Ab initio studies of Interparticle Coulombic Electron Capture

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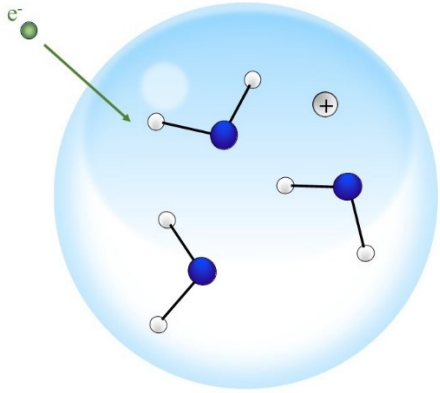

Project highlights:

- 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 capture by molecules is an important process that can be significantly enhanced or even enabled by the presence of an environment (other molecules or atoms). The environment mediated process is known as Interparticle Coulombic Electron Capture (ICEC) [1] and was first predicted theoretically in 2010 [2]. In ICEC, an electron is attached to the target atom or molecule; the excess energy is then transferred to a nearby particle leading to its ionization. ICEC therefore leads to both a change in the species present in the medium and in the kinetic energy of free electrons. ICEC is part of a family of non-local processes mediated by the exchange of energy between neighbours in weakly bound systems [3].

Much is yet to be understood about ICEC and quantifying its effect could be crucial to model many processes of applied relevance and to guide and analyse experiments. Free electrons are present in a range of physical environments, from natural and man-made plasmas to matter subject to ionizing radiation. In many processes of applied relevance (e.g. radiation used in medicine for imaging and treatment [4]), molecules are not isolated and the environment affects their interaction with the free electrons present.

Only a few *ab initio* theoretical studies of ICEC with molecules as the electron acceptor have been carried out so far [1] and ICEC is yet to be confirmed experimentally. The aim of this project is to study ICEC for different systems (target molecule and surrounding particles) in order to understand its fundamental properties, provide data of applied relevance and guide experiments. We will use the R-matrix approach and the UKRmol+ suite [5] a well-established software suite developed by the OU group and collaborators. 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 [6] have shown a rich, and sometimes unexpected, resonance structure.

References:

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6. A. Molle et al, Phys. Rev. A 103, 012808 (2021)