Large-scale simulations of molecular self-assembly on epitaxial graphene on Ru(0001)

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Epitaxial graphene on metals, in analogy to ultra-thin films of alkali-halides and oxides,[1,2] can be used to decouple the electronic states of molecular adsorbates from the substrate, and allow the visualization of their orbitals with intramolecular resolution.[3,4] In the case of a strong interaction with the underlying metal, however, the electronic structure of graphene is strongly perturbed,[5] and such modification can have unexpected consequences on the properties of the molecular overlayer. As a prototypical example of this situation, we have studied the adsorption of the electron acceptor 7,7',8,8'-tetracyanoquinodimethane (TCNQ) on monolayer graphene grown on Ru(0001). Using large-scale calculations based on Density Functional Theory (DFT),[6,7] we have characterized the role of charge-transfer at the interface, as well as the nature of the lateral interactions that are at the origin of the formation of highly ordered molecular monolayers.

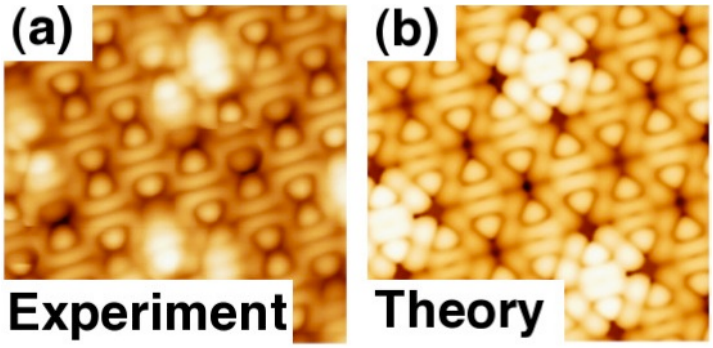

Figure: Measured (a) and simulated (b) scanning tunnelling microscopy (STM) topographies at a bias voltage of -1 V for TCNQ monolayer deposited on graphene/Ru(0001).

References:

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