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Une vue sur la catalyse hétérogène par la chimie quantique: nature des sites actifs et mécanismes réactionnels

The nature of the surface active site, and the molecular reaction mechanisms are the two complementary pillars of fundamental catalysis. In this lecture we will explore the duality between these two aspects by first principle calculations. Selective hydrogenation of unsaturated molecules will be the central reaction. We will first show that the reactant itself might modify the surface of the catalyst^{1,2}, with the formation of a surface carbide phase that has strong implications on the selectivity of the catalyst. In a second part, the mechanism of the hydrogenation of butadiene will be presented and we will show how modeling can explain why Pt is not selective for these reactions, while the PtSn alloy is^{3,4}. New C-H bond formation pathways, where the C=C bond is not coordinated to the surface, play a central role for the specific selectivity of the alloy. The mechanism of glycerol transformation on a Rh catalyst will also be explored.⁵

References

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