Theoretical material and surface science: From method development to applications

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Material properties are mainly determined on the first principle level applying density functional methods. In several cases these methods yield sufficient accuracy to predict the most stable allotropes. Here I will present results for aluminium oxide/fluoride mixtures [1] and their interaction with water [2]. Using the results of first principle calculations and the methods of surface thermodynamics, it is also possible to predict the structure of nanocrystals depending on the pressure and temperature. We apply this method to nanoscopic magnesium fluoride [3] and aluminium fluoride.
But there exists materials, where present-day density functionals reveal problems, e.g. the weak interaction of adsorbed molecules on surfaces. Two examples will be presented, one is the adsorption of water and hydrogen fluoride on magnesium fluoride [4] a second one the interaction of water with graphene and different carbon nanotubes [5]. In the later one the method of increments for adsorption energies [6] on the coupled cluster level is applied and yield qualitative different results in comparsion to dispersion corrected density functional methods.

[1] J. Budau, B. Paulus, K. Steenbergen, Chem. Phys. **491**, 112-117 (2017).
[2] J. Wirth, J. Schacht, P. Saalfrank, B. Paulus, J. Phys. Chem. C **120**, 9713-9718 (2016).
[3] E. Kanaki, S. Gohr, C. Müller, B. Paulus, Surf. Sci. **632**, 158-163 (2015).
[4] E. Kanaki, G. Sansone, L. Maschio, B. Paulus, Phys. Chem. Chem. Phys. **17**, 18722-18728 (2015).
[5] S. Lei, B. Paulus, S. Li, B. Schmidt, J. Comp. Chem. **37**, 1313-1320 (2016)
[6]B. Paulus, Phys. Rep. 428, 1 (2006); C. Müller, B. Paulus, Phys. Chem. Chem. Phys., **14**, 7605-7614 (2012).