Danish researchers design virtual nano-catalyst

January 28 2005

Research offers new opportunities in the fields of renewable energy, pollution control and in the chemical industry.
On January 28th 2005 *Science* features a paper by researchers from the Technical University of Denmark (DTU) and Haldor Topsøe A/S. The paper demonstrates that by applying the quantum theory you can calculate the performance of catalysts to be used in everything from cars to the future production of hydrogen.

So far the development of new catalysts have been based on very expensive experiments where you test a myriad of different substances. The research now published in Science forms a whole new scientific basis for the understanding of catalytic processes, and consequently for the development of new technology.

”This research is a perfect example of how in the field of nano-technology the gap between basic research and industrial production is very short indeed.” says the Chairman of Nano•DTU, professor Jens Nørskov.

Catalysis forms the basis of more than 20% of the world’s industrial production as well as a whole range of technologies that work towards creating a safer environment. One example is the catalytic converters that remove most of the pollution from today’s cars. We still need to design even better catalysts to remove more pollution from e.g. the exhaust from diesel engines.

The results of the scientists open the way towards designing new effective energy technologies. The production of hydrogen and fuel cells are thus directly dependent on the catalytic processes that we can now create models for – atom by atom.

According to Director of Research, Jens Rostrup-Nielsen from Haldor Topsøe A/S the researchers' discovery proves "that by intelligently using the advanced calculations which we are able to perform today, we will soon be capable of reducing the number of experiments necessary to develop new heterogeneous catalysts".

Professor Jens Nørskov and his group including Dr. Karoliina Honkala (now at the University of Jyväskylä, Finaland) and Dr. Ioannis Remediakis (now at the University of Crete, Greece) at the Department of Physics at DTU have developed new theoretic approaches based on quantum physics, enabling them to predict the catalytic activity for any catalyst. Together with professor Claus Hviid Christensen of the Department of Chemistry at DTU and researchers at Haldor Topsøe A/S, headed by Dr. Søren Dahl, the calculations have been tested in detailed experiments on technical catalysts made up of nanometer sized metallic particles.

Publication: www.sciencemag.org/cgi/data/307/5709/555/DC1/1

Source: Technical University of Denmark (DTU)