Canadian Association of Physicists

Association canadienne des physiciens et physiciennes

Contribution ID: **572** Type: **Invited Speaker / Conférencier(ère) invité(e)**

(I) Ionization of biologically relevant molecules studied with an independent atom model including geometric overlap

Monday 7 June 2021 12:45 (5 minutes)

If one wishes to understand and successfully simulate the radiation damage of biological tissue one needs to understand the fundamental ionization processes of molecules in the gas or vapour
phase first. The latter problem has been addressed in a number of studies in recent years, but experimental data have remained scarce and accurate cross-section predictions based on first-principles quantum-mechanical calculations challenging due to the complexity of the molecules of interest. There is thus a role to be played by simplified modelling - provided the models used
can be shown to work for simpler systems for which reliable theoretical and experimental data are available for comparison.

We have recently developed one such model. It is based on the independent atom model (IAM) according to which a cross section, e.g., for electron removal from a molecule can be obtained from atomic cross sections for the same process. Instead of simply adding up the cross sections for all the atoms that make up the molecule we take geometric overlap into account, which arises when the atomic cross sections are pictured as circular disks surrounding the nuclei in the molecule. The overlapping areas are calculated using a pixel counting method (PCM) and, accordingly, we label our model IAM-PCM.

The IAM-PCM has been applied to a number of ion-impact collision problems with target systems
ranging from relatively simple molecules, such as water and methane to complex biomolecules,
such as the RNA and DNA nucleobases [1], and also including atomic and molecular clusters [2].
In this talk, I will explain the model, present a selection of recent results and discuss what can be learned from them.

[1] H. J. Lüdde et al., J Phys. B 52, 195203 (2019); Phys. Rev. A 101, 062709 (2020); Atoms 8, 59 (2020).

[2] H. J. Lüdde et al., Eur. Phys. J. B 91, 99 (2018).

Primary author: Prof. KIRCHNER, Tom (York University)

Presenter: Prof. KIRCHNER, Tom (York University)

Session Classification: M2-1 Interaction between matter and light (DAMOPC) / Interaction entre matière et lumière (DPAMPC)

Track Classification: Atomic, Molecular and Optical Physics, Canada / Physique atomique, moléculaire et photonique, Canada (DAMOPC-DPAMPC)