

Abstract Submitted
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Merging quantum-chemistry with B-splines to describe molecular photoionization¹ L. ARGENTI², C. MARANTE, M. KLINKER, I. CORRAL, J. GONZALEZ, F. MARTIN, UAM, Madrid (Spain) — Theoretical description of observables in attosecond pump-probe experiments requires a good representation of the system's ionization continuum. For polyelectronic atoms and molecules, however, this is still a challenge, due to the complicated short-range structure of correlated electronic wavefunctions. Whereas quantum chemistry packages (QCP) implementing sophisticated methods to compute bound electronic molecular states are well established, comparable tools for the continuum are not widely available yet. To tackle this problem, we have developed a new approach that, by means of a hybrid Gaussian-B-spline basis, interfaces existing QCPs with close-coupling scattering methods. To illustrate the viability of this approach, we report results for the multichannel ionization of the helium atom and of the hydrogen molecule that are in excellent agreement with existing accurate benchmarks. These findings, together with the flexibility of QCPs, make of this approach a good candidate for the theoretical study of the ionization of poly-electronic systems.

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