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Control of ionization and dissociation of $\text{H}_2^+$ by elliptically polarized ultra-short VUV laser pulses.

Alejandro de la Calle$^*$, Alicia Palacios$^\dagger$, Fernando Martín$^1$, Daniel Dundas$^*$

* Atomistic Simulation Centre, School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, Northern Ireland, UK.
$^\dagger$ Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain

Synopsis Resonance-enhanced multiphoton ionization of $\text{H}_2^+$ exposed to elliptically polarized VUV laser pulses is investigated. Differential cross sections for nuclei and electron are obtained using numerical solutions of the time-dependent Schrödinger equation. In this work in progress, we explore the dependence of the dissociative ionization observables with the polarization of the light.

The hydrogen molecular ion represents the simplest molecule in which correlations between electronic and ionic motion can be studied in a full quantum mechanical fashion. Understanding the interplay between electronic and ionic motion is fundamental in a wide range of areas such as condensed matter, plasma physics, medicine and biochemistry. Studying the interaction between the hydrogen molecular ion and the ultrashort VUV pulses therefore provides important insights into how these pulses interact with more complex molecules.

Since nowadays ultrafast intense radiation from sources such free-electron lasers and high-order harmonic generation are currently available in many laboratories around the world, the interest of photoionization of atoms and molecules by femto and sub-femtosecond laser pulses in the VUV and XUV frequency regime, has grown in the past years. Differential (in proton and electron energy) ionization cross sections have been theoretically obtained for $\text{H}_2^+$ [1] and $\text{H}_2$ [2] exposed to radiation polarized parallel to the molecular axis. Those studies show that, taking into account the vibrational motion of the molecule, it is possible to control the ratio between dissociative and non-dissociative ionization. In addition, photo-angular distributions (PAD) has been studied recently for linear [3] and elliptically polarized laser pulses [4, 5]. For fixed in space molecules, linearly polarized radiation oriented parallel to the molecular axis can only excite $\sigma_u/\sigma_g$ states ($\Delta M = 0$), whereas perpendicular oriented one will populate $\sigma_u$ in one-photon absorption ($\Delta M = \pm 1$), and subsequent photon absorptions may reach $\sigma_g/\delta_g$ and so on. Elliptically polarized light is viewed as a combination of parallel and perpendicular oriented fields, therefore can simultaneously excite all those symmetries. Recently, it has been shown that the rotational symmetry of PAD with respect to the molecular and the polarization axis are strongly dependent of the interplay between intermediate resonant states [6].

All the available work using circular or elliptical polarizations has been performed within the fixed nuclei approximation. In our study, the electronic and vibrational degrees of freedom are described exactly through the solution of the Time-Dependent Schrödinger Equation (TDSE), assuming that the laser light can have elliptical polarization. In such case, as there is no longer a symmetry around the internuclear axis, the TDSE is solved in cartesian coordinates, with all the degrees of freedom treated using scaled finite-difference meshes [7, 8, 9]. This approach has been implemented in a massively parallel code called HYThMIC (vibrating Hydrogen Molecular Ion in Cartesians) that allows the first full-dimensional studies of the hydrogen molecular ion in circularly polarized laser pulses for hundreds of femtoseconds in large grids.

References


$^*$E-mail: a.delacalle@qub.ac.uk