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Spectral Signature of Molecular Charge Migration[1] RUBEN FERNANDEZ, Burnett School of Biomedical Sciences, University of Central Florida, FL 32816, LUCA ARGENTI, Dept. of Physics and CREOL, University of Central Florida, FL 32816 — Attosecond laser technology has opened the way to study ultrafast charge-transfer processes at their natural time scale and at the molecular level. Interpreting these processes is a challenge due to i) correlation in excited electronic states, ii) the loss of electronic coherence caused by entanglement with nuclear degrees of freedom within the same molecule as well as with other molecules in the matrix, and iii) the non-perturbative character of light-matter interaction. Here employ a new ab initio method to simulate the evolution of N-Methlyacetamide under the action of arbitrarily polarized non-ionizing light pulses, in the presence of decoherence. The electronic states are obtained from MCSCF calculations while the effects of the driving pulses and decoherence are taken into account by solving the time-dependent Lindblad equation for the molecular electronic density matrix. We reconstruct the susceptibility from the dipolar response of the molecule, which is experimentally observable, and use Beckes charge-partitioning algorithm to predict the migration of charge associated to each spectroscopic signal.

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