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Ab Initio Simulation of Photoinduced Ring Currents in Benzene¹ TENNESSE JOYCE, AGNIESZKA JARON-BECKER, JILA and Department of Physics, University of Colorado, Boulder — A circularly polarized femtosecond laser can induce ring currents within a single molecule on the order of microamps that are expected to remain coherent for several picoseconds. Photoinduced ring currents have not yet been observed experimentally, and most theoretical studies have assumed weak laser intensitybelow about 10^{12} W/cm² 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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