



# TRR 80 Sonderseminar

Am Mittwoch, den 18. November um 10:15 Uhr

spricht

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über das Thema

***First principles electron transport simulations of organic radical molecules in the Kondo regime***

Stable organic radicals have a molecular orbital with an unpaired electron and therefore correspond to molecular magnets with a spin of one half. When brought into contact with metals the electron-electron interaction on the molecule leads to the appearance of the correlated Kondo state at low temperatures, as indeed found in recent experiments [1-3]. While the results in those conductance measurements are explained in terms of a single impurity Anderson model, in this talk I will present a description of the electron transport properties that takes into account atomic structures of the metal/molecule interfaces from first principles. The theoretical framework is implemented in the Smeagol [4] electron transport code, and integrates the density functional theory (DFT) with Anderson impurity solvers within the continuum time quantum Monte Carlo (CTQMC) and numerical renormalization group (NRG) approaches. Results for the STM measurements of 1,3,5-triphenyl-6-oxoverdazyl (TOV) organic radicals on Au [1], as well as recent Au break junction experiments with polychlorotriphenylmethyl (PTM) radicals [3] will be presented, with atomic structures obtained including van der Waals interactions [5]. In particular the effect of the contact geometry on the Kondo temperature will be evaluated. Possible future applications of such framework for systems including spin-orbit interaction and non-collinear spins will be discussed.

[1] J. Liu, J. Isshiki, K. Katoh, T. Morita, B. K. Bredlove, M. Jamashita, and T. Komeda, J. Am. Chem. Soc. 135, 651(2013)

[2] Y. H. Zhang, S. Kahle, T. Herden, C. Stroh, M. Mayor, U. Schlickum, M. Ternes, P. Wahl, and K. Kern, Nature Comm. 4, 2110 (2013)

[3] R. Frisenda, R. Gaudenzi, C. Franco, M. MasTorrent, C. Rovira, J. Veciana, I. Alcon, S. T. Bromley, E. Burzurí, and H. S. J. van der Zant, Nano Lett. 15, 3109 (2015)

[4] A. Rocha et al., Nature Mater. 4, 335 (2005); A. Rocha et al., Phys. Rev. B 73, 085414 (2006); I. Rungger et al., Phys. Rev. B 78, 035407 (2008)

[5] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffler, and A. Tkatchenko, Phys. Rev. Lett. 108, 146103 (2012)

Gäste sind herzlich willkommen.

Der Vortrag findet im Raum T-2003, Hörsaalzentrum Physik, Universität Augsburg statt.

Gastgeber: Prof. Dr. Liviu Chioncel

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