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Quantum dynamics of H2+ in an atto-second laser pulse NICHOLAS VENCE, ROBERT HARRISON, University of Tennessee, PREDRAG KRSTIC, Oak Ridge National Laboratory — We demonstrate a highly-accurate numerical procedure to investigate the quantum dynamics of single electron, single- and two-center wave functions in a strong, sub-femtosecond, few-cycles laser pulse. The non-perturbative time evolution does not rely on an eigenfunction basis set. The multiresolution numerical techniques from [Harrison et. al., J. Chem. Phys. 121, 2866 (2004)] are used for spatial discretization. These calculations observe excitation and ionization in the hydrogenic systems up to lithium++ along with the molecular hydrogen ion. This study will serve as a benchmark for future multielectron calculations. This research is supported by the U.S. Department of Energy.

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