Computational Spintronics

A. Droghetti, N. Baadji, A. Hurley, I. Rungger and S. Sanvito
School of Physics and CRANN, Trinity College, Dublin 2, Ireland

e-mail: drogheta@tcd.ie

INTRODUCTION

The field of *spintronics* broadly concerns the study of all spin-related phenomena occurring in materials and, more specifically, the study of spin-polarized electron transport problems. Its ultimate goal consists in designing devices, which, by exploiting both the charge and the spin degrees of freedom of the electrons, would implement new functionalities.

In this context, computational studies play a fundamental role in providing a valuable support to the work of experimentalists. In fact, on the one hand, the development of accurate electronic structure methods, such as Density Functional Theory and Diffusion Monte Carlo, together with the increasing availability of large supercomputing facilities, allows for a detailed description of novel materials and nano-devices. On the other hand, the complex equations deriving from the formalism of quantum many-body theory can be numerically solved thus leading to a better understanding of several fascinating quantum effects.

MOLECULAR SPINTRONICS

Historically spintronics effects have been firstly studied in transition metals and inorganic semiconductors. However interest for devices incorporating organic molecules has recently grown very rapidly leading to the birth of organic and molecular spintronics [1], [2], [3]. In fact organic molecules exhibit a large range of properties, which can be finely tuned in order to search for new functionalities, with no analog in world of inorganic materials.

In parallel, experimental advances in scanning tunneling microscopy have made it possible the detailed characterization of the conductance spectra of magnetic molecules and atoms [4], [5]. These spectra are characterized by a competition between the Kondo effect and spin-flip inelastic electron tunnelling.

MANIPULATING AND READING SPINS

We will discuss the intriguing idea of using magnetic molecules, mainly Fe(II) complexes and cobalt dioxolene [6], [7], in order to implement single-molecule spintronics devices. In such systems, the magnetic moment can be changed by an external stimulus, such as optical irradiation or a static electric field. We will show that a direct control over the molecule spin is in principle possible. Then, through quantitative transport simulations performed with the SMEAGOL code [8], we will demonstrate that the molecule magnetic moment can be inferred by an electrical readout [9]. In fact, the current-voltage characteristic curve depends drastically on the molecule magnetic moment (see Fig. 1).

INELASTIC SINGLE-SPIN TRANSPORT THEORY

We will also present a perturbative approach to the calculation of the inelastic spin-flip spectra of magnetic adatoms and small magnetic clusters on surfaces. The theory is based on the non-equilibrium Green's function formalism combined with a model spin Hamiltonian. By expanding the self-energy describing the electron-spin interaction to the third order, we are able to account for both inelastic spin-flip events and signatures of the Kondo resonances [10], [11]. The results obtained are in extremely good quantitative agreement with published experimental data (see Fig. 2).

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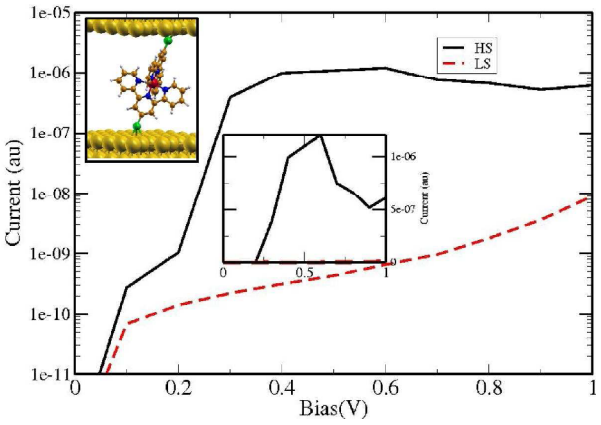

Fig. 1. Calculated $I-V$ curve for the Fe(II) molecule (shown in the inset and attached to gold electrodes) for the two different spin values $S = 0$ (LS) and $S = 2$ (HS). The current is plotted on a logarithmic scale only for positive currents. The inset shows the spin-crossover magneto-resistance ratio, $RSCMR = (G_{HS} - G_{LS})/G_{LS}$, where G_{LS} (G_{HS}) is the conductace for the molecule with spin $S = 0$ ($S = 2$)..

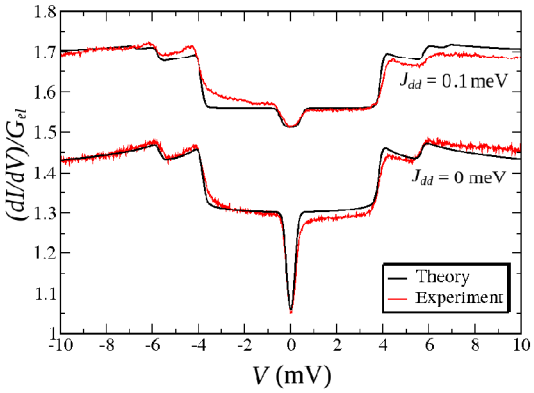

Fig. 2. Normalized conductance spectrum for a Fe adatom on CuN surface when it is exchange coupled to Co adatoms (J_{dd} represents the exchange coupling between Co and Fe). The calculated spectra are in black, while the corresponding experimental data from Ref. [5] are in red.