Trends in reactivity for transition metals.

Thomas Bligaard and Jens K. Nørskov
Center for Atomic-scale Materials Physics,
Department of Physics,
Technical University of Denmark.

We present a detailed database of adsorption energies for a number of atoms and molecules on transition metal surfaces\(^1\). The database is calculated using density functional theory\(^2\) on periodically repeated transition metal slabs in a plane-wave pseudopotential approach. It has been shown that there is a simple, universal relationship between adsorption energies and reaction barriers for a number of important surface processes\(^3\). The surface thermo-chemistry database can therefore be used to estimate activation energies for a number of surface elementary reactions taking place over transition metal surfaces.

Using a recently developed interpolation principle\(^4\), the database can also be used to estimate the reactivity of surface alloys. This gives a large amount of reactivity information, but avoids laborious experimental and computational effort. Using the Pareto-optimization method\(^5\) for materials design with respect to multiple criteria, we can screen a large number of hypothetical catalyst surfaces for their usefulness as catalysts.

References