Implementation of the multiresolution method for the calculation of inner-shell excitations on OCTOPUS

Report

We made significant progress regarding the main objective of the visit, i.e. implementing and improving the multiresolution method for OCTOPUS code. Advances for Poisson solver and especially the integration routines now make multiresolution calculations possible. Also an implementation of various multiresolution levels was carried out during the visit. As an example, in the calculation of methane molecule with inner-shell electrons, the number of grid points could be decreased by more than one order of magnitude while accurately retaining the ground state electron density, energy, and orbital eigenvalues. The extension of the method to excited state properties is now under development.

Regarding the simulation of the vibronic coupling, we made intriguing discoveries. We found out that when the ions are allowed to move during time propagation, the calculated absorption spectrum shows new features as fingerprints of the vibrational modes. The now appearing side peaks are separated by the vibrational mode energy from the main absorption peak. The effect is also known from experimental work. The interpretation of the calculated intensity of the side peaks is however lacking.

During the visit we also studied how the simulation of the electronic excitations to continuum can be modeled in the time propagation framework. This will enable e.g. the study of photoelectron spectroscopy. We started a work to compare the so-called mask method (i.e. at each time step multiplying the wavefunction by a specific mask function at the outer region of the simulation box) and transparent boundaries (that have been typically used for simulating quantum transport). Preliminary results show that the methods provide similar absorption spectra.