

Seminář odd. 26

Tenkých vrstev a nanostruktur

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

datum: 14. 10. 2014 úterý

čas: 10:00

mítnost: knihovna, budova A, 1.p.

TÉMA

A theoretical description of water splitting on metal decorated oxide surfaces

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Efficient, sustainable production of molecular hydrogen - a promising alternative to batteries in terms of energy storage - is still an unsolved problem. Implementation of direct water splitting using only sunlight and suitable metal-oxide photo-catalysts so far has been hampered by poor photon absorption properties of the materials and low reaction efficiencies. In order to understand the microscopic processes involved in photo-catalytic hydrogen production we implemented an implicit solvent model and a solid state QM/MM embedding scheme based on ChemShell into the all electron DFT and beyond code FHI-aims.[1] This allows us to study defects and charged systems - as occurring in electron-hole driven water splitting - without any spurious interaction between periodic images, while at the same time yielding the correct electrostatic potential and solvent screening in the QM region.

In order to overcome the limitations of current water splitting setups we study the use of small metal clusters as co-catalysts, the microscopic effect of which is still poorly understood in literature. We develop an enhanced version of the thermodynamic approach pioneered by Nørskov and Rossmeisl,[2] of water oxidation reactions on metal clusters in the non-scalable size regime (less than 55 atoms) and compare with the bare extended oxide surface.[3] On top of these results we discuss the influence of solvent on the reaction as well as the stabilisation of electron holes necessary for the reaction.

[1] V. Blum et al., *Comp. Phys. Commun.* 180, 2175 (2009)

[2] A. Valdes et al., *J. Phys. Chem. C* 112, 9872 (2008)

[3] H. Oberhofer, K. Reuter, *J. Chem. Phys.* 139, 44710 (2013)