

Abstract Submitted
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Time-dependent density functional theory calculation of strong field ionization rates of H₂ XI CHU, The University of Montana — We first report a detailed numerical comparison of strong field ionization rates of the H₂ molecule using two TDDFT methods, the molecular ADK (MOADK) method, and an *ab initio* complex scaling (CS) method. The two TDDFT methods are TDSIC and TDLB_α, respectively, and they both contain the correct long-range limit of the exchange-correlation potential. The comparison covers different internuclear distances, molecular orientations, and laser intensities. The two TDDFT methods give consistent results. In the DC field limit, they agree with the MOADK and the CS results when the laser intensity is relatively small. At larger intensities the TDDFT results are lower and present a knee structure when plotted against the intensity. We think this difference is due to the ionization of the ion, which is not considered by the MOADK or the CS methods. We further explore the influence of the photon energy. The rates for 800 nm lasers are significantly larger than the values predicted by the slow varying field approximation at lower intensities. This difference diminishes with increasing laser intensity. With a lower intensity DC field, TDDFT methods predict an anisotropy similar to the MOADK prediction. However, we find that both the photon energy and the laser intensity play a role in the anisotropy, which the MOADK method does not describe.

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