UNIVERSITÄT OSNABRÜCK

Seminar NanoScience
Vortragsankündigung

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„The method of increments applied to the adsorption energy of physisorbed molecules on ionic surfaces“

Freitag, 11.02.2011
10:00 Uhr
Raum 32/372

The method of increments [1] for the correlation energy in solids is based on the expansion of the correlation energy in terms of localized orbital groups. Any size-extensive correlation method like coupled cluster can be used for the correlations, the Hartree-Fock treatment is performed for the extended systems. The method of increments is now extended to adsorption processes on surfaces. The standard density functional methods have their difficulties with describing dispersion forces, especially the long-range van der Waals interactions and therefore there is a need of highly accurate results especially for physisorbed systems. Here we want to present as application the adsorption of CO, N_2O, NO and metallic atoms on ionic surfaces, especially ceria surfaces [2], and first results for the surface energies of MgF_2 surfaces. The method is also applicable for H_2S and H_2O on graphene as example for a purely van der Waals bound system [3] and preliminary results for metallic surfaces like the adsorption of Xe on magnesium will be presented.

[1] H. Stoll, Phys. Rev. B 1992, 46, 6700; B. Paulus, Phys. Rep. 2006, 428, 1 (review); E. Voloshina, B. Paulus, Z. Phys. Chem. 2010, 224, 369.
[2] C. Müller, B. Herschend, K. Hermansson, B. Paulus, J. Chem. Phys. 2008, 128, 214701; C. Müller, K. Hermansson, B. Paulus, Chem. Phys. 2009, 362, 91; C. Müller, B. Paulus, K. Hermansson, Surf. Science 2009, 603, 2619.
[3] K. Rosciszewski, B. Paulus, Int. J. Quantum Chem. 2009, 109, 3055.

gez. M. Reichling