Tailoring surface chemical properties using electronic structure theory

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Electronic structure methods based on density functional theory have reached a level of sophistication where they can be used to describe complete catalytic reactions on transition metal surfaces. This opens the possibility that computational methods can be used to tailor surfaces with desired chemical properties. Recent progress in this direction for transition metal catalysts will be discussed. First, it will be shown that certain catalytic reactions can be described in semi-quantitative detail on the basis of calculations. The accuracy of present theoretical methods will be discussed on this basis. Next a number of developments that are necessary in order to be able to treat complex reactions on a large number of different catalysts are treated. Correlations between activation energies and reaction energies (BEP relations) and between adsorption energies of different species (scaling relations) are introduced and explained in terms of the d-band model. The d-band model is also used to explain trends in adsorption energies and activation energies for alloys. These methods allow the understanding of the trends in reactivity of complete catalytic reactions. Finally, it is shown how these concepts can be used to identify the factors determining the catalytic activity of a given transition metal surface, and how this can form the basis for screening of a large number of metals and alloys for catalytic properties.