326b Heterogeneous Catalysis from First Principles

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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 transitional metal surfaces. This gives an unprecedented insight in these processes, and it allows us to pinpooint the origin of the catalytic activity of a metal in terms of its electronic structure. The ammonia synthesis is used to exemplify this approach. It will be shown that by combining densitiy functional calculation with kinetic modelling we can now predict relative catalytic activities of different metals. The generality of the approach is illustrated by including a number of other catalytic reactions into a universal property-activity scheme, which identifies the surface properties that determine the catalytic activity for a whole class of reactions.