Abstract Submitted
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The Kondo effect in molecular magnets from first principles DAVID JACOB, Max Planck Institute of Microstructure Physics Halle, MICHAEL KAROLAK, ALEXANDER I. LICHTENSTEIN, University of Hamburg, MARIA SORIANO, JUAN JOSE PALACIOS, Universidad Autonoma de Madrid — When a magnetic molecule is deposited on a metallic substrate or attached to metallic contacts its magnetic moment may actually be screened by the conduction electrons due to the Kondo effect. In view of possible applications of molecular magnets such as nanoscale spintronics and magnetic storage devices, it is important to being able to predict whether the Kondo effect will take place or not in a given system. Also one would like to understand in detail how the Kondo effect emerges in a given situation and how it is controlled by the various parameters such as the molecular conformation and the type of substrate. Using a recently developed ab initio approach for molecular devices [1,2] that explicitly takes into account the strong electronic correlations that give rise to the Kondo effect, we have calculated the electronic structure and transport properties of different magnetic molecules coupled to nanocontacts [3] and surfaces [4]. Our calculations shed light on the complex nature of the Kondo effect in molecular-scale devices. [1] D. Jacob *et al.*, PRL **103**, 016803 (2009); [2] D. Jacob *et al.*, PRB **82**, 195115 (2010); [3] M. Karolak *et al.*, PRL **107**, 146604 (2011); [4] K. J. Franke *et al.*, Science **20** 940 (2011)

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