Study of the first excited $B^1\Sigma_u^+$ state of H_2 exposed to intense laser fields

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Abstract

Ionization, excitation, and deexcitation to the ground state is studied theoretically for the first excited state $B^1\Sigma_u^+$ of H_2 exposed to intense laser fields assuming a parallel orientation of a linear polarized laser and the molecular axis. Within the dipole and fixed-nuclei approximations the time-dependent Schrödinger equation describing the electronic motion is solved in full dimensionality for different laser parameters. The validity of different single-active-electron approximations in the single-photon ionization regime is investigated. The results for a large range of laser wavelengths (400 nm to 3000 nm) will be shown. It is shown that due to the close spacing of the $B^1\Sigma_u^+$ state to other excited states it is difficult to find even in this large range of laser parameters the typical signatures of tunneling ionization.

The time-dependent Schrödinger equation is solved by expanding the time-dependent electronic wavefunction in terms of a superposition of field-free eigenstates. The field-free eigenstates are calculated in two ways. In the first approach, which is applicable to two electron systems like H_2, fully correlated field-free eigenstates are obtained in complete dimensionality using a configuration-interaction calculation where the one-electron basis functions are built from B splines [1]. In the second approach, which is even applicable to larger molecules, the field-free eigenstates are calculated within the single-active-electron (SAE) approximation using density functional theory [2]. Another single-active-electron approach is developed by using a restricted basis in the configuration-interaction method. In this approach only those configurations are taken where one electron is fixed in the ground state of the ion ($H_2{}^+$). Using these three approaches results for various laser parameters are obtained and the validity of the single-active-electron approximation is investigated.

Another single-active-electron approach for the $B^1\Sigma_u^+$ state of H_2 was recently proposed in [3]. This approach is based on time-dependent extension of Koopmans' picture for the ionization in a laser pulse. The validity of this approach is also tested. It is shown that the single-active-electron approximation is not suitable for the description of single-photon ionization from the $B^1\Sigma_u^+$ state of H_2.

References

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