

Abstract Submitted
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Coupled electronic and vibrational dynamics of a molecular ion in a strong laser field¹ NICHOLAS VENCE, University of Tennessee, ROBERT HARRISON, PREDRAG KRSTIC, Oak Ridge National Laboratory — We study a response of a hydrogen molecular ion to the strong 2-cycle 800-nm laser pulse, using highly accurate numerical solution of the time-dependent Schrodinger equation in 4 spatial dimension. We use a computational approach which employs an adaptive, discontinuous spectral element basis as well as multiresolution analysis and separated representations of operators for efficient computation in multiple dimensions (MADNESS). The basis (tensor product of Legendre polynomials) automatically adapts to meet the requested precision, while the time-dependent evolution of the system is considered using an efficient Chin-Chen propagator. We vary the laser polarization with respect to the fixed molecular axis, while the coupled electron and vibrational dynamics enables calculation of the ionization, dissociation and high-harmonic generation at the “same footing”.

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