On behalf of the

Science College CMS

Vienna Computational Materials Laboratory

and Center for Computational Materials Science

we cordially invite you to the following seminar

Mag. Florian Göltl

University of Vienna, Faculty of Physics, Computational Materials Physics

Alkane adsorption in chabazite – The influence of dispersion forces

In this work we investigate the performance of different levels of theory to describe the adsorption of alkanes in chabazite, a mineral from the zeolite family. Modeling this problem is an especially challenging task, since, even though there is a very weak bond between the adsorption site (in our case an H- or Na- atom) and the alkane, the bonding is dominated by van der Waals (vdW) interactions between the alkane and the zeolite wall.

Even though vdW-interactions are not included in standard density functional theory (DFT), several ways to include them in DFT and post-DFT methods were proposed. In this work we compare the performance of (i) DFT in its generalized gradient approximation after Perdew, Burke and Ernzerhof (PBE), (ii) PBE with an added forcefield after Grimme (PBE-d), (iii) the van der Waals density functional after Dion et al. (vdW-DF), (iv) the Adiabatic Connection Fluctuation Dissipation Theorem in its Random Phase Approximation (RPA), (v) a modified form of the RPA, where the Hartree-Fock exchange contribution is evaluated self-consistently (RPA-HF) and (vi) 2nd order Møller Plesset perturbation theory (MP2).

We give a critical discussion of differences in structural parameters, charge distribution and energetics and propose an improved way to compare the theoretically obtained results with experiment.

Date: Monday, Dec 13, 2010 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10