Interface constraints leading to 2D-quasicrystalline fullerene structures

Silvia Karthäuser[1], Michael Paßens[1], Nicolae Atodiresei[2], Vasile Caciuc[2]

[1]*Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany*

[2]*Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH and JARA, D-52425 Jülich, Germany*

s.karthaeuser@fz-juelich.de

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. Moreover, C_{60} has the ability to form self-assembled monolayers that mirror impressively the electronic properties of the respective substrate. Most interestingly, in the case of a $Pt_3Ti(111)$-single crystal alloy [1] used as substrate the influence of subsurface Ti-atoms on the self-assembly behaviour of fullerenes leads to the formation of a 2-dimensional quasicrystalline structure [2].

Conventional crystals have a periodic structure whose elementary cells are repeated at regular intervals and can be joined together without gaps. Quasicrystals, in contrast, also enable other symmetries – for example fivefold symmetries or the here determined dodecagonal structure which is formed by triangular and quadrangular basic elements consisting of fullerenes.

Using low-temperature UHV-STM and STS and employing density functional theory calculations, we identify the complex adsorption energy landscape of the Pt-terminated Pt_3Ti-surface that is responsible for the quasicrystal formation. The LT-STM images with highly resolved orbital structure allow a distinct assignment of the C_{60} adsorption orientation and geometry with respect to the underlying substrate (Figure 1) and thus, provide a detailed insight into an interface-driven formation mechanism of the dodecagonal quasicrystalline structure.

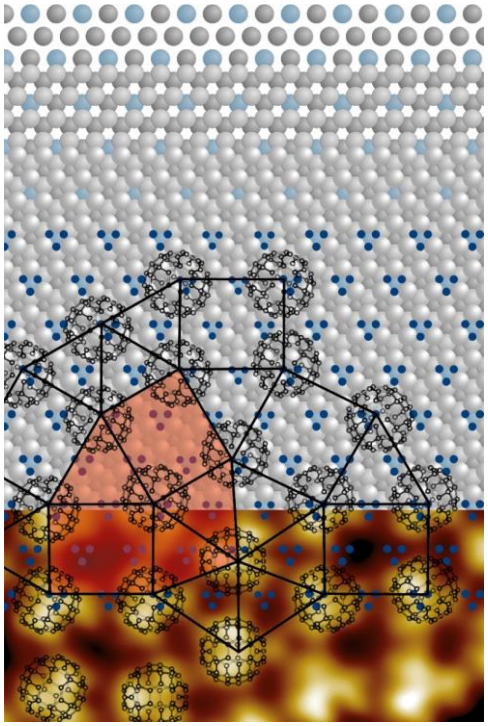

Figure 1: From top to bottom it is shown how the platinum–titanium alloy initially forms, where the energetically preferred spaces are (blue dots), and how the fullerene molecules arrange themselves into triangles and squares. At the bottom a high-resolution scanning tunnelling microscopy image of the fullerene quasicrystalline structure is depicted.

References:

[1] Michael Paßens, Vasile Caciuc, Nicolae Atodiresei, Marco Moors, Stephan Blügel, Rainer Waser, Silvia Karthäuser, Nanoscale **8**, 13924 (2016).

[2] Michael Paßens, Vasile Caciuc, Nicolae Atodiresei, Michael Feuerbacher, Marco Moors, Raphal E. Dunin-Borkowski, Stephan Blügel, Rainer Waser, Silvia Karthäuser, Nat. Commun. **8**, 15367 (2017).