Magnetic functionalities in epitaxial graphene structures by means of molecular deposition

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Abstract

Cryogenic scanning tunneling microscopy (STM) measurement and large-scale density functional theory (DFT) calculations are used to provide evidence that the deposition of electron acceptor molecular species can be employed to add magnetic functionalities to otherwise non-magnetic epitaxial graphene surfaces. DFT calculations predict that the 7,7',8,8'-tetracyano-p-quinodimethane (TCNQ) molecule develops a finite magnetic moment upon adsorption on epitaxial graphene on Ru(0001) [1,2,3] due to single electron transfer from the substrate, which is subsequently verified by the appearance of a prominent Kondo resonance in the measured STS spectra. At larger coverage, the self-assembled monolayer formed by the charged TCNQ molecules develops spatially extended spin-split electronic bands (see Fig. 1), whose predicted spin alignment is verified by spin-polarized STM measurements [4]. Furthermore, by co-depositing TCNQ and its fluorinated derivative 2,3,5,6-Tetrafluoro-7,7',8,8'-tetracyano-p-quinodimethane (F4-TCNQ) on the same surface, it is shown that while the charged TCNQ molecules spontaneously self-assemble to form molecular oligomers, F4-TCNQ oligomers are not formed because of the reduced delocalization of the extra electrons transferred from the surface. This makes it possible to control the spatial selectivity of the two distinct radical anions on the surface, thus paving the way for the creation of two-dimensional heteromolecular arrays of purely organic magnetic molecules on epitaxial graphene surfaces [5].

References

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Figures

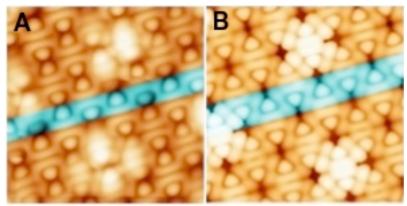


Figure 1: Intermolecular organic band formed by self-assembled TCNQ molecules on epitaxial graphene on Ru(0001). Panels A and B show an experimental STM topography at 4K (V_b = -0.8 V) and the corresponding simulated STM topography.