Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Quantum mechanical simulation of the dissociation dynamics of the N_2 (N_2^+, N_2^{++}) and O_2 (O_2^+, O_2^{++}) molecules* MAIA MAGRAKVELIDZE, IRINA BOCHAROVA, IGOR LITVINYUK, UWE THUMM — The nuclear dynamics of molecular nitrogen and oxygen in intense laser fields was studied by analyzing their fragment kinetic energy release (KER) spectra as a function of time[1]. Typically, several intermediate states contribute to the same KER. Based on a quantum mechanical model, we calculated the time evolution of an initial (ground state) nuclear wave packet in N_2^+ and N_2^{++} (O_2^+ and O_2^{++}) separately, for given adiabatic molecular potential curves, in order to assess the relevance of individual potential curves during the laser-induced fragmentation. By Fourier transformation of the nuclear probability density with respect to time, we derive internuclear distance (R) dependent power spectra[2] that allow us to identify vibrational frequencies associated with the bound motion of the vibrationally excited molecular ion. To include laser-induced dynamical couplings between molecular potential curves we are in the process of modeling (non)adiabatic transitions near curve crossings based on Landau-Zener transition rates and will compare our numerical results with existing measured KER- spectra. [1]I. Bocharova et al., to be published. [2]M. Magrakvelidze et al., PRA 79, 033410 (2009) *Supported by the US DOE.

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Date submitted: 22 Jan 2010 Electronic form version 1.4