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First principles electron transport simulations in the Kondo regime IVAN RUNGGER, National Physical Laboratory, MILOS RADONJIC, WILHELM APPELT, LIVIU CHIONCEL, University of Augsburg, ANDREA DROGHETTI, Universidad del Pais Vasco — When magnetic atoms, molecules or thin films are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state at low temperatures. In this talk we will present results for the electronic structure and conductance in the Kondo regime of recent STM and break junction experiments for stable radical molecules[1], which correspond to spin half molecular magnets. We will outline the methodological approach to evaluate the conductance of such systems from first principles, as implemented in the Smeagol electron transport code[2]. The method combines the density functional theory (DFT) with Anderson impurity solvers within the continuum time quantum Monte Carlo (CTQMC) and numerical renormalization group (NRG) approaches.

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[2]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)

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