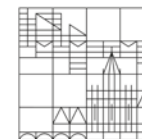


SFB 767 Seminar

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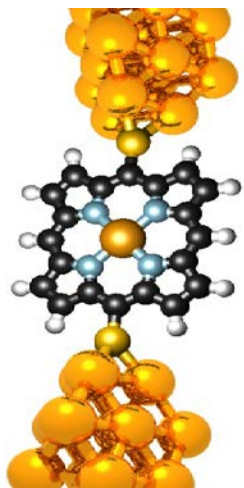


Fr 22 June 2018
10:00
P 602



Prof. Dr. Carmen Herrmann
Institute of Inorganic and Applied Chemistry
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Spin-dependent effects in molecular and nanoscale electron transport: challenges for first-principles descriptions



Using the spin degree of freedom offers fascinating options for nanoscale functionality, and also provides new data for improving our insight in fundamental aspects of nonequilibrium physics at that scale. For interpreting experimental data and for suggesting new experiments, theoretical simulations and concepts are often necessary. First-principles theoretical approaches have the advantage of being independent from system-specific fit parameters and therefore in principle predictive, but in practice, compromises between accuracy and computational feasibility imply that for molecular and nanoscale spintronics, a reliable first-principles description may be elusive [1]. We illustrate the resulting challenges as well as successes for examples such as chiral induced spin selectivity [2] and related spin-orbit effects [3], and structure—property relationships for the Kondo effect of $\text{Co}(\text{CO})_n$ molecules on a Cu surface [4,5].

[1] C. Herrmann, *Atomistic modeling for molecular electronics and spintronics: successes and challenges*. In: M. Springborg, J.-O. Joswig (Eds.), *Chemical Modelling* 14, 43-70 (2018) [2] R. Naaman, D. H. Waldeck, *Spintronics and chirality: spin selectivity in electron transport through chiral molecules*. *Annu. Rev. Phys. Chem.* 6, 263-81 (2015) [3] M. M. R. Moayed, T. Bielewicz, M. S. Zöllner, C. Herrmann, C. Klinke, *Towards colloidal spintronics through Rashba spin-orbit interaction in lead sulphide nanosheets*, *Nature Commun.* 8, 15721 (2017) [4] P. Wahl, L. Diekhöner, G. Wittich, L. Vitali, M. A. Schneider, and K. Kern, *Phys. Rev. Lett.* 95, 166601 (2005) [5] M. P. Bahlke, M. Karolak, C. Herrmann, *Interplay between strong correlation and adsorption distances: Co on Cu(001)*, *Phys Rev. B* 97, 035119 (2018)

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