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Ab Initio Simulation of Photoinduced Ring Currents in Benzene[1]

TENNESSE JOYCE, AGNIESZKA JARON-BECKER, University of Colorado Boulder — A circularly polarized femtosecond laser can induce electronic ring currents within a single molecule on the order of microamps that are expected to persist for as long as nanoseconds. Photoinduced ring currents have not yet been observed experimentally, and most theoretical studies have assumed weak laser intensitybelow about 10^{12} W/cm^{2}which limits the strength of the induced current. To accurately model ring currents in benzene generated by high-intensity femtosecond laser pulses, we have used Time-Dependent Density Functional Theory, a direct ab initio method for molecular calculations. Our results indicate that ionization plays a larger role than previously expected at high intensities, because of a Resonance Enhanced Multiphoton Ionization (REMPI) process.

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