A dressed harmonic study in laser-assisted photoionization of water molecules by attopulses

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Synopsis We study theoretically the laser-assisted photoionization of water molecules by attopulses by using a separable Coulomb-Volkov model [1, 2, 3]. We analyze the effect of varying the delay between the attopulse and the assistant laser field on the dressed harmonics lines.

Since organic matter is composed mostly of water, the reactions involving this molecule are essential to understand the interaction between the radiation and the biological tissue. In this work, we study theoretically the photoionization of water molecules by extreme ultraviolet (XUV) attopulses assisted by lasers in the near-infrared (NIR) range.

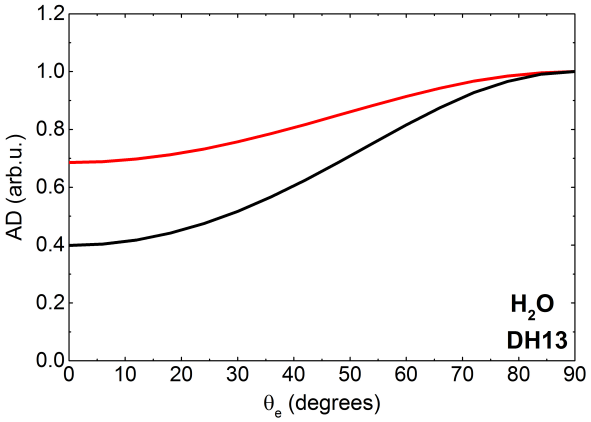

Figure 1. Angular distribution (AD) for the outermost water orbital $1b_1$ as a function of the emission angle θ_e for the 13th dressed harmonic (DH13) line computed using the Moccia's wavefunction for water, for the delays $\phi_L = 0.188\pi$ (—) and $\phi_L = 0.688\pi$ (—).

Firstly, we obtain monochromatic total cross sections in the framework of the dipole approximation within the velocity gauge. We use a simple model where the final state wavefunction is given by a Coulomb continuum wavefunction with optimized effective charges and we employ Moccia's monocentric wavefunctions to representate the H_2O molecule orbitals. We compute total cross sections for randomly oriented molecules and we compare our predictions with more elaborated theoretical results [4, 5] and experimental data (see [4, 5] and references there in). A very good agreement is obtained with the available experiments especially at high enough energies where there is a lack of elaborated results due to their high computational cost.

Secondly, the main objective of our work, we consider the photoionization reaction by XUV attopulses assisted by NIR lasers. We analyze photoelectron angular distributions (AD) for different delays between the attopulse and the assistant laser field. To this end, we use a separable Coulomb-Volkov model in which the temporal evolution of the system can be divided into three stages that allows spatial and temporal separation for the Coulomb and Volkov final state wavefunction. We compare our results for water and Ne atoms as they belong to the same isoelectronic series (results for water are shown in Figure 1 as an example). Furthermore, we contrast our calculations with previous theoretical and experimental work for Ar atoms due to the similarities of the orbitals involved in the reaction [2]. It is expected that these studies promote progress on the control of the chemical reactivity of water molecules.

References

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