Influence of interface constraints on the assembly of two-dimensional fullerene quasicrystals

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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. 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, which can be described in terms of a square-triangle tiling [2].

Using low-temperature UHV-STM and STS and employing density functional theory calculations, we identify the complex adsorption energy landscape of the Pt-terminated $Pt_3Ti(111)$-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 (Fig. 1). Thus, a detailed insight into an interface-driven formation mechanism of the dodecagonal quasicrystalline structure is provided.

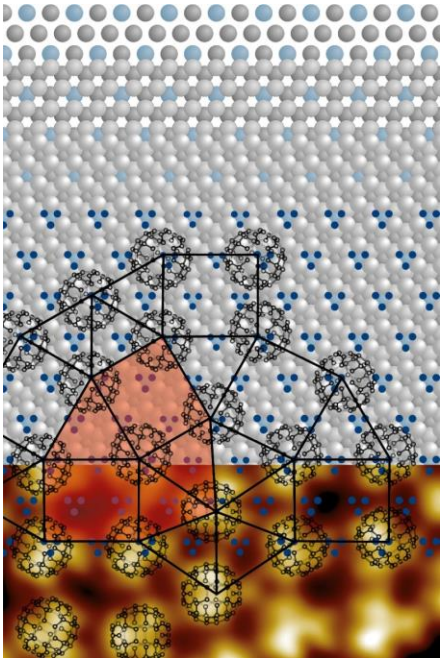

Figure 1. From top to bottom it is shown how the platinum–titanium alloy initially forms, where the energetically preferred spaces are (blue dots), and how the fullerene molecules arrange themselves into triangles and squares. At the bottom a high-resolution scanning tunnelling microscopy image of the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

Furthermore, quasicrystal-specific phason strain is identified to enable the accommodation of the quasicrystalline structure on the periodic substrate. Finally, it will be shown that this general concept, to generate quasicrystalline structures by tuning the adsorption energy landscape as a consequence of the introduction of suitable atoms in subsurface layers of a periodic substrate, can be successfully applied [3].

1. M. Paßens, V. Caciuc, N. Atodiresei, M. Moors, S. Blügel, R. Waser, S. Karthäuser, *Nanoscale* **8**, (2016), 13924.

2. M. Paßens, V. Caciuc, N. Atodiresei, M. Feuerbacher, M. Moors, R. E. Dunin-Borkowski, S. Blügel, R. Waser, S. Karthäuser, *Nat. Commun*. **8**, (2017), 15367.

3. S. Karthäuser, M. Paßens, M. Feuerbacher, R. E. Dunin-Borkowski, R. Waser, ready for submission.