Theoretical Study of low electron scattering from CS and Rb$_2$

This visit took place from the June 22 up to July 12.

1. Electron Scattering by CS

During this visit which is part of an ongoing collaboration between the groups of Bordeaux and Romawe did a complete study of the elastic scattering of electrons by CS. All the contributions to the interaction potential were computed using a SCF wave function of the target calculated for the experimental equilibrium geometry of CS using a 6-311G** Gaussian basis set analytically expended in Legendre polynomials. In this basis set the dipole moment of CS is found to be 0.63 a.u. which is in fair agreement with its experimental value of 0.79 a.u. We used a separable form of the exchange potential and a local density functional form of the correlation polarisation potential. We first compared for the three symmetries Σ, Π and Δ the partial elastic cross sections between 1 and 100 eV with the theoretical results available obtained by Sobrinho and Lee [1] using a complex potential. Our results illustrated in Figure 1 exhibit a Π resonance around 14 eV in good agreement with theirs.
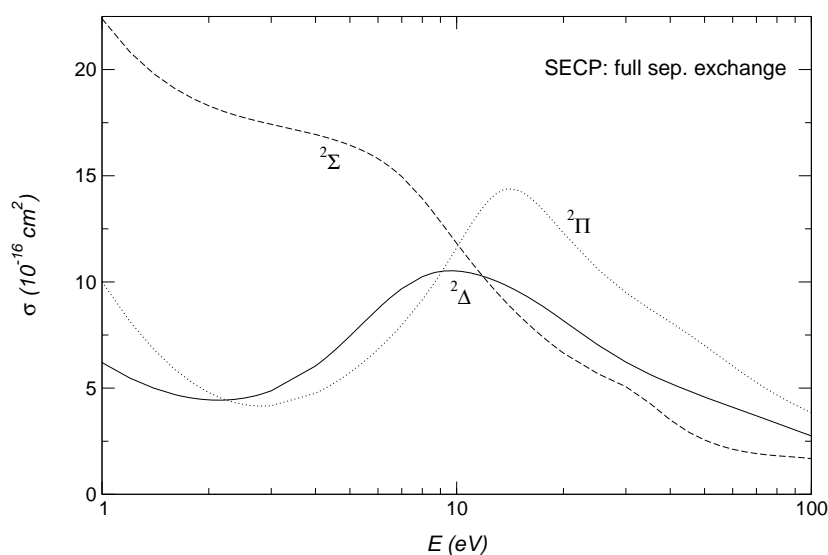

Figure 1: Partial cross sections for elastic scattering of electrons by CS as a function of collision energy.

The second issue that we considered is the existence of a lower energy Π resonance which was identified around 0.5 eV by the team of Roma using a Hara free electron gas exchange potential [2]. Another important result of this recent work where they studied the effects of bond stretching is that no bound anionic state exists for CS at its equilibrium

geometry. Our results using a separable form of the exchange potential limited to the valence molecular orbitals exhibit a very similar resonance illustrated in Figure 2.
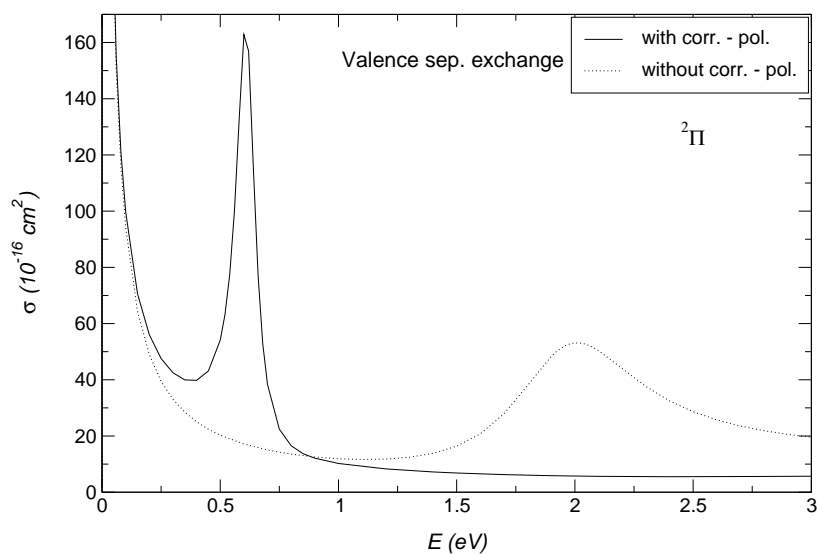

Figure 2: Comparison of the cross sections for elastic scattering of electrons by CS in the Π symmetry as a function of collision energy with and without correlation polarisation potential and including exchange only with the Valence molecular orbitals.

We found however that when the separable exchange potential includes also the contributions from all the core orbitals this resonance disappears as illustrated in Figure 3 and becomes a bound state.
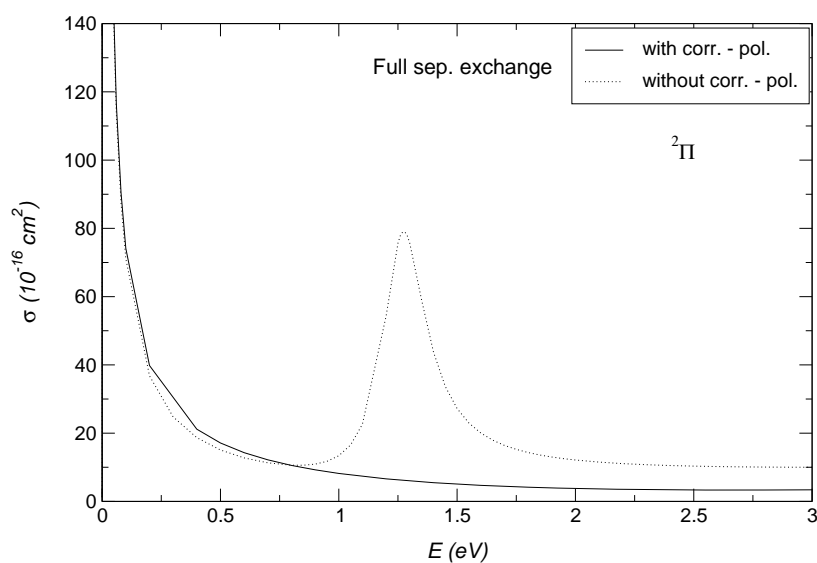
Figure 3: Cross sections for elastic scattering of electrons by CS in the Π symmetry as a function of collision energy and including exchange with all the occupied molecular orbitals.

These results which complement the study done in Roma will be submitted to publication and show that the existence of the low energy Π resonance is strongly dependent on the model of exchange potential. These results also suggest that some experimental study at low collision energy is needed for this system in order to check the existence of this resonance. We also calculated the differential cross sections for several energies ranging between 0.5 and 100 eV using Born Corrections of the scattering amplitude. These results will be published in a separate publication.

1. Electron Scattering by Rb_2:

As there are no theoretical data available for this system we decided to compare results obtained using Core Potentials and full basis sets. This diatomic molecule includes 37 occupied molecular orbitals and four of them are of Δ symmetry. During my stay I developed and implemented in the Bordeaux' code the analytical expansion around the center of mass of Δ type molecular orbitals in symetrised spherical harmonics as well as the corresponding contributions to the static potential. The calculation of the associated contributions to the exchange potentials as well as the scattering calculations will be implemented in Bordeaux in the near future and these results will also be the object of a future publication.

During this period I also gave a seminar concerning a recent work which was entitled:

Spin depolarisation of N_2^+ ($^2\Sigma^+$) in ultra cold collisions with ^{3}He and ^{4}He in a magnetic field

1. A. M. C. Sobrinho and M. T. Lee, Int. J. Quantum. Chem. 103, 703 (2005)
2. F. Carelli, F. Sebastianelli, I. Baccarelli and F. A. Gianturco, to be published in Int. J. Mass. Spectr.