Manipulating the torsion of molecules by strong laser pulses

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Synopsis In recent years the manipulation of molecules by strong laser pulses has attracted much attention. Non-resonant laser fields apply torques on molecules, due to the interaction between the induced dipole moment and the laser field itself. This has proven very useful for controlling both external and internal degrees of freedom of molecules. We extend the use of strong non-resonant laser fields to manipulation of the torsion in a molecule. Specifically, we consider the laser induced dynamics of the two phenyl rings of a biphenyl molecule.

Many studies during the last decade have shown that strong non-resonant laser fields can effectively manipulate the external degrees of freedom of isolated gas phase molecules. The manipulation results from laser-induced forces and torques due to the interaction between the induced dipole moment and the laser field itself. Examples of manipulation include deflection, focusing and slowing of molecules through the dependence of the non-resonant polarizability interaction on the intensity distribution in a laser focus. Likewise, the dependence of the induced dipole interaction on molecular orientation has proven highly useful for controlling the rotation of a variety of molecules. In particular, the spatial orientation of molecules can be sharply confined with respect to axes that are fixed in the laboratory. Molecular manipulation by induced dipole forces extends beyond the external degrees of freedom and has also been demonstrated for the internal degrees of freedom such as vibrational motion in molecular hydrogen.

In the case of larger molecules control of the lowest frequency vibrational modes attracts special interest since some of these modes correspond to motion along well-defined reaction coordinates separating two conformational minima (conformers). Although many molecules contain large number of conformers it is often just two conformers that dominate important chemical properties, for instance chirality. A particularly important example is found in axially chiral molecules such as biaryl systems. In these molecules rotation about a single stereogenic carbon-carbon (C-C) bond axis changes the molecule from one enantiomer into the opposite enantiomer (mirror image).

We demonstrate that the laser-induced non-resonant polarizability interaction can also be used to influence the internal rotation of an axially chiral molecule around the stereogenic C-C bond axis (cf. Fig. 1). In particular, we show that by fixing the C-C bond axis of a substituted biphenyl molecule in space, using laser induced alignment by a long laser pulse, it is possible to initiate torsional motion of the two phenyl rings by a short laser pulse polarized perpendicular to the fixed axis.

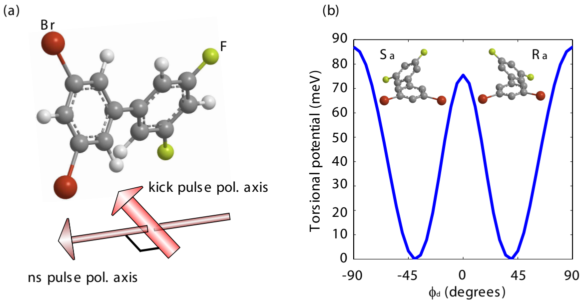

Fig. 1. (a) Model of the substituted biphenyl and the laser geometry of the experiment. (b) The torsional potential as a function of the dihedral angle, ϕ_d, between the two phenyl rings. The minima at $\phi_d = \pm 39^\circ$ result in the R$_a$ and S$_a$ enantimomers.

On the basis of these results we discuss future applications of laser induced torsion, viz., time-resolved studies of de-racemization and laser controlled molecular junctions based on molecules with torsion.

References

[1] Madsen et al. PRL **102**, 073007 (2009).

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