ENI AWARD 2022

Energy Frontiers

Ib Chorkendorff and Jens Nørskov

Winners

Sustainable production of fuels and chemicals – electrochemical ammonia synthesis at low temperature and pressure

Research Description

Chorkendorff
The pivotal approach of Chorkendorff's research has been utilizing surface science to establish a fundamental understanding of heterogeneous catalysis on the atomic level and to capitalize on this understanding to develop new and efficient catalysts/processes for conversion of sustainable energy and environmental protection. Almost all the interesting action on a catalyst is occurs at the outermost atomic layer and by applying surface science methods it is possible to establish an insight, on the atomic level, on what the individual atom or molecule is doing during a given reaction. Being able to extract essential parameters such as limiting barrier or determining bonding energies it is possible to also start modifying these surfaces to obtain new catalysts with higher rates for the reactions. In this process Chorkendorff has been developing new routes for electrifying catalysis and methods for exploring his field. He has built a laboratory with most of the modern surface science methods and on top of that developed new equipment for making mass selected clusters and testing their reactivity and catalytic activity, whether it be electrochemical or thermal catalysis. This as well as innovative development of new measurements methods has led to several patents and has been the foundation for several spinout companies.

Chorkendorff has studied the interaction of reactants with surfaces of relevance for large-scale industrial processes. For example, methane interaction with surfaces/catalysts relevant for the steam reforming process, CO_2 and H_2 relevant for the methanol synthesis and the N_2 and H_2 relevant for the ammonia process. The information gained from these studies along with information from theoretical modelling has been used to modify such catalysts and test them, improving their process conditions for the good of society. Chorkendorff's work has not been limited to thermal catalysis but broadened to electrocatalysis and photoelectrocatalysis. Here he has been working on water splitting for generating hydrogen by using either electricity or light directly as the energy source. He has been heavily involved in CO and CO_2 electrocatalysis into hydrocarbons and lately together with his co-workers pioneered the N_2 electro-hydrogenation into ammonia to use sustainable energy directly to make fuels and chemicals i.e., Power-to-X. Such new processes will ease the largest current challenge humankind is facing: the transition to a fossil free society. In addition, they will allow for a more secure and decentral production.

Norskov

An important milestone in Nørskov's work in the last ten years is the formulation of a coherent theory of transition metal surface catalysis. Catalysis is an inherently complex phenomenon where many reaction steps and many catalytic sites can contribute to the observed catalytic rate. Scaling relations between transition state energies and adsorption energies have been found to be ubiquitous in surface chemistry, and Nørskov has shown how they can be used to project the extremely high-dimensional space of activation energies and reaction energies than can contribute to the rate onto a few descriptors – typically adsorption energies of key intermediates. This has allowed a systematic understanding of many trends in transition metal heterogeneous catalysis. This includes the dependence on active transition metal and the role of alloying. It also includes the structure dependence, which is key to understanding the nature of the active sites in catalysis. The work has formed the basis for development of design strategies for catalysts.

The success of the approach raises the question about the reliability of the computational methods and the accuracy of the scaling relations. The conclusion from an analysis of uncertainties in calculated results is that scaling relations are considerably more accurately determined than data for a single catalytic system, and that catalytic activity trends are considerably more reliable than the absolute magnitude of the calculated rates. An underlying theme in all of Nørskov's work is an understanding of the electronic structure factors governing surface chemical properties (the d-band model). Nørskov has also been active in developing a theory of surface electrocatalysis.

One of the major recent insights form the Nørskov group is that limitations in our ability to design new, better catalysts for many heterogeneous (chemical and electrochemical) reactions can be traced back to the scaling relationships that restrict our capability to control activation energies for different steps in a catalytic process independently. This leads to the formulation of a new set of catalyst design rules aiming at "breaking" the scaling relations.

A major aim of Nørskov's research is to contribute to the scientific underpinning of new chemical and electrochemical processes and catalysts for sustainable production of fuels and chemicals.