Towards Computational Design of Solid Catalysts

Thomas Bligaard

Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark
bligaard@fysik.dtu.dk

Electronic structure methods based on density functional theory have reached a level of accuracy and speed where they can be used to treat surface processes on transition metal surfaces semi-quantitatively. A number of recent developments enabling the treatment of complex reactions on a large number of different catalysts will be introduced. Correlations between activation energies and reaction energies (BEP relations) and between adsorption energies of different species (the so-called scaling relations) are explained in terms of the d-band model. In combination with experiments on model systems and nano-particle catalysts these methods allow the understanding of the trends in catalytic activity for a number of catalytic reactions including ammonia synthesis, methanation, Fischer–Tropsch synthesis, and hydrogen production by reforming of hydrocarbons and alcohols. Finally, it is shown how these concepts can be used to identify descriptors determining the catalytic activity of a given transition metal surface, and how this can form the basis for screening a large number of metals and alloys for catalytic properties. Examples will be given of computational searches for alloys with improved catalytic rates and selectivity.