COST P9 STSM Report: Chiara Piccarreta

Electron collisions with water are very important for the understanding of radiation damage in biological systems.

In the context of the study of collisions between an electron and a water molecule, the determination of the resonance potential surface is very important for a full-dimensional study of dissociative attachment.

During this first period of my PhD, I am focusing on electron-water scattering using the R-matrix method and the UK R-matrix polyatomic code. I have performed calculations for 735 geometries of water and I have obtained resonance positions and widths for each of these geometries.

In order to determine the potential surface wanted, I now need to fit these ab initio points. Studying similar systems and using a different R-matrix code, some researchers within the group of Professor Nestmann have developed a program for solving the fit problem I am currently facing.

During the period that I spent in Bonn in the group of Dr. B. Nestmann (starting from the 1st of December 2004 and finishing the 12th of the same month) I was able to carry out at least partially the following:

- fitting the ab initio points obtained by the UK code using the algorithm developed in Nestmann's group, to obtain the desired surface; this was the main objective for me to achieve while in Bonn;
- using the Bonn R-matrix code for this problem and then comparing the results with previous results;
- performing some calculations in order to compute the energy depending width of resonance states.

After some discussions about our different R-matrix codes we analysed my results of electron-water scattering calculations obtained for 735 geometries of water using the UK R-matrix polyatomic code.

As a consequence we decided to perform additional calculations for a specific geometry of the molecule: particularly for a value of the bond angle close to the equilibrium geometry. This is important in order to have a reliable fit in the Franck-Condon region.

At the same time we used the above-mentioned algorithm for solving the problem of the fitting ab initio data calculated for the potential surface of the target molecule. Next step will be to use it with the full grid of data for the resonance potential surface, which will be done at UCL in discussion with Brems and Nestmann from Bonn.