PHOTOINDUCED RING CURRENTS IN MOLECULES

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Circularly polarized laser pulse can induce electronic ring currents within a single molecule, that are expected to persist for as long as nanoseconds. Photoinduced ring currents in molecules have not yet been observed experimentally, and most theoretical studies have considered rather weak laser intensity - below 10^{12} W/cm^2, which limits the strength of the induced current.

We study the properties of the ring current that can be induced in benzene, over the range of laser pulse frequencies and intensities. Simulations within Time-Dependent Density Functional Theory (TDDFT) are compared to results obtained within Tight Binding method. In the regime of the excitation of the persistent ring current one can observe influence of the resonance enhanced ionization (REMPI) on the current.

Our results indicate that circularly-polarized femtosecond laser pulse can be used to control ionization and efficient ionization leads to a persistent hole current. Consequently for higher intensities of the laser pulse the leading contribution from the hole current induces the change of the direction of the total ring current (see Figure 1). Furthermore we present how the mechanism can be used to switch between the two regimes of co- and counter propagating ring currents during the laser pulse and discuss properties of ring currents in other molecules.

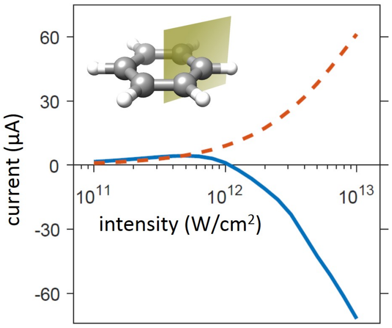

Figure 1: Induced current as a function of the peak laser intensity. Tight binding method (dashed red line) versus TDDFT (solid blue line) results.