Ab initio Studies of Interparticle Coulombic Electron Capture

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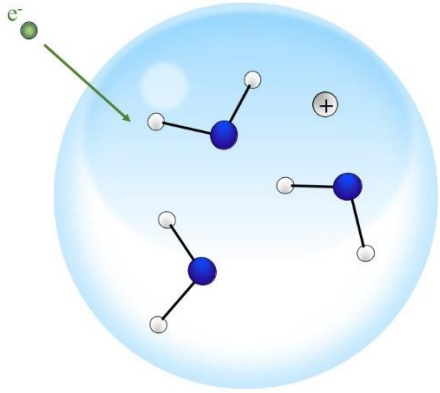

Project highlights:

- Investigate Interparticle Coulombic Electron Capture, a novel atomic and molecular process of applied importance
- Provide the first quantitative insight into its mechanism
- Develop an in depth understanding of how to model collision induced processes in molecules as well as gaining skills in high-performance computing and, optionally, software development.
- Interact with international collaborators in France and Germany.

Project description:

Electron-molecules collisions take place in many environments, both natural (e.g. the interstellar medium) and man-made (e.g. plasmas used for industrial applications) [1]. Understanding them, and being able to quantify their effect, is crucial to model processes of applied relevance and to guide and analyse experiments. A particularly interesting example is the potential biological damage caused by low energy electrons produced when radiation used for medical imaging and treatment interacts with the cells in our bodies [2].

Until relatively recently, most electron collision studies were done in gas phase (experiment) or assuming the molecular target is isolated (calculations). However, many of the environments mentioned above involve molecules surrounded by other molecules or atoms. These surrounding particles can modify the collision (for example, by increasing/reducing the likelihood of a specific collisional outcome) and can also lead to new phenomena like Interparticle Coulombic Electron Capture (ICEC).

ICEC is part of a family of processes mediated by the exchange of energy between neighbours in weakly bound systems. In ICEC, an electron is attached to the target atom or

molecule; the excess energy is then transferred to a nearby particle (as a virtual photon) leading to its ionization. The process was first predicted theoretically in 2010 [3] and the first *ab initio* calculations of ICEC cross sections were performed a few years later [4]. ICEC has been theoretically shown to also take place in quantum dots. Currently, experiments are being carried out to validate the calculations. A related process, Interparticle Coulombic Decay (ICD) was predicted a couple of decades before ICEC and confirmed experimentally within 10 years, leading to a still growing field of research [5]. ICEC is following a similar trajectory, partly due to its expected relevance to low energy electron interaction with biological matter.

The aim of this project is to study ICEC for different systems (target molecule and surrounding particles) in order to understand its fundamental properties and as well as provide data of applied relevance. We will use the R-matrix approach and the UKRmol+ suite [6], a well-established software suite developed by the OU group and collaborators for the treatment of low energy electron and positron collisions with molecules and molecular clusters as well as photoionization. We plan to study the effect of the target + environment system geometry on ICEC, how an increased number of neighbouring particles affects it and whether the total charge of system influences the process significantly. In addition, we plan to investigate how the formation of resonant states affects ICEC: initial calculations [7] have shown a rich, and sometimes unexpected, resonance structure.

References:

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