The role of computations in catalysis

This chapter examines the successes and the challenges of computational design of catalysts. It explores and learns from a crude example of experimental screening for catalysts for an exothermic reaction. There are several rules that make such rapid computational screening possible: the Sabatier principle, linear-scaling, and the Brensted-Evans-Polanyi (BEP) relation. Scaling relations can be developed for larger molecules, which make two bonds with the solid surface, through two different atoms. Oxide catalysts have numerous applications. The chapter discusses few rules discovered through computations. It illustrates many of the problems faced by most large-scale catalytic processes. A useful catalyst must be cheap to make and it should not contain expensive or rare ingredients. Another important property of a good catalyst is its resistance to poisoning. Density functional theory (DFT) is the only practical option. DFT is approximate, especially when calculating activation energies.