Magnetic functionalities in nanostructured epitaxial graphene by means of molecular deposition

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Abstract: Cryogenic scanning tunneling microscopy (STM) measurement and 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]. A more systematic analysis of the Kondo resonance observed for the isolated molecules adsorbed on the graphene moiré further reveals that the Kondo response of the system is strongly inhomogeneous, as only those molecules adsorbed on specific low areas of the moiré present a well-defined Kondo resonance in the STS spectra. DFT calculations trace back this behavior to the existence of a surface resonance whose amplitude at the surface depends on the precise geometry of the moiré pattern [5].