Electron and positron scattering data for radiation bio-matter modelling

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Scattering cross section data are required as inputs for modelling software devised to quantitatively assess radiation dose and radiation induced damage in biological matter. Monte Carlo simulations that describing charged-particle interactions within the human body (e.g. GEANT4, PENELOPE, LEPTS) rely on the availability of these data to provide information that could improve the application of radiation-based medical treatment and imaging techniques. STFC’s Healthcare Futures Programme recognizes the important contribution of computational research to the development and improvement of radiotherapy.

Recent developments in the UKRmol+ software suite (https://ccpforge.cse.rl.ac.uk/gf/project/ukrmol-in/) have made it possible to perform more accurate calculations of electron and positron scattering cross sections from molecules and small molecular clusters than ever before. Exploiting current high performance computing capabilities, it is now possible to determine integral and differential cross sections for \(e^-/e^+\) scattering for targets relevant in the modelling of biological radiation damage/track structures. A methodological gap remains, however, related to how to use this data to model the effects of radiation on soft-condensed material.

Description:

The project will involve:

1) Determining cross sections for a range of small and mid-size molecules using HPC facilities, liaising with track structure and non-equilibrium charged particle transport modellers (Prof. Ron White, Australia, Prof. Garcia, Spain) to establish greatest data needs.

2) Develop an approach to adapting the gas phase/cluster data to the modelling of \(e^-/e^+\) scattering from molecules in gases and soft-condensed (disordered) materials.

3) Implement required software developments in the UKRmol+ and related suites in collaboration with members of the R-matrix community and the support of members of the STFC’s Scientific Computing Department already involved in parallel developments via CCPQ (http://www.ccpq.ac.uk/) and the software development Flagship project R-MADAM.

4) This project provides an opportunity to develop programming and high performance computing skills while investigating fascinating molecular physics phenomena. It is therefore particularly suitable for a student interested in scientific software development and the use of atomic and molecular data in medical applications.

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Qualifications required:

Applicants must have graduated (or be about to graduate) with an honours degree in Physics, Chemistry or a related discipline and possess good undergraduate-level knowledge of atomic and molecular physics and/or theoretical chemistry. Furthermore, the applicant should have some experience of writing software and/or the use of Linux or high performance computing environments.