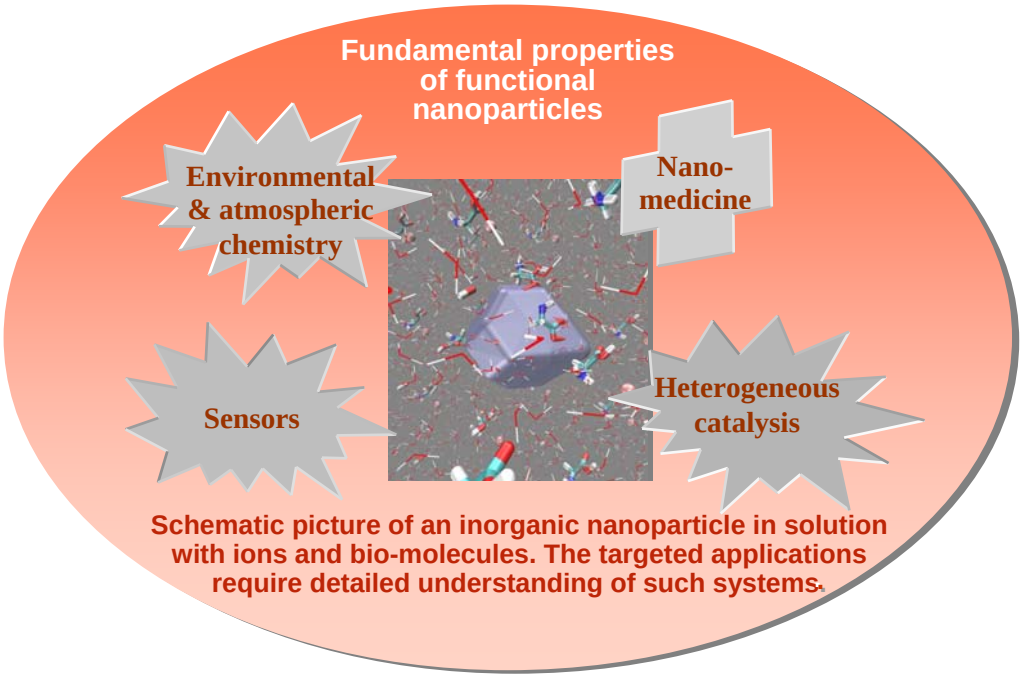
Four Ph.D. positions in "Computer simulations in Materials Chemistry"

at the Ångström Laboratory, Uppsala University

For more info and the application procedure – see http://www.uu.se/jobb/phd-students

The overall vision of these Ph.D. projects is to solve important scientific questions in the fields of nanoscience and inorganic materials chemistry, and at the same time address challenging technological and environmental problems. We therefore work with two of the most important materials and chemicals that exist – *metal oxides* and *water* – and study how molecules interact with the surface ions of the nanoparticle. In short, we want to find the relations between the atomic-level structure and dynamics of functional oxide nanoparticles and their properties under realistic (dry or aqueous) environments.

Functional nanoparticles. Nature can produce inorganic nanoparticles in various sizes and shapes, and today, also new experimental synthesis methods can do it. Here large-scale computer simulations open up new opportunities. They can provide a fundamental atomic-level understanding of how the particles' properties vary with their *sizes and shapes* and allow the design of nanoparticles with pre-defined, tailored chemical functionalities or explain the role of nanodroplets in the atmosphere. This is valuable knowledge that is difficult to acquire in any other way! The picture below illustrates some applications of nanosystems that we are particularly interested in in our research group.



Schematic picture of an inorganic nanoparticle in solution with ions and bio-molecules. The targeted applications require detailed understanding of such systems.

How shall we do it? Our research group has several decades of experience in using, developing and adapting models and tools for our needs. In addition to using state-of-the-art methods in quantum chemistry and molecular dynamics (MD) simulations, we improve upon these methods, or combine them in new ways. For small molecules or nanoclusters one can use very detailed and accurate models with explicit electrons. But the motion of many thousands of atoms during long times is impossible to calculate today. Therefore we need to gradually remove "unneeded" detail from the model as we go to larger length and time scales. This process is known as "multi-scale modeling". *Which details shall we remove*? Our dream is to "make our calculations meet experiments". On our way towards this goal we perform very large-scale simulations on computers with several hundreds or thousands of cores. We are therefore strongly involved in the national e-Science initiative eSSENCE and in the SNIC (Swedish National Infrastructure for Computing), and in many international collaborations.

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