

THE ROLE OF MOLECULAR ROTATION FOR H_2^+ AND ITS ISOTOPES IN INTENSE, SUB-10 fs LASER PULSES

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By including nuclear rotation in our solution of the time-dependent Schrödinger equation for H_2^+ and D_2^+ in an intense laser pulse, we show that alignment effects are important even for sub-10 fs pulses. We will explore the interplay of nuclear rotation and vibration, along with electronic excitation, on the dynamics of these fundamental molecular ions.

Impulsive alignment, for instance, results from the fact that these pulses populate a broad range of angular momentum states, leading to the alignment of the molecules at the end of the pulse and to clear revival structures — rotational as well as vibrational. We will discuss our results in the context of the recent D_2 impulsive alignment experiment of Lee *et al.* [1] and compare our predictions for the vibrational revivals to the experiments in Ref. [2], looking especially for evidence of the influence of rotation.

Just as the bound molecules evolve freely after the pulse, becoming periodically aligned, any molecules that dissociated will also continue to evolve. This evolution tends to further align the fragments with the laser polarization in a manner similar to that predicted for ionizing fragments by Tong *et al.* [3]. Most experimental analyses, however, utilize the axial recoil approximation in which this post-pulse alignment is neglected. We will discuss the validity of this approximation for dissociation within our fully quantum mechanical treatment.

We will also present results for a broad range of intensities, comparing them with those obtained from the standard field-aligned, two-channel model that neglects rotation. In particular, we will show that this standard approach systematically over estimates the dissociation fraction at any given intensity relative to the more

complete calculations including rotation.

With the ability to treat the H_2^+ system including all physical processes save ionization, we will begin to work towards quantitative comparisons [4] with the detailed experimental spectra now available [5, 6].

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References

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