The report of the academic visit to Madrid, Spain

My visit to Madrid to work with Prof. G. Garcia and Prof. F. Blanco was very successful and met the objectives I set for the visit. My main aim was to develop an understanding of the theoretical methods used by these colleagues to develop a model of electron scattering from biological molecules a major objective of Working Group 1 of the COST RADAM Action.

One of the goals of radiation biology is to develop a model of how ionizing radiations interact with living tissues, from the initial energy deposition event at the molecular level, through to the longer term consequences for the whole organism. Theoretical track structure modelling is used to stimulate the distinctive patterns of ionizations produced by wide range of ionizing radiations. Such methods show us that penetrating radiations produce a significant number of nanometre-sized clusters of ionization at the low energy track-ends of secondary electrons. Similarly, ions produce an abundance of clustered ionization along the path of the particle track both by the ions themselves and low energy secondary electrons. Such clusters can induce complex strand breaks in DNA, which are less easily repaired than the predominantly simple breaks produced by energetic electrons. The low energy electrons therefore have an important role in determining overall radiobiological effect of ionizing radiations and the mechanisms by which they damage DNA.

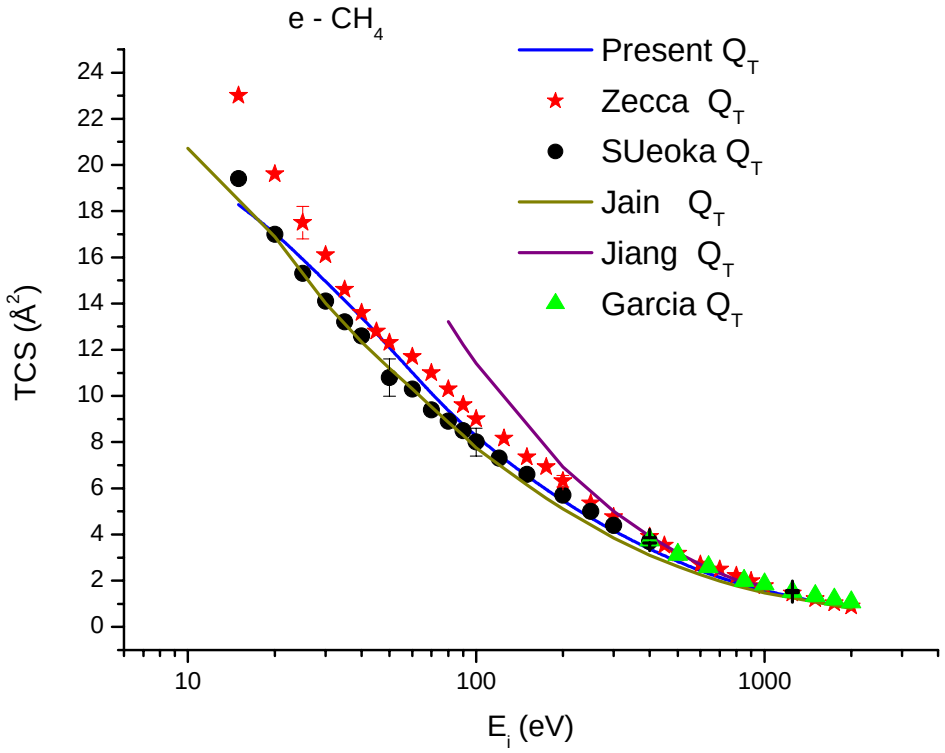
Prof. Garcia and his group have recently applied a method to reproduce the energy deposition pattern of secondary electrons generated by high energy photons in free air ionisation chambers. The input parameters for this model are the fundamental electron scattering cross sections (derived both experimentally and theoretically) and the angular resolved energy loss spectra obtained with standard electron spectroscopy techniques. During my visit I was able to learn their methods and explore how they may be adapted/addedc to my own theoretical technique. In particular they have developed an ab-initio procedure for incorporating the screening correction (resulting from the overlap of the atoms

in the molecule) into the scattering problem. Even though it is based on the semi-classical arguments this correction gives more reliable results on the scattering cross section and extends the range of validity of the model to lower energies. This is in contrast with my own independent atom model (using simple additivity rule) which is over estimates the cross section at the low energies.

During my visit we successfully incorporated the screening correction factor resulting from the overlap of the atoms in the molecule into my own scattering model. We also incorporated the polarization model of Zhang et al [1]. Having Incorporated these changes we calculated the total cross sections for e – CH_4 scattering (methane is a widely studied molecule both theoretically and experimentally and has several applications in industry). As shown in Figure 1, our total cross sections are in very good agreement with the experimental results of Sueoka and Mori [2] across the whole energy range. The experimental results of Zecca et al [3] are somewhat higher at lower energies (below 30 eV) but are are in good agreement with the present results for all higher energies up to 2000 eV. The present results are also in good accord with the theoretical values of Jain et al [4] while the values of Jiang et al [5] are higher for the energies up to 300 eV. The present results are also in very good agreement with experimental values of Garcia [6].

In future development of this collaboration we intend to calculate the total cross sections for ethane and propane molecules. I will then develop the method to investigate electron scattering from larger more biologically relevant molecules.

Finally I would like to thank the COST Programme (RADAM action) for the opportunity to undertake this visit.



References

[1] Xianzhou Zhang, Jinfeng Sun and Yufang Liu, J. Phys. B: At. Mol. Opt. Phys. **25** (1992) 1893.
[2] O. Sueoka and S. Mori J. Phys. B: At Mol. Phys. **19** (1986) 4035.
[3] Antonio Zecca, Grzegorz Karwasz, Roberto S Brusa and Czeslaw Szmytkowski , J. Phys. B: Mol. Opt. Phys. **24** (1991) 2747.
[4] Ashok Jain and K. L. Baluja, Physics Rev. A **45** (1992) 202.
[5] Yuhai Jiang, Jinfeng Sun and Linde Wan, Physics Rev. A **52** (1995) 398.
[6] G. Garcia and F. Manero, Physical Review A **57** (1998) 1069