New theoretical approaches to describe single- and multi-photon processes in atoms and molecules

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Résumé

The optical response of atoms and molecules induced by an intense ultra-short laser field is a subject of increasing interest since the advent of attosecond (10–18 s) laser pulses. In the last decades, impressive advances in laser technology have introduced new time resolved spectroscopies, offering the opportunity to investigate electron dynamics in atoms and molecules with an unprecedented time resolution.
However, the mechanism that control electron dynamics of complex systems in strong fields is still a challenge that requires to be interpreted by advanced theory. Development of accurate theoretical and computational methods, able to provide a precise treatment of the fundamental processes generated in the strong field regime, such as above-threshold ionization (ATI) or high-harmonic generation (HHG), is therefore crucial. In general, the accuracy in describing single- or multi-photon processes is strictly related to two aspects : the representation of the continuum energy spectrum and the description of the correlation effects.

In this seminar, these two aspects are explored in simple atomic and molecular systems. We are going to analyze the numerical performance of three different basis sets (Gaussian/Grid/Bsplines) in order to reproduce a good continuum spectrum in molecules [1], and, in a second step, we present a new linear-response range-separated time-dependent density functional theory to study photoexcitation and photoionization processes in atomic systems [2].

F. Zapata, M. Labeye, E. Coccia, V. Véniard, J. Toulouse, J. Caillat, R.Taïeb and E. Luppi, J. Chem. Theory Comput. 14 (11), 5846-5858 (2018).

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