

Topic 1: Computer Simulations of Metal oxide surfaces and catalysis

Topic 2: Computer Simulations of Metal ions in solution

We have some open positions for *examensarbete* (with a possibility to continue for a *Ph.D.* degree afterwards). Some part of the project might be carried out together with one of our collaborating research teams in Europe.

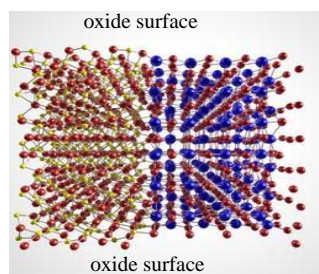
RESEARCH TOPIC 1: METAL OXIDE SURFACES AND CATALYSIS

Almost all chemical reactions of importance in our daily lives occur at surfaces and interfaces. Metal oxide surfaces are used in car catalysts to help remove toxic NO and CO from the exhaust gas, according to $2\text{CO} + 2\text{NO} \rightarrow \text{N}_2 + 2\text{CO}_2$.

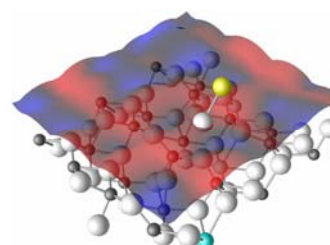
This is the net formula, but the molecular-level mechanism for this process is not well known. For example, one knows that the car catalyst needs a temperature of at least 200 °C to function efficiently. So one knows that the temperature has an effect on these surface reactions - but what exactly goes on at a molecular level at these elevated temperatures? We study the properties of catalyst surfaces using theoretical computer simulation techniques to find some of the answers.



Car catalysts destroy the toxic exhaust gases CO, NO_x and hydrocarbons and form CO₂, H₂O and N₂. The catalyst consists of metal particles and metal oxides (such as CeO₂ and Al₂O₃).



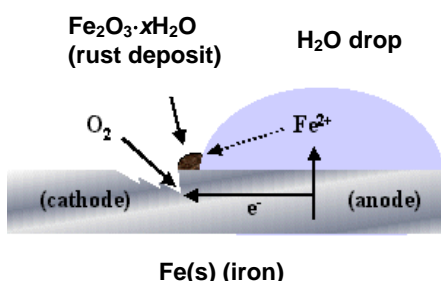
How is the catalytic activity related to the surface properties? This picture shows a "snapshot" from a molecular dynamics (MD) simulation at 700 K of an oxide film with two surfaces. The film consists of two different oxides: Al₂O₃ (red and yellow atoms) and CeO₂ (red and blue atoms).



Where do the molecules want to adsorb at the surface? Quantum-chemical calculations can help us find the answer. The red & blue colour scheme illustrates the molecule's adsorption probability.

RESEARCH TOPIC 2: SIMULATIONS OF METAL IONS IN SOLUTION

Metal ions solvated in aqueous or non-aqueous solvents and in mixtures of solvents play an important role in *electrochemical applications* and in *solvent separation technologies*. Solvated ions also appear in high concentrations in *living organisms*, where their presence or absence can fundamentally alter the functions of life. In fact, the structure and dynamics of the solvation shells have a large impact on any *chemical reaction* of metal ions in solution.

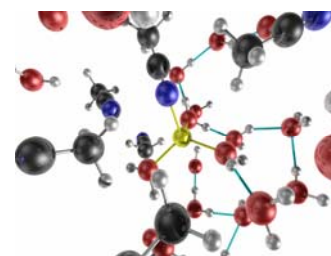


Corrosion: Solution chemistry at the interface between a solid and a liquid.

Kemiska reaktioner



When CrCl₃ salt is dissolved in water, the green [Cr³⁺(H₂O)₄(Cl)₂]⁺ complex is formed. The Cl⁻ ions surrounding the Cr³⁺ ion then gradually exchange with the water molecules in the solution. After about a day the solution becomes blue, because the [Cr(H₂O)₆]³⁺ complex is blue.



A snapshot from an MD simulation of a metal ion (Li⁺, yellow) in a mixture of 10% acetonitrile (CH₃CN) and 90% water at room temperature. The H₂O molecules can be seen to point their negative ends (red O) towards the positive ion. How are the CH₃CN molecules oriented? (C is black, H is white, N is blue).

Some molecular-level questions that we want to answer in this project are for example: *How far out in the solution do the solvent molecules feel the strong influence from the positive cation? And, conversely, how much are the ions affected by the surrounding solvent molecules? In a mixed solvent, which type of solvent molecules will win the competition for the places around the ion?* We are trying to find the answers to questions like these using theoretical simulations of different kinds.

WHY DO WE PERFORM THEORETICAL CALCULATIONS?

Experiments usually give information which is averaged over a large number of atoms/molecules and averaged over some timespan. Therefore there is a built-in limitation in the detail of molecular-level information that experiment can give. **Computational chemistry** and physics give perfect detail. The interplay between experiment and theory is very challenging - and very valuable!

YOUR PARTICULAR EXAMENSARBETE

We offer different diploma projects where you will perform Molecular Dynamics simulations to generate time-dependent structural and dynamical data and/or perform *ab initio* calculations to generate the electronic structure and bonding properties at the surface of a metal oxide, at a metal/oxide interface, in a solid or in an ionic solution. Your diploma work will be focussed around one or two relevant chemical systems and processes and around a few specific scientific problems. Some of the projects involve writing computer programs to perform parts of the data analysis.

You will participate in the daily research work of our group. It is desirable that you have taken some course in quantum chemistry *or* chemical bonding *or* statistical thermodynamics *or* computational chemistry/physics. We use both home-written computer codes and commercial ones; some are the very same ones they use in industry. We have had several examensarbetare working in the two areas described here, with successful results (for example carstenm@mkem.uu.se, whom you are welcome to contact).

For more information, see www.teoroo.mkem.uu.se. If you are interested in an examensarbete, please contact Professor Kersti Hermansson (kersti@mkem.uu.se, Room 2410 at the Ångström Laboratory, tel. 471 3767) or any of the group members. We belong to the Department of Materials Chemistry at the Ångström Laboratory.