Density functional theory for spin-transport

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9.7 cm

Density functional theory has revolutionarized our way to do materials science and it is now a fundamental asset for research in Physics, Chemistry, Biology and Nanoscience. This is mainly due to a combination of conceptual simplicity, rigorous theoretical foundation and efficient numerical algorithms. The Smeagol [1,2] project (www.smeagol.tcd.ie) has the ambitious goal of setting the same revolution in the field of ab initio quantum transport.
In this talk I will present our recent results for the bias-dependent transport of various spin-devices. I will first start from Fe/MgO (001) tunnel junctions and demonstrate how the magnetoresistance depends on the presence of resonant tunneling through surface states, how it is affected by bias and how it is reduced by FeO allowing at the interfaces. I will then move to discuss spin-effects in organic materials, and demonstrate that molecules offer the unique possibility to engineer the magneto-transport response of spin-valves. Finally I will present some very recent results on electron transport across Mn_{12} magnetic molecules and demonstrate that the magnetic state of the molecule can be inferred by a detailed analysis of the I-V characteristics.

[1] Towards Molecular Spintronics, Alexandre Reily Rocha, Victor Garcia-Suarez, Steve W. Bailey, Colin J. Lambert, Jaime Ferrer and Stefano Sanvito, Nature Materials **4**, 335 (2005).
[2] Spin and Molecular Electronics in Atomically-Generated Orbital Landscapes, Alexandre Reily Rocha, Victor Garcia-Suarez, Steve W. Bailey, Colin J. Lambert, Jaime Ferrer and Stefano Sanvito, Phys. Rev. B. **73**, 085414 (2006).

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