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Fragmentation dynamics in O_2^{q+} and CO^{q+} molecules in intense laser pulses[1] M. MAGRAKVELIDZE, J. R. Macdonald Laboratory, Kansas State University, C.M. AIKENS, Department of Chemistry, Kansas State University, U. THUMM, J. R. Macdonald Laboratory, Kansas State University — We investigate influence of non-adiabatic couplings on the dissociation and Coulomb-explosion (CE) dynamics of diatomic molecules in intense laser fields. To identify electronic states that contribute to the molecular dynamics, we first calculate adiabatic potential curves and electric dipole-coupling (DC) elements with the quantum chemistry code GAMESS.[2] Next we calculate fragment-kinetic-energy-release (KER) spectra as a function of time and quantum-beat frequency[3] for one molecular potential curve at a time and compare calculated revival times and beat frequencies with experimental data.[4] After identifying relevant electronic states we include laser-induced DCs in improved wave-packet propagation calculations including two (or more) electronic states and again compare KER spectra with experimental results.[5] We apply this scheme to O_2 and CO.

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[2]M. W. Schmidt et al., J. Comput. Chem. 14, 1347-1363(1993)
[3]M. Magrakvelidze et al., PRA 79, 033410 (2009)
[4]S. De et al., PRA 82, 013408 (2010)
[5]Ibid.

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