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New determination of structure parameters in strong field tunneling ionization theory of molecules[1] SONG-FENG ZHAO, CHENG JIN, ANH-THU LE, T.F. JIANG, C.D. LIN, Physics Department, Kansas State University — In the strong field molecular tunneling ionization theory of Tong et al. [Phys. Rev. A 66, 033402 (2002)], the ionization rate depends on the asymptotic wavefunction of the molecular orbital from which the electron is removed. The orbital wavefunctions obtained from standard quantum chemistry packages in general are not good enough in the asymptotic region. Here we construct a one-electron model potential for several linear molecules using density functional theory (DFT). We show that the asymptotic wavefunction can be improved with an iteration method and after one iteration accurate asymptotic wavefunctions and structure parameters are determined. With the new parameters we examine the alignment-dependent tunneling ionization probabilities for several molecules and compare with other calculations and with recent measurements, including ionization from inner molecular orbitals.

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