Abstract

The center of excellence of computational molecular science will work towards the realization of the following interrelated goals. This requires an interdisciplinary collaboration between the groups of the CoE. The knowledge gained in one of the goals will help the realization of the others.

Goal 1. *Development and application of new theoretical and computational methods in molecular science.* Both nuclear and electronic dynamics are important. For the former, the optimum or even the correct molecular Hamiltonians are often unknown. From a computational point of view, the choice of coordinates and molecule-fixed axes matters. The electronic part, necessary for high-resolution spectroscopic data, requires the most advanced treatments of electron correlation. Subtle mechanisms like non-Born-Oppenheimer, relativistic corrections and quantum electrodynamic (QED) effects may also become significant.

Involved senior scientists: Halonen, Pesonen, Pyykkö, Straka, Sundholm, Vaara.
Special hot topic: Introduction of *geometric algebra* to nuclear dynamics in molecules.

Goal 2. *Prediction and identification of new chemical species and nanoclusters. Calculation of their properties.* State-of-the-art quantum chemistry methods will be used to search for new molecules and small nanoclusters, and predict properties by which they could be experimentally observed. Analytical force models, parametrized from the quantum chemistry calculations, will be employed to examine the formation mechanisms of large nanoclusters. Optical and magnetic properties for various applications will be calculated. New theoretical methods from robotics will be developed to model and control motions of large molecular units in systems, such as DNA.

Involved senior scientists: Hakala, Halonen, Khriachtchev, Lundell, Nordlund, Pesonen, Pyykkö, Räsänen, Straka, Sundholm, Vaara.
Special hot topic: Neon and helium chemistry.

Goal 3. *Multiscale modelling of the reactions of atoms and small molecules with each other and with surfaces.* First principles quantum chemistry, as well as semi-empirical and kinetic Monte Carlo models, parametrized against the first principles results, will be used to study chemical reactions of importance in environmental sciences. Different ionization methods in mass spectroscopy will be used to identify Criegee biradicals in atmospheric ozone oxidation. The knowledge gained will lead to better understanding of atmospheric chemistry, molecular processes in low-temperature solids, combustion chemistry, and fusion reactor boundary plasmas.

Involved senior scientists: Halonen, Khriachtchev, Lundell, Nordlund, Räsänen, Seetula, Sundholm, Timonen.
Special hot topic: Materials problems preventing controlled fusion.

Goal 4. *Quantum chemistry of extended systems: solid materials, surfaces, and solutions.* We will extend the application of first-principles electronic structure methods by developing and using genuinely periodic methods, based both on plane-wave and localised basis function expansions, for realistic predictions and modeling of novel species, optical and magnetic resonance spectroscopy, and reactions occurring in molecular solids, adsorbates on the external and internal surfaces of solids, and in the solution state. Periodic methods for magnetic properties near the nucleus do not yet exist. Computationally expedient models will be parametrized for the purpose of large time- and length-scale simulations, based on the first principles data. Time-dependent optical and magneto-optical excitations will be particularly emphasized.

Involved senior scientists: Hakala, Halonen, Khriachtchev, Lundell, Nordlund, Räsänen, Seetula, Timonen, Vaara.
Special hot topic: Understanding how xenon works as materials NMR probe and as anaesthetic.

The focus of the activity of all CoE partners will be on the aforementioned goals. They will also maintain their core competence in their fields of expertise. A significant effort in software development will be necessary and it will result in computer-program packages, made available for both academic and industrial use.
An important part of the CoE activity will be education, which will be in the form of already begun interdisciplinary (chemistry and physics) graduate student seminars as well as basic and graduate courses.