Environment effects in electron scattering from molecules

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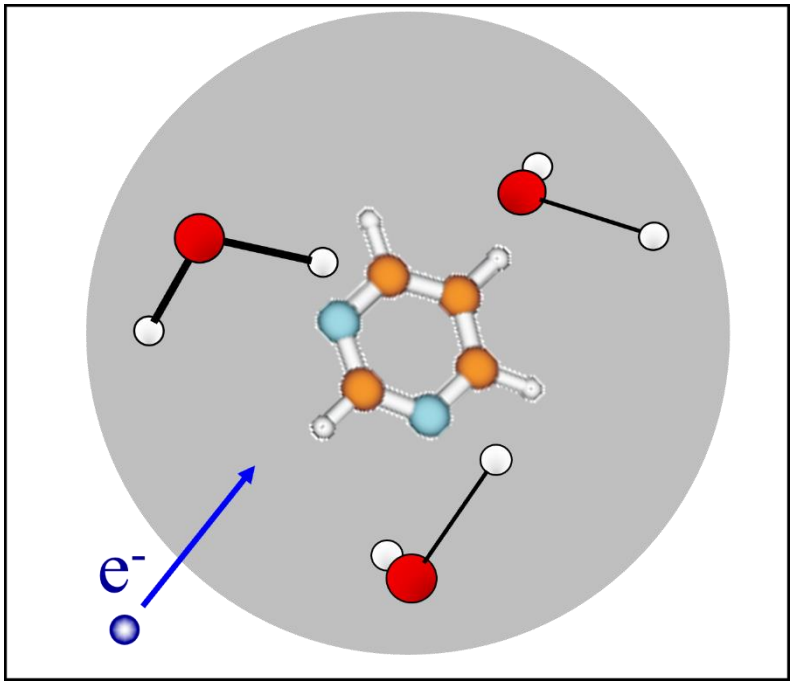

Project highlights:

1. Determining cross sections for a range of molecules embedded in water clusters using current high performance computing facilities, liaising with track structure and non-equilibrium charged particle transport modellers and experimentalists to establish greatest data needs.
2. Investigating ICEC to biologically relevant molecules, looking at the effect of improving correlation description and of cluster geometry.
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.

Project description:

Electron collisions with molecules take place in a wide range of 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 particular example is understanding how low energy electrons, produced by radiation used for medical treatment or imaging, interact with the cells in our bodies and can damage biological material [2].

Some electron-molecule collisions take place in the gas phase, but many do not: biomedical applications involve interactions with molecules in a condensed environment as does

radiation interaction with atmospheric and astrophysical ices. A way to bridge the gap between gas phase investigations and the processes in the condensed medium is to examine scattering from molecular clusters. The environment due to other molecules in the cluster will affect the collision process both quantitatively and qualitatively. An example of this is the environment assisted process known as Interatomic Coulombic Electron Capture (ICEC)[3]. Investigating the collision with a molecule embedded in a water cluster allows us to understand the effect of hydration.

UKRmol+ [4], a software suite developed by the OU group and collaborators, is the only ab initio code that can provide accurate insight into processes with targets of these sizes, not only into how scattering processes are enhanced or quenched, but also into ICEC.

References:

1. S. Schippers et al, J. Phys. B: 52 (2019) 171002 (https://iopscience.iop.org/article/10.1088/1361-6455/ab26e0)
2. J. D. Gorfinkiel and S. Ptasinska, J. Phys. B 50 (2017) 182001 (https://iopscience.iop.org/article/10.1088/1361-6455/ab26e0)
3. A. Molle et al, Phys. Rev. A 104, 022818 (2021) (https://doi.org/10.1103/PhysRevA.104.022818)
4. Z. Mašín et al, CPC 249 (2020) 107092 (https://arxiv.org/abs/1908.03018)