ID de Contribution: **83** Type: **Contribution orale**

Calculation of molecular ionization cross-sections using complex Gaussian representations of the continuum

lundi 3 juillet 2023 17:20 (15 minutes)

The theoretical study of molecular ionization processes requires an efficient description of the electronic continuum states. Because of their very interesting mathematical properties, Gaussian basis sets are widely exploited for bound states calculations, while their use is far less developed in the context of fragmentation processes where continuum states play a leading role.

In a series of recent papers [e.g. A. Ammar et al, 2021 J. Comput. Chem. 42, 2294], we have explored the possibility of representing the continuum state associated with the outgoing electron with complex Gaussian-type orbitals (cGTOs), i.e. Gaussian orbitals with a complex exponent. While nodeless real GTOs usually fail in representing oscillating wavefunctions, their complex counterparts perform better, leading to sufficiently accurate expansions (up to ~ 30 a.u. using typically 30 cGTOs), reliable enough for physical applications. Based on such Gaussian orbitals, we have derived analytical, closed-form expressions for all the integrals involved in cross-section calculations, either in the case of molecular photoionization, or in the more challenging case of electron-impact ionization.

The method has been first applied to the calculation of photoionization cross-sections and asymmetry parameters for ammonia, water and methane, using angular-averaged potentials and a monocentric approximation for the initial states of the target. We will also present triple differential cross-section calculations for the electron-impact ionization (e,2e) of methane with two sets of kinematic parameters corresponding to recent experiments [E. Ali et al 2019, J. Chem. Phys. 150, 194302].

Affiliation de l'auteur principal

LPCT, Université de Lorraine et CNRS, 57000 Metz

Auteur principal: Dr LECLERC, Arnaud (Université de Lorraine)

Co-auteurs: Dr AMMAR, Abdallah (Université de Toulouse); Prof. ANCARANI, Lorenzo Ugo (Université de Lorraine)

Orateur: Dr LECLERC, Arnaud (Université de Lorraine)

Classification de Session: Mini-colloques: MC07 Les 100 ans de l'effet Compton : des sources aux applications

Classification de thématique: MC7 Les 100 ans de l'effet Compton : des sources aux applications