Theoretical approach for simulating single photon double core ionization of small molecules

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Résumé

We present a theoretical approach for simulating single photon double core ionization of small molecules in the dipolar approximation. Our method couple a selected CI computation of wave functions to reduce the number of slater determinants needed to converge the peak relative energies and the use of non-orthogonal molecular orbital basis set for the neutral and the ionised system in order to speed up the convergence of the peak intensities.

Mots-Clés: Applied quantum chemistry, Spectroscopy, Core electrons, Chemical physics, Non orthogonal basis sets

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