

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Transient magnetization of core excited organic molecules adsorbed on graphene¹ ABHILASH RAVIKUMAR, ANU BABY, HE LIN, GIAN PAOLO BRIVIO, Department of Materials Science, University of Milano-Bicocca, Milano, Italy, GUIDO FRATESI, Department of Physics, University of Milano, Milano, Italy — This work presents a density functional theory based computational investigation of electronic and magnetic properties of physisorbed and chemisorbed organic molecules on graphene in the ground state and core excited one at low molecular coverage. For physisorbed molecules, where the interaction with graphene is dominated by van der Waals forces and the system is non-magnetic in the ground state, it is found that the valence electrons relax towards a spin polarized configuration upon excitation of a core-level electron. The magnetism depends on efficient electron transfer from graphene on the femtosecond time scale. On the contrary, when graphene is covalently functionalized, the system is magnetic in the ground state presenting two spin dependent mid gap states localized around the adsorption site. At variance with the physisorbed case upon core-level excitation, the LUMO of the molecule and the mid gap states of graphene hybridize and the relaxed valence shell is not magnetic anymore.

¹This project has received funding from the European Union Seventh Framework Programme under grant agreement n° 607232 [THINFACE]

Abhilash Ravikumar
University of Milano-Bicocca, Milano, Italy

Date submitted: 28 Oct 2015

Electronic form version 1.4