THEORY OF MAGNETIC NANOPARTICLES ON 2D MATERIALS FOR NOVEL TRANSPORT PROPERTIES

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The main objective of this thesis is to induce tailored magneto-transport properties in graphene by proximity effect of well-defined assemblies of nanomagnets. It is of high importance to explore from a theoretical point view what are the induced spin polarized states due to various types of nanomagnets. We are interested in particular by FePt nanoclusters coupled magnetically on top of graphene. The objective of both theoretical and experimental efforts within the ANR project (submitted) is to cross-link the predictive power of the computational modeling for revealing the magnetic properties at the atomic scale with the experimentally determined microstructure and magnetic characteristics. Such a synergy between theory and experiment will help to extract those parameters from the atomic scale that could affect the macroscopic magnetic properties and help us identify new magnetic nanocluster candidates **to induce tailored magneto-transport properties in graphene by proximity effect of well-defined assemblies of nanomagnets.**

The magnetic nanoclusters on top of graphene will be modeled using slab geometry. It will be interesting to study the tuning of magnetic coupling of the magnetic nanocluster induced magneto-transport in graphene as a function of the number of layers. Our approach of computer simulation is based on methods for obtaining a reliable description, at the atomic scale, of the electronic structure and transport properties of materials from first principles. This task will be carried out by means of the state-of-the-art spin-dependent Density Functional Theory (DFT) with various approximation to the exchange-correlation potential. The quantum transport will be conducted using the transiesta code, which is a fully spin-polarized code, which combines DFT with the non-equilibrium Green's functions (NEGF) transport method [1]. Transiesta uses Siesta as DFT platform exploiting the fact that the operators calculated by Siesta (density matrix and Hamiltonian) are in tight-binding-like form and can be easily interfaced to the NEGF method. The NEGF method splits up a two-terminal device into three regions, a scattering region and two semi-infinite leads (see the figure below). Bias voltage V_b is applied by setting the chemical potential of the left and right leads to $\mu_L=E_F+eV_b/2$ and $\mu_R=E_F-eV_b/2$, respectively, where E_F is the common Fermi level of both leads. The current through the atomic scale system can be calculated from the corresponding Green's function and lead's self-energies using the Landauer formula.

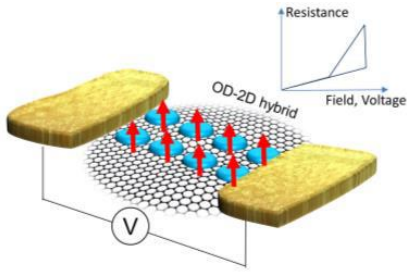

Figure: *Arrangements of well-defined nanomagnets on a 2D material in contact with two gold electrodes (figure from ANR COM2D, submitted).*

References

[1] M. Brandbyge et al, Phys. Rev. B, «Density-functional method for nonequilibrium electron transport", 65, 165401 (2002) and references therein.