Ab initio design of spintronics devices and their materials

A talk by Stefano Sanvito
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In nanoscale devices every atom matters! In fact the electrical response of a nano-device depends sensitively on the atomistic details of the various interfaces, to a point that small perturbations can generate large changes. As atomic features are often difficult to capture by experiments, theoretical tools are rapidly becoming a crucial asset for device design. In the last few years we have created a sophisticated atomistic device simulation package based on density functional theory and the non-equilibrium Green's function method, the *Smeagol* code [1], capable of modelling atomic scaled devices. This has been employed in multitude of applications ranging from molecular junctions, phase-coherent transistors, spin-valves for magnetic recording, sensors for DNA sequencing etc. As a specific example I will discuss proposals for a multi-state memory and logic element based on magnetic tunnel junctions incorporating a ferroelectric tunnel barrier [2,3]. In particular I will demonstrate that asymmetric tunnel junctions may display tuneable magneto- and electro-resistance.

Designing the concept of a device is however only the first step towards the realization of its practical implementation. A second, crucial, aspect is that of selecting the most appropriate materials. Here I will present preliminary results on our recent effort of combining density functional theory with high-throughput materials screening. In particular I will address the issue of discovery new magnetic Heusler alloys specifically designed for magnetic sensors and magneto-electronics.

[1] A.R. Rocha, V.M. Garcia Suarez, S.W. Bailey, C.J. Lambert, J. Ferrer and S. Sanvito, *Spin and Molecular Electronics in Atomically-Generated Orbital Landscapes*, Phys. Rev. B **73**, 085414 (2006); www.smeagol.tcd.ie.
[2] Nuala M. Caffrey, Thomas Archer, Ivan Rungger and Stefano Sanvito, *Prediction of large bias-dependent magnetoresistance in all-oxide magnetic tunnel junctions with a ferroelectric barrier,* Phys. Rev. B **83**, 125409 (2011).
[3] Nuala M. Caffrey, Thomas Archer, Ivan Rungger and Stefano Sanvito, *Coexistance of giant tunneling electroresistance and magnetoresistance in an all-oxide magnetic tunnel junction,* Phys. Rev. Lett. **109**, 226803 (2012).