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Progress in ab initio methods for spin transport¹

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Numerical simulations have an important role in spintronics, here one envisages the use of the spin as well as the electron charge for electronic applications. In this talk I will present our code *Smeagol* [1] which combines the non-equilibrium Green function formalism with density functional theory and it has been specifically designed for magnetic devices. With *Smeagol* I will first investigate the possibility of large ballistic magnetoresistance in nickel point contacts, addressing the effects of local exchange and correlation functionals as well as the possible presence of oxygen impurities. Then I will describe an attempt to integrate the fields of spin- and molecular-electronics by constructing spin-valves using organic molecules. I will demonstrate that it is possible to obtain different transport behaviour, large magnetoresistance [1] as well as current rectification and spin-diode effects by simply selecting the molecule and the anchoring groups. Finally I will show how *Smeagol* is a valuable tool for simulating spin-polarised STM images.

References

- [1] A. R. Rocha, *et al.*, Phys. Rev. B **70**, 085414 (2006), Nature Materials, **4**, 335 (2005).

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