Scientific report

During my visit in the Laboratoire de Chimie et Physique Quantique, IRSAMC, Toulouse, we have considered the approaches providing relativistic data of potential energies and molecular properties of the ground and lowest excited states of HI and HI^- systems that could be possibly used in building up non-local resonance model for the description of dissociative electron attachment.

The calculation strategy was determined for the HI and HI^- molecules: First, accurate non-relativistic high-level correlation ab initio calculations with the use of extended basis sets and effective core potentials will provide potential energies and corresponding wave functions at large interval of internuclear distances. These will be followed, in the second step, by relativistic spin-orbit calculations with the use of the EPCISO method employing the relativistic core potentials and moderate carefully chosen basis sets. We have collected and checked all data, already published as well as an unfinished work from the Laboratory. In collaboration with Prof. C. Teichteil and Prof. T. Leininger the input data, i.e., relativistic effective core potential parameters and corresponding basis sets - were prepared for series of calculations. These will be run in following weeks at the J. Heyrovský Institute in Prague and the work will result in common publication. We have as well discussed the possibility how to incorporate EPCISO program into R-matrix code: though this is possible and it would provide the necessary relativistic data required in scattering calculations, a very important programming work is necessary to join the two codes.

The visit enabled me to gain valuable experiences from Prof. Christian Teichteil concerning the relativistic calculation and to get better understanding of the EPCISO code and its performance, a promising tool for providing missing data in theoretical studies of scattering processes.