Independent-atom-model pixel counting method calculations for proton collisions from biologically relevant molecules

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Synopsis The recently introduced independent-atom-model pixel counting method is used to calculate net ionization cross sections of complex biomolecules bombarded by energetic protons. Scaling relations are examined and a simple parametrization of the cross section results in terms of an analytical formula is suggested.

The growing interest in collisions involving large biomolecules, coupled with the complexity of the problem, calls for the development of simplified theoretical models for the calculation of charge-changing cross sections. In recent work, we have introduced a variant of an independent atom model (IAM) which is easily applicable to a wide range of systems [1, 2]. It is based on a geometrical interpretation of an ionization or electron capture cross section as an effective area composed of overlapping circular disks. The latter represent the cross sections of the atomic constituents of the molecule of interest and are calculated using a well-tested density-functional-theory framework. The effective area calculation is carried out using a pixel counting method (PCM).

If the atomic cross sections are small and do not overlap the IAM-PCM results coincide with standard independent-atom-model additivity rule (IAM-AR) cross sections. However, at not too high impact energies atomic cross sections for ionization and electron transfer tend to be large and the overlap reduces the IAM-PCM cross section significantly compared to the IAM-AR result.

At the conference we will present IAM-PCM (and IAM-AR) net ionization cross sections for proton impact on a large class of systems including amino acids and nucleotides. We will discuss scaling relations with respect to the number of (active) electrons and suggest a parametrization of our results in terms of a simple analytical formula.

References

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