**Article in Nature Materials on nano-scale catalyst design**

In the February issue of the world-leading scientific journal Nature Materials, scientists from the Interdisciplinary Nanoscience Center (iNANO) at the University of Aarhus, from NANO-DTU at the Technical University of Denmark, and from Haldor Topsøe A/S report on a new approach to improve catalyst surfaces for industrial chemical processes and environmental use. In their article, “Controlling the catalytic bond-breaking selectivity of Ni surfaces by step blocking”, the team of scientists demonstrate how the catalytic properties of nickel surfaces can be controlled by selectively blocking the atomic defects on the surface. The approach may lead to an important breakthrough in the efficiency and lifetime of catalyst materials.

**Heterogeneous catalysis**

Heterogeneous catalysis plays a tremendous role in the modern society; both for the entire chemical industry (e.g. fertilizer production and oil refinement) and for environmental use (e.g. exhaust cleaning). Despite their great importance, very little is known about the detailed atomic mechanisms of most catalytic processes, and so far new catalysts have mainly been developed by the so-called “trial and error” approach.

**Nano-scale design of new catalysts based on fundamental studies**

The scientists from the University of Aarhus have used a scanning tunnelling microscope (STM) to study catalytically relevant reactions on a nickel surface. The STM, which was developed in the iNANO group headed by Professor Flemming Besenbacher, makes it possible to see the single atoms on metal surfaces. As such the STM is an ideal tool to gain insight into details at the atomic level. PhD students Ronnie Vang, and Ebbe K. Vestergaard, and postdoc Joachim Schnadt were able to observe by STM that ethylene molecules decompose with a much higher rate at step edge atoms than on regular atoms on the flat nickel surface, i.e. the step edge atoms are so-called “active sites” for the decomposition of ethylene on nickel.

Karoliina Honkala from the group of Professor Jens K. Nørskov at the Technical University of Denmark in Lyngby, used large-scale quantum mechanical calculations to study the reactivity of different surface structures. She found that step edge atoms on a nickel surface have a higher reactivity than regular atoms, in agreement with the STM findings. Furthermore, the step edge atoms are the only sites where dissociation (breaking of a C-C bond) can take place, whereas dehydrogenation (breaking of a C-H bond) may also take place at the regular atoms. The relative ratio of different products (known as the catalytic selectivity) is a very important factor in heterogeneous catalysis, and the ability to control this selectivity is highly desirable in order to avoid unwanted side products. The calculations showed that a blocking of the steps enables us to control the selectivity. The Aarhus STM group demonstrated how they were able to block all the free step edge atoms on the nickel surface by depositing small amounts of silver, and they confirmed that this does indeed prohibit the decomposition of ethylene at the step edges.

The ideas were exploited in the synthesis of a high surface-area, oxide-supported Ag/Ni catalyst, which was shown, by Bjerne Clausen and Søren Dahl at Haldor Topsøe A/S, to have the properties predicted from the STM experiments and the quantum mechanical calculations.

**Perspectives**

If we are to deal with future problems, like the increasing demand for energy produced in a sustainable way, the development of new and improved catalysts is crucial. In order to do so we need to understand the fundamental properties of catalytic reactions, and we need to exploit this knowledge to rationally design new materials with specific catalytic properties.
The work described in the article shows that fundamental studies on model systems is a method that can be used for this purpose.

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