Some aspects of magnetism, charge transfer and anomalous transport in functional graphene quantum dots and heterostructures

Rajarshi Roy
David Holec, Lenka Zajickova, Jennifer Gomez Inmaculada, Saikat Sarkar, Gundam Sandeep Kumar, David Necas, Meena Dhankar, Preeti Kaushik, Petr Lepcio, Nazdezda Pizurova, Dusan Hemzal, Lukas Michal, Phillipp Muenzer, Markus Kratzer, Christian Teichert
Institute of Physics of the Czech Academy of Sciences, Cukrvarnicka 10/112, Czechia.
Contact@E-mail (Century Gothic 10)

Abstract

Graphene quantum dots have attracted a lot of due to superior optoelectronic and functional properties applicable in diverse domains of cutting-edge research from energy to optoelectronics and biomedical and beyond. However low temperature magnetism and electrical transport of these functional or doped GQDs and their heterostructures still remain elusive thus far. In this work, we demonstrate the prospect of chemically synthesizing transition metal (Ni) doped magnetic graphene quantum dots (GQDs) with the sole aim of shedding light on their magnetic properties. Our results show that adsorption of nickel hydroxide on predominantly paramagnetic GQDs reveals antiferromagnetic ordering in the M–T profile around 10 K with change of the spin exchange coupling deviating from J = 1/2 to J = 1, mainly arising from the d–p mixing hybridization between the p orbital of carbon from the GQD and the d orbital of Ni. Our results are well complemented by ab initio simulations showing asymmetry of the up and down spins around the Fermi level for nickel hydroxide-doped GQDs with long-range spin polarization. The magnitude of the net magnetic moment generated for doped GQDs on the carbon atoms is found to be site-dependent (surface or edge). [1] Moreover, we highlight on the abrupt change of resistance (T1 ~ 213K, T2 ~ 325K) in a 0D−2D van der Waals (vdW) heterostructure comprising of single layer graphene (SLG) and functionalized (amine) graphene quantum dots (GQD). Using Kelvin probe force microscopy (KPFM) measurements and ab-initio simulations, we confirm that the incorporation of functional GQDs leads to a charge transfer induced p-type doping in graphene. [2] Finally, we elucidate the interplay between electron-electron and electron-phonon interactions to substantiate high temperature EPC driven charge ordering in the heterostructure through analyses of magnetotransport and weak anti-localization (WAL) framework. [3]

References

[1] L Michal, R Roy*, D Holec, I Jennifer Gomez, N Pizurova, D Necas, J Medalova, A Doleckova, P Lepcio, L Zajickova, J. Phys. Chem. Lett. 2022, 13, 49, 11536–11542.

[2] R Roy*, D Holec, M Kratzer, P Muenzer, P Kaushik, L Michal, G S Kumar, L Zajickova, C Teichert, Nanotechnology 33 (2022) 325704.

[3] R Roy* et al. Possible charge ordering and anomalous transport in graphene/graphene quantum dot heterostructure (communicated)