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

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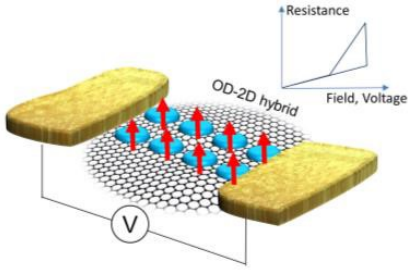
This thesis aims to theoretically investigate the induction of tailored magneto-transport properties in graphene through the proximity effect of well-defined nanomagnet assemblies. Specifically, we will explore the spin-polarized states arising from the interaction of graphene with FePt nanoclusters and rare-earth magnetic atoms. A key objective, in collaboration with the ANR-funded project, is to establish a synergistic approach that integrates predictive atomic-scale computational modeling with experimental characterization of microstructure and magnetic properties. This integration will enable the extraction of critical atomic-scale parameters influencing macroscopic magnetic behavior, ultimately guiding the identification of novel magnetic nanocluster candidates for achieving desired magneto-transport functionalities in graphene.

We will employ slab geometry models to simulate magnetic nanoclusters on graphene, focusing on the influence of layer number on the magnetic coupling and resulting magneto-transport properties. Our computational approach leverages first-principles methods to provide a robust atomic-scale description of electronic structure and transport. This will be achieved using spin-dependent Density Functional Theory (DFT) with various exchange-correlation potential approximations. Quantum transport calculations will be performed using the Transiesta code, a fully spin-polarized implementation that combines DFT with the non-equilibrium Green's function (NEGF) formalism [1]. Transiesta utilizes Siesta code as its DFT platform, exploiting the tight-binding-like representation of the density matrix and Hamiltonian for seamless integration with the NEGF method.

The NEGF method partitions a two-terminal device into a central scattering region and two semi-infinite leads (see Figure below). A 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 is then calculated from the Green's function and lead self-energies using the Landauer formula. This work will be under the supervision of M. Alouani and Benjamin Bacq-Labreuil.

Figure: *Arrangements of well-defined nanomagnets on a 2D material in contact with two gold electrodes.*



Reference

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