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Ab Initio Simulation of Fragmentation in Polyatomic Molecules by Short Intense Laser Pulses ARTHUR RUSSAKOFF, SERGIY BUBIN, KALMAN VARGA, Vanderbilt University — We study ionization and fragmentation of polyatomic molecules induced by short intense laser pulses by performing ab initio simulations within the formalism of Time Dependent Density Functional Theory. Within this formalism we investigate intra-molecular electron dynamics during a fragmentation reaction on a pre-chemistry time-scale. The time-scale of the dynamics bridges the time-domain of sub-femtoseconds, on which the electrons move, and that of the much slower motion of the heavier ions (e.g. carbon ions), which proceeds on a time-scale of tens to hundreds of femtoseconds. The kinetic energy spectrum of the fragments and the charge state of the molecule prior to fragmentation are calculated and compared to experiment.

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