

Abstract Submitted  
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**Smeagol: the ultimate computational tool for spin transport at the nanoscale** STEFANO SANVITO, Trinity College Dublin — The ability of manipulating electron spin in organic molecular materials offers a new and extremely tantalizing roadmap for both spin and molecular electronics. The modeling of molecular spin-devices however requires a level of sophistication never reached before since both accurate electrostatics and the description of the magnetic state are needed. In this talk I will present our newly developed *ab initio* quantum transport code *Smeagol* (Spin and Molecular Electronics in an Atomically-Generated Orbital Landscape. [www.smeagol.tcd.ie](http://www.smeagol.tcd.ie)), which has been specifically constructed for dealing with these issues. *Smeagol* combines density functional theory in the numerical optimization contained in SIESTA, with non-equilibrium Green's function transport method. It has been completely designed for dealing with magnetic systems including both non-collinear spin, spin-orbit interaction and strong correlated functionals (LDA+U and LDA+SIC). A demonstration of its capabilities will be presented.

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