Topic number

Challenges in the kinetic modelling of electrons and ions in gaseous and liquid matter

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Modelling of electron and ion induced processes in plasma medicine and radiation damage is reliant on accurate self-consistent sets of cross-sections for electrons in tissue. These cross-sections (and associated transport theory) must accurately account not only the charged particle-biomolecule interactions but also for the soft-condensed nature of tissue. In this presentation, we report on recent swarm experiments for electrons in gaseous water and tetrahydrofuran using the pulsed-Townsend experiment, and the associated development of self-consistent cross-section sets that arise from them. We also report on the necessary modifications to the transport theory and gas-phase cross-sections required to accurately treat electron transport in liquids. The accuracy of the ab-initio theory is highlighted through comparison of theory and experiment for electrons in liquid Ar/Xe.

1. Introduction

Accurate modelling of electron and ion transport in plasmas, plasma-liquid and plasma-tissue interactions is dependent on (i) the existence of accurate and complete sets of cross-sections, (ii) an accurate treatment of electron/ion transport in these phases, and (iii) accurate description of other processes e.g. localization (trapping), bubbles, etc.

Modelling of electron/ions transport in gases, liquids and soft-condensed matter is considered through appropriate generalisations of Boltzmann's equation to account for spatial-temporal correlations present in liquids including self-trapping of electrons into bubble states, and combined localised-delocalised nature of transport. Unified solutions of Boltzmann's equation for electrons and ions are made within a multi-term framework, avoiding the well-known restrictions associated with the 'two-term' approximation.

2. Self-consistent electron-biomolecule cross-section sets

The accuracy and completeness of electron-biomolecule cross-section sets can be assessed by comparison of calculated transport coefficients with those measured using a pulsed-Townsend swarm experiment of de Urquijo and co-workers. In this presentation we will present results from our recent studies of electrons in water, as the natural surrogate for human tissue. In addition, while DNA is currently not convenient to study, tetrahydrofuran (THF – C_4H_8O) has been investigated as a close analogue for low-energy electron interactions with 2-deoxyribose, a sugar that links phosphate groups in the DNA backbone.

3. Electron transport in dense atomic gases and liquids

As detailed above the treatment of electron transport in liquids involves distinctly more complicated physical processes than in the gas and crystalline phases. The randomness assumption inbuilt in the treatment of gases is no longer present, and neither is the long-range order generally present in crystalline materials. Rather in liquids there exists some short range order, where the scattering centres are spatially and temporally correlated. The impact of the screening of the electron interaction potential within the liquid is treated using an ab-initio solution of the Dirac-Fock equation, with a fully non-local treatment of exchange and accurate multipole polarisability in the electron-atom potential. We should emphasize that there are no adjustable parameters in the calculation [1]. In the presentation we will highlight our results for the transport of electrons in liquid argon and liquid xenon. Furthermore, we will highlight our preliminary results for electron capture into bubble states for atomic liquids [2].

[1] G J Boyle, R P McEachran, D Cocks, and R D White. J. Chem. Phys. , 142:154507, 2015
[2] D Cocks and R D White. arXiv:1602.07834v1