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Comparison of the strong field ionization of N_2 and F_2: A TDDFT study[1] XI CHU, MELISSA MCINTYRE, The University of Montana — We compare strong field ionization probabilities of N_2 and F_2 molecules using time-dependent density functional theory (TDDFT) calculations. Accurate nuclear potentials and ground vibrational wave functions are incorporated into our study. For both molecules, the effect of molecular vibration is small, while that of the molecular orientation is significant. When compared to the ionization probability of a molecule at the equilibrium geometry, we estimate the effect of the ground state vibration to be within 3% for N_2 and within 6% for F_2, in the intensity range from 1 to 5×10^{14} W/cm^2. The molecular orientation dependent ionization probabilities for both molecules at various intensities are presented. They are strongly dependent on the laser intensity, and the anisotropy diminishes when the laser intensity is high. For laser intensities of 1.6 and 2.2 $\times 10^{14}$ W/cm^2 we find ionization probability ratios of 5.9 and 4.3, respectively, for the parallel versus perpendicular orientation of N_2. This is reasonably consistent with experimental measurements [1,2] For randomly oriented molecules, the ratio of the probabilities for N_2 and F_2 increases from about 1 at 10^{14} W/cm^2 to 2 at 4×10^{14} W/cm^2, which agrees well with experimental results [3]. [1] I. V. Litvinyuk *et al.*, Phys. Rev. Lett. **90**, 233003 (2003). [2] D. Pavicic *et al.*, Phys. Rev. Lett. **98**, 243001 (2007). [3] M. J. DeWitt *et al.*, Phys. Rev. Lett. **87**, 153001 (2001).

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