THE CHALLENGES OF COMPUTATIONAL MOLECULAR SPINTRONICS

S. Sanvito

School of Physics and CRANN, Trinity College, Dublin 2, IRELAND

The injection and manipulation of electron spins at the molecular level is giving a novel intriguing twist to the already burgeoning field of spintronics. The computational challenges associated to such a research area are rather demanding, since one has to describe on the same footing spin-polarized transport, accurate electrostatics, and should employ a reliable but scalable electronic structure theory.

In this talk I will present the most recent advances in the development of the *Smeagol*[1] code. *Smeagol* is our state of the art density functional theory code for quantum transport. It has been specifically designed to investigate two-probe spin-devices and it has optimized to yield extremely accurate electrostatics and to be scalable to large systems. In this talk I will review recent results on Fe/MgO/Fe single and double tunnel junctions[2], where I will discuss the importance of ultra-accurate electrostatics and of the treatment of bound states. Then I will show how a delicate balance between molecular levels re-hybridization in an electric field and localization can generate negative differential conductance in magnetic molecules. This is shown to depend on the magnetic state of the molecule itself, opening the opportunity for the electrical readout of the molecular state[3].

[1] A.R. Rocha et al., Phys. Rev. B. **73**, 085414 (2006); Nature Materials **4**, 335 (2005). See also: www.smeagol.tcd.ie

[2] Ivan Rungger, Oleg N. Mryasov and Stefano Sanvito, arXiv:0808.0902

[3] C.D. Pemmaraju, I. Rungger and S. Sanvito, in preparation