHV-STM image of C_{60} on 2Pt- $Pt_3Ti(111)$ (scale bar: 3 nm). One dodecagon and two local

structures are indicated in white. (b) Square-triangle tiling extracted from a), with color-coded decomposition into different types of approximants.

Recent Publications

- Paßens M, Waser R, Karthäuser S (2015) Enhanced fullerene-Au(111) coupling in $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ -superstructures with cooperative intermolecular interactions. *Beilstein J. Nanotechnol.* 6: 1421-1431.
- Paßens M, Karthäuser S (2015) Interfacial and intermolecular interactions determining the rotational orientation of C_{60} adsorbed on Au(111). *Surf. Sci.* 642: 11-15.
- Paßens M, Caciuc V, Atodiresei N, Moors M, Blügel S, Waser R, Karthäuser S (2016) Tuning the surface electronic structure of a $Pt_3Ti(111)$ electro catalyst. *Nanoscale* 8: 13924-13933.
- Paßens M, Moors M, Waser R, Karthäuser S (2017) Energy level alignment at the fullerene/titanium oxide ultrathin film interface. *J. Phys. Chem. C* 121: 2815-2821.
- Paßens M, Caciuc V, Atodiresei N, Feuerbacher M, Moors M, Dunin-Borkowski R E, Blügel S, Waser R, Karthäuser S (2017) Interface-driven formation of a two-dimensional dodecagonal fullerene quasicrystal. *Nat. Commun.* 8: 15367.

Biography

Silvia Karthäuser has her expertise in the self-assembly of organic molecules and nanomaterials on surfaces; surface analysis and electronic transport phenomena with spectroscopic and scanning-probe methods; design, fabrication and electronic characterization of novel nano-electronic test devices. Special interest: phenomena at organic-metal or organic-semiconductor interfaces; chemical structure – electronic property relationship of functional organic molecules; addressing molecular structures by external triggers, e. g. electronic or photonic.

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