

A molecular view of heterogeneous catalysis

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The development of sustainable energy systems puts renewed focus on catalytic processes for energy conversion. We will need to find new catalysts for a number of processes if we are to successfully synthesize fuels and chemicals from solar or wind electricity. Insight into the way the catalysts work at the molecular level may prove essential to speed up the discovery process. The lecture will outline a theory of heterogeneous catalysis that allows a detailed understanding of elementary chemical processes at transition metal surfaces and singles out the most important parameters determining catalytic activity and selectivity. It will be shown how scaling relations allow the identification of descriptors of catalytic activity and how they can be used to construct activity and selectivity maps for both thermal and electro-catalytic processes. The maps can be used to define catalyst design rules and examples of their use will be given.