Modeling the nanoscale: the *Smeagol* project

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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.

Smeagol, in its present form, calculates the I-V characteristics of nanoscale two-probe devices from first principles. It combines a non-equilibrium transport algorithm capable of evaluating the effects of a steady state current on the electronic structure of the device with density functional theory implemented on a localized atomic orbital basis set. *Smeagol* is constructed with three main goals in mind. First it must be accurate. For this reason exchange and correlation potentials including strong correlation corrections (LDA+U or LDA+SIC) have been implemented and demonstrated effective for the transport. Secondly, it must be able to scale, and therefore capable of accessing massive parallel machines. Finally it must be reasonably user friendly to serve a large community.

In this talk I will review the basic ideas behind quantum transport and density functional theory, and introduce the *Smeagol* project. Then I will present results for two currently "hot" problems. First I will discuss transport through simple molecules attached to Au leads, and demonstrate that a computational undemanding method for self-interaction correction can yield results in good agreement with experiments. Then I will tackle the problem of the conductivity of DNA

and demonstrate that simulations of devices exceeding several thousands atoms are in the reach of *Smeagol*'s computational capabilities.

[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).