standing Nanomaterials from a Quantum Perspective" (Sundholm) and "Quantitative Spectroscopy for Atmospheric and Astrophysical Research" (Halonen), the Nordisk Forskerakademi (NorFA) network for research and research training on "Quantum Modeling of Molecular Materials" (Sundholm) and in the COST Action D26, "Integrative Computational Chemistry" (Pyykkö).

In Germany, the Deutsche Forschungsgemeinschaft (DFG) have five CoE:s. One of them is the "Center for Functional Nanostructures" at Karlsruhe. Pyykkö is a member of its Advisory Board. This opens an excellent link to a large foreign CoE.

1.2 Participants

- Prof. **Pekka Pyykkö** (chairman 2006-2008), Department of Chemistry, Laboratory for Instruction in Swedish.
  Prof. Pyykkö is internationally a leading person in the theoretical chemistry of heavy elements, especially on relativistic effects. The strong intersection with Inorganic Chemistry includes understanding of the metallophilic attraction and prediction of numerous new species. Pyykkö is former chairman of ESF/REHE and COST D9 and former Academy Professor in 1995-2000.
  Added value: This group both develops their own computational chemistry approaches and provides contacts to cutting-edge developments in newest quantum mechanical methods. This includes new physical contributions that are just becoming observable with improved accuracy, such as QED. These are needed for producing potential energy surfaces for spectroscopic problems and molecular simulations. The development work provides tailored computational tools for studies of large molecules, clusters, and quantum dots.
  Other senior scientists: Dr. Dage Sundholm.

- Prof. **Lauri Halonen** (chairman 2009-2011), Department of Chemistry, Laboratory of Physical Chemistry, Molecular Spectroscopy and Theoretical Chemistry Group.
  Prof. Halonen works in computational and theoretical optical spectroscopy. He with his group also develops advanced laser spectroscopic methods and collaborates with Drs. Timonen and Seetula on gas phase reaction kinetics.
  Added value: This group will provide theoretical and computational foundations for the treatment of nuclear motion. When quantum mechanical Hamiltonians are needed, our group will help. Molecular potential energy surfaces play a key role in many areas of chemistry. Our group is able to offer high-level expertise on this topic. Computational results have to be compared with experiments. Our group can supply accurate spectroscopic, kinetic and thermodynamic data for these purposes.
  Other senior scientists: Drs. Raul Martinez, Janne Pesonen, Jorma Seetula and Raimo Timonen.

- Prof. **Kai Nordlund**, (vice chairman), Department of Physical Sciences, Accelerator Laboratory, Computational Physics Group.

Prof. Nordlund is a generation younger than chairman Pyykkö. He recently chaired the 7th International Conference on Computer Simulation of Radiation Effects in Solids (COSIRES 2004), held in Helsinki.
Added value: This group applies the deep quantum chemistry knowledge of the other CoE groups to problems in materials science and nanotechnology. The knowledge of the Pyykkö group on molecular interactions at short interatomic distances, in nonequilibrium configurations and for heavy elements has proven valuable in studies of ion beam modification of materials and fusion reactor surface chemistry. Recently a collaboration with the Vaara group on the properties of water has also been initiated. The CoE will enable additional collaborations on electronic effects in surface chemistry and Si optoelectronics. The group brings a link to high-energy inelastic x-ray spectroscopy, which gives complementary information on the chemical bonds, structural properties and radiation-matter interaction of the molecular systems, in particular in the liquid phase.
Other senior scientists: Dr. Mikko Hakala.

- Prof. **Markku Räsänen**, Department of Chemistry, Laboratory of Physical Chemistry, Solid-State Spectroscopy and Photochemistry Group.
Prof. Räsänen is a prominent matrix spectroscopist and perhaps the World leader on new noble-gas molecules.
Added value: This group has a comprehensive expertise in noble-gas chemistry[1]. It will also be used for applications, including medical ones and the use of xenon for materials studies. Light-controlled chemical reactions in solids are a further aspect. Theoretical challenges for others and theoretical input from the rest of the CoE are important.
Other senior scientists: Drs. Leonid Khriachtchev and Jan Lundell.

- Doc., lecturer **Juha Vaara**, Department of Chemistry, Laboratory of Physical Chemistry, Computational Chemistry and Molecular Physics Group.
Dr. Vaara represents the youngest independent generation. He is internationally prominent in the theories of NMR and ESR parameters.
Added value: This group provides a link to magnetic resonance spectroscopy, NMR and ESR. Methods development work in relativistic and parity violation effects, as well as laser-matter interactions provide concepts, tools and modelling aid for high-resolution spectroscopic studies. NMR and ESR theories for periodic systems open new avenues in nano- and materials sciences. The interest in noble gas chemistry within the CoE is supplemented with the different perspective of using noble gases as inert agents spying upon the microstructure of their surroundings, in both materials-oriented and life-science applications.
Other senior scientists: Dr. Michal Straka.

[1]We shall systematically call Group-18 elements 'noble gases'.