



NIC Seminar

Topic: **Optical Properties Using Explicitly Correlated Coupled Cluster Theory**

Speaker: Christian Neiß, Institute of Nanotechnology,
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Contents: For many-electron systems, the CCSD and CC3 models are today the only methods that yield frequency-dependent polarizabilities, first and second hyperpolarizabilities and some magneto-optical properties to within a few percent. Unfortunately, because of the slow convergence of the electron-correlation contributions, which for nonlinear properties often add up to several tens of a percent, one has to use a large one-electron basis which makes the methods applicable only for small molecules. The use of explicitly-correlated basis sets within the R12-Ansatz makes it possible to reduce the number of required basis functions considerably. The additional excitations into R12 correlation functions can be written as an extension of the cluster operator, making them fitting smoothly into the CC framework. Optical response functions are computed as derivatives of the coupled cluster Lagrangian. We implemented the additional expressions needed for CC2-R12 and CCSD(R12) into the DALTON program package. Some results for (hyper)polarizabilities are presented, and necessary extensions of the R12 pair functions are also discussed.

Time: Tuesday, 3 February 2009, 14:00

Venue: Besprechungsraum 1, Jülich Supercomputing Centre

Anyone interested is cordially invited to participate.

sgd Dr. Sabine Höfler-Thierfeldt