

Short Autobiography of Jens K. Nørskov

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I received a PhD in physics from Århus University, Denmark, under the inspiring supervision of Bengt Lundqvist. After postdoc experiences at Århus University, IBM Yorktown Heights Research Laboratories, and the Nordic Institute for Theoretical Physics in Copenhagen, I found it hard to find a faculty position in Denmark in the early 1980s. There simply were no openings. Fortunately, I was offered a position at the Haldor Topsøe Research Laboratories—strongly supported by Haldor Topsøe, Henrik Topsøe, and Bjerne Clausen. The involvement with the Topsøe company, one of the world's largest suppliers of catalysts and technology for the chemical and energy industry, influenced my career in many ways. Most importantly, it became clear to me that a theory of heterogeneous catalysis was essential to further advance this important area of science and technology. I kept that focus when starting an academic career, and kept the association with the Topsøe company, now serving on its Board of Directors.

In the late 80s the Danish government started to realize that they were about to lose a whole generation of scientists and instituted some special professorships with applicants competing in all fields and at all universities in the country. That got me started at the Technical University of Denmark building up a research group with the funding that came with the professorship. The focus was on understanding surface reactivity as well as impurities in bulk metals.

The impurity work started an extremely fruitful collaboration with Flemming Besenbacher at Århus University that continued for the next decades. With Besenbacher, I founded the Center for Atomic-scale Materials Physics with large-scale funding from the first round of grants from the Danish National Research Foundation. Here my group established the beginning of an understanding of the surface chemical bond. It started with simple models like the effective medium theory. Later, as more accurate density functional calculations became possible, it formed the foundation of the d-band model, or Hammer–Nørskov model, of chemisorption. The model allowed an understanding of trends in bond energies of adsorbates on transition metal surfaces including variations from metal to metal, the effect of alloying, the effect of structure and defects, and the effect of strain. The interplay with the experimental groups of Flemming Besenbacher, Ib Chorkendorff and Anders Nilsson became extremely important in supporting the theory efforts.

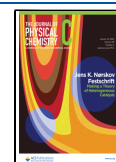
Combining DFT calculations of trends in adsorption energies and transition state energies of elemental surface processes with microkinetic modeling opened the possibility of

calculating trends in full catalytic rates, for the first time. This also opened the possibility of making predictions for new catalysts, several of which were synthesized and tested in the groups of Claus Hviid Christensen and of Ib Chorkendorff.

I established a Center for Atomic-scale Materials Design with Karsten Jacobsen, Kristian Thygesen, Thomas Bligaard, and Jan Rossmeisl in the late 2000s with funding from the Lundbeck Foundation. An important new effort was aimed at an understanding electrocatalysis. The theory of electrocatalysis was not nearly as developed as the theory of heterogeneous catalysis in terms of a quantitative description of processes and trends in reactivity. One aspect that makes the theoretical description of adsorption and reaction processes at the solid–liquid interface extremely demanding is the description of the solvated reactants. We developed the so-called computational hydrogen electrode, which opened up for a description of thermo-chemical trends in electrocatalysis. Our first application provided an understanding of trends in reactivity of different catalysts for the oxygen reduction reaction (ORR) providing insights into why Pt is the best elemental electrocatalyst for the cathode process in fuel cells, and how it can be made even better by alloying.

The discovery of scaling relations between adsorption energies of different intermediates and between transition energies and adsorption energies opened the possibility of reducing the enormous complexity associated with the calculation of trends for full catalytic rates. We found that many adsorption energies of CH_x species scaled and it took us some time to understand the physical basis for this amazing effect well enough to publish the result. Later, we found that this is extremely general. The fact that many activation energies scale with reaction energies, known as Brønsted–Evans–Polanyi relations, have been realized for many years. The scaling we discovered of adsorbed species is considerably more general than that. First, it includes scaling between adsorption energies of intermediates, and therefore transition state energies not only scale with reaction energies but with any chosen representative adsorption energy. This gives an enormous simplification.

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Moving to Stanford and SLAC in 2010, DOE funding to a new Catalysis center, SUNCAT, allowed a large expansion of the theory efforts, and Thomas Bligaard, Frank Abild Petersen, Felix Studt, and Alexandra Vojvodic moved along to SLAC to form the core theory group in this center. The Center also included a number of outstanding experimentalists, in particular Anders Nilsson, Tom Jaramillo, Matteo Cargnello, Stacey Bent, and Zhenan Bao.

A systematic theory of transition metal catalysis was developed in those years. We showed that the scaling relations are extremely general for many surfaces and reactions, and eventually you can plot the rate as a function of a few adsorption energies, or descriptors, for any reaction in a volcano plot directly identifying the optimum catalyst. Sabatier had postulated such a relationship between a bond energy and the rate many years before. The scaling relations directly showed that a single or a few bond energies can in fact be used as a descriptor, it defined what the descriptor should be, and most importantly, it made volcano relations quantitative, allowing its use to search for new catalysts. Many reactions were analyzed including hydrogenation reactions and methane activation reactions.

Another development that accelerated considerably during the time at Stanford was the description of electrochemical processes for energy conversion, including models of activation energies in electrocatalysis. This included the oxygen evolution reaction, the CO and CO₂ reduction reactions and the N₂ reduction reaction. For the latter we developed an understanding of the requirements for a high ammonia selectivity, something that laid the foundation for the thinking in the experimental groups we worked with (Ib Chorkendorff at DTU and Tom Jaramillo and Matteo Cargnello at Stanford).

In 2018 I moved back to DTU in a Villum Kann Rasmussen Chair and with good funding from the Villum Foundation. I also took on the position as Chair of the Danish National Research Foundation. The work on electrochemical ammonia synthesis became a cornerstone. Additional work on thermal ammonia synthesis resulted in the discovery of a new promotion mechanism. Surfaces with a spin moment bind adsorbates weaker than the non spin polarized surface of the same metal, and certain adsorbates quench the spin in their vicinity and thus act as promoters by lowering the energy of transition state of important elementary steps. Experimental work in the Chorkendorff and Kibsgaard groups validated the effect for several ammonia synthesis catalysts. Another new effort was in translating the theory we developed to understand trends in heterogeneous catalysis to homogeneous catalysts. All of this work continues

In all my career I have been fortunate to have worked with outstanding students and postdocs as well as some of the best

scientists in the field. I have mentioned some of the colleagues in the above but it would be completely impossible to do all students and postdocs justice in this short piece. Let me just thank everyone profoundly. The picture above, taken at a conference celebrating my 70th birthday, shows many of the students and postdocs I have worked with over the years.

Jens K. Nørskov

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Notes

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