O 81: Invited talk (Bligaard, Thomas)

Time: Friday 10:15–11:00 Location: H36

Invited Talk O 81.1 Fri 10:15 H36

Towards the computational design of heterogeneous catalysts

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Electronic structure methods based on density functional theory have reached a level of speed and accuracy where they can be used to describe complete catalytic reactions on transition metal surfaces. Simulations now complement experiments to give unprecedented insight into surface processes, allowing one to pinpoint the origin of catalytic activity of a metal in terms of its electronic structure. The use of electronic structure theory as a tool for directly designing or searching for new materials is a computationally rather expensive process, though, and has until now been quite limited. For a limited number of catalytic processes the underlying reactivity trends have been understood well enough that they could subsequently successfully be used to seek out new catalysts. The computational search for such potentially useful catalysts will be discussed. The focus will be on showing the generality of such a trend- and descriptor-based approach by linking a few specific case stories to more fundamental underlying linear-energy relations for the adsorbate-surface bonds [1].

[1] J.K. Nørskov, T. Bligaard, J. Rossmeisl, C.H. Christensen, Nature Chemistry 1, 37 (2009)