Electron and positron scattering data for biological radiation damage modelling

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**Description:** Electrons and positrons play a role in the interaction of radiation with biological material: electrons are generated in large quantities by the ionizing radiation used in medical treatment and imaging; positrons are used for sophisticated medical imaging (PET scans). Understanding the mechanisms and effect of electrons and positions on biological molecules can help improve how we use radiation both for treatment and imaging. In particular, scattering data are required as input for software that models quantitatively radiation dose and radiation induced damage in biological matter [1].

Recent developments in the UKRmol+ software suite [2] have made it possible to perform more accurate calculations of electron and positron scattering for molecules and small molecular clusters than ever before. We are now able [3] to determine integral and differential cross sections for electron and positron scattering for targets relevant in the modelling of biological radiation damage/track structures as well as provide insight into, for example, the mechanisms by which radiosensitizers may enhance damage. A methodological gap remains, however, related to how to use these data to model the effects of radiation on soft-condensed material (i.e. a cellular environment) where the relevant target molecules are not isolated.

The project will involve:
1) Determining cross sections for a range of small and mid-size molecules using high-performance computing facilities, liaising with track structure and non-equilibrium charged particle transport modellers and experimentalists to establish greatest data needs.
2) Developing an approach to adapt the gas phase/cluster data to the modelling of electron and positron scattering from molecules in soft-condensed (disordered) materials.
3) Implementing required software developments in the UKRmol+ and related suites in collaboration with members of the CCPQ (http://www.ccpq.ac.uk/) and UK-AMOR (https://www.ukamor.com/) communities.

The project is linked to a collaboration with several Australian universities entitled **Positrons in biosystems** and provides an opportunity to investigate fascinating molecular physics phenomena of relevance in medical applications while developing high performance computing skills.

**References:**


**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 use of Linux or high-performance computing environments; some software writing experience is also desirable but not essential.