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Ab inito **study of molecular spin valves** ALEXANDRE REILY ROCHA, STEFANO SANVITO, Trinity College Dublin, Dublin 2, Dublin, IRELAND — The combination of spin and molecular electronics poses exciting perspectives both for basic science and technological applications. By manipulating the spin degree of freedom at the atomic level we enter a new and exciting era where entire spin devices can be substituted by single a molecule performing analogous tasks. In this talk, we will present a through theoretical study of electronic transport through molecular spin valves [1] obtained by sandwiching a molecule between two Ni electrodes. The calculations are performed with our novel code Smeagol (www.smeagol.tcd.ie), which combines density functional theory with non-equilibrium Green function transport method. We will show results for two types of molecules with distinct transport mechanisms, namely: tunneling and metallic conductance. In both cases we analyze the effects of the contacts on the molecule and the particular states contributing to the transport. We will demonstrate that it is not only possible to obtain large magnetoresistance effects in both types of molecules, but also to engineer the signal by an appropriate choice of end-groups.

[1]Towards Molecular Spintronics, A. Reily Rocha, V. M. Garcia Suárez, S. W. Bailey, C. J. Lambert, J. Ferrer and S. Sanvito, submitted to Nature Materials.

Alexandre Reily Rocha
Trinity College Dublin, Dublin 2, Dublin, IRELAND

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