Computer predicts reactions between molecules and surfaces, with 'chemical precision'

November 6 2009

Good news for heterogeneous catalysis and the hydrogen economy: computers can now be used to make accurate predictions of the reactions of (hydrogen) molecules with surfaces. An international team of researchers, headed by Leiden theoretical chemist Geert-Jan Kroes, published on this subject this week in the journal *Science*.

The team developed a new method of modelling what happens when hydrogen molecules separate on a copper surface. The way is now open for calculating the interaction between more complex molecules and surfaces.

Kroes: 'It's amazing how little we actually know about chemical processes on surfaces. Processes that take place openly and under our very noses.' Even the interaction between hydrogen - with its two atoms, the simplest of all molecules - and metal surfaces is so complex that it has so far never been possible to describe what happens with quantitative precision.

Yet at the same time the reaction of molecules with surfaces is highly important for society. Their interaction plays a crucial role in heterogeneous catalysis whereby surfaces function as an intermediary allowing two other substances to react with one another. This is what happens with catalysers in cars, for example, and also in the production of the majority of synthetic compounds.

In the specific case of hydrogen, the interaction between a metal surface and hydrogen molecules also has an important function in the storage of hydrogen, in its turn one of the mainstays in the use of hydrogen as a clean fuel. Separation of hydrogen molecules into two atoms is generally the first step in chemical hydrogen storage methods.

Research into chemical reactions is no longer restricted to the lab; complex computer calculations have become an essential element of this research. Since the sixties, theoreticians have tried to find methods of calculating the forcefield between the atoms of the molecules that are involved in the reactions of molecules with surfaces. The forces between the atoms and therefore the barriers for the activation of energy exert an exponential influence on reaction speed.

The more precise the calculations of the inter-atomic forcefield, the more precise the prediction of the reactions that take place between molecules and surface. However, it is very difficult to calculate the force field, because it calls for an accurate description of two totally different subsystems: that of individual molecules and that of complete metal surfaces.

Kroes and his team members have now developed a method of making computer models of an important class of molecule-surface reactions, namely the dissociation of hydrogen on a metal surface, with so-called chemical precision.

Kroes: ' "Chemical precision" means that we can calculate the energy of the interaction between molecules and surface with a margin of error not greater than 1 kilocalorie per mol. The kilocalorie is the unit of energy familiar to us from diet lists, and a mol is the unit that expresses the number of molecules. There are about 6 x 1023 molecules in one mol. To give you an idea: 1 mol of water weights approximately 18 grams.'

To achieve "chemical precision" an advance first had to be made in so-called density function theory (DFT). In this theory, the Hohenberg-Kohn theorems state that the energy of the system (and therefore also the reaction barrier) is determined by the density of the electrons in the system. However, the theory does not explain how exactly the energy is determined from the electron density. The trick that the Leiden researchers applied is to take a so-called functional with a parameter that could be fitted to one experiment on the reaction of 'heavy hydrogen' (D_2) with copper. The functional gives the energy as a function of the electron density. Subsequent calculations showed that other experiments on the reaction of H_2 on that copper surface could be reproduced accurately using the same functional.

More information: Chemically accurate simulation of a prototypical surface reaction: H2 dissociation on Cu(111).
C. Díaz, E. Pijper, R.A. Olsen, H.F. Busnengo, D.J. Auerbach, G.J. Kroes. *Science* 6 November 2009.

Source: Leiden University

Citation: Computer predicts reactions between molecules and surfaces, with 'chemical precision' (2009, November 6) retrieved 13 April 2024 from https://phys.org/news/2009-11-reactions-molecules-surfaces-chemical-precision.html

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.