TECHNISCHE UNIVERSITÄT CHEMNITZ

PHYSIKALISCHES KOLLOQUIUM

Mittwoch, den 19.05.2010, um 15:30
Reichenhainer Str. 90; Neues Hörsaalgebäude, Raum :2/N013

From molecular magnetism to magnetic molecules on surfaces

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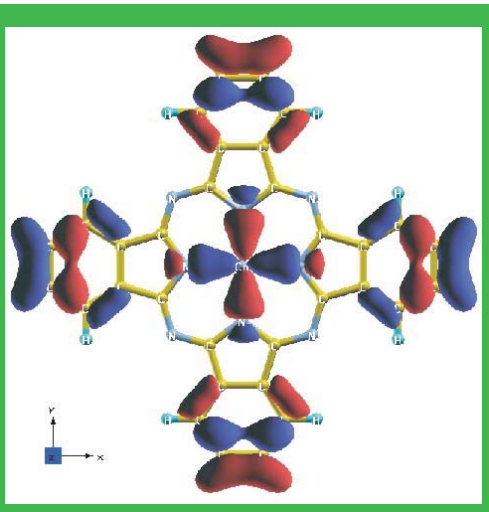

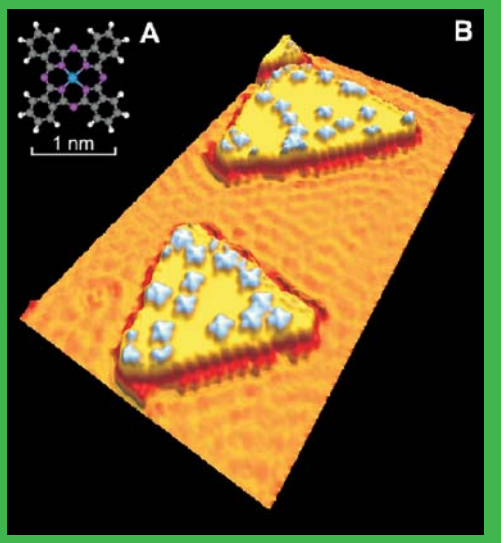

In order to store information in any magnetic material one needs an energy barrier preventing the flip of the direction of the magnetization. The height of the barrier determines the temperature up to which the device will function properly. Therefore one of the major hopes in the field of molecular magnetism is the rational design of this magnetic anisotropy barrier, which depends on the total magnetic moment of the molecule and the magnetic anisotropy, by means of electronic structure calculations [1]. There is considerable knowledge about the magnetic exchange coupling which determines the total spin. In contrast there is not much known about magnetic anisotropy which is mainly determined by the spin-orbit coupling. Only recently it became possible to predict the value of the magnetic anisotropy by means of electronic structure calculations. I will discuss the interplay of the magnetic anisotropy and magnetic exchange interaction in case of two Mn6 complexes. The results suggest that large magnetic anisotropy is not favoured by a high spin state of the ground state [2]. In the second part I will focus on electronic properties of magnetic molecules on surfaces, where electronic structure calculations can provide information required for interpretations of experimental data [3].

[1] J. Cirera, E. Ruiz, S. Alvarez, F. Neese, J. Kortus: Chem.-Eur. J. 15 (2009) 4078
[2] E. Ruiz, J. Cirera, J. Cano, S. Alvarez, C. Loose, J. Kortus: Chem. Commun. 1 (2008) 52
[3] C. Iacovita, M. V. Rastei, B. W. Heinrich, T. Brumme, J. Kortus, L. Limot, J. P. Bucher: Phys. Rev. Lett. 101 (2008) 116602-1

Alle Zuhörer sind ab 15:15 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt Prof. Dr. PeterHäussler, Tel. 0371/531-33140