STOCHASTIC PULSE OPTIMIZATION FOR SURFACE MOUNTED CHIRAL MOLECULAR SWITCHES

Dominik Kröner

Theoretische Chemie, Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Straße 24-25, D-14476 Potsdam, Germany
E-mail: Dominik.Kroener@uni-potsdam.de

The model system 1-(2-cis-fluoroethenyl)-2-fluorobenzene supports two chiral and one achiral atropisomers upon torsion around the C-C single bond connecting phenyl ring and vinyl group. Linearly polarized IR pulses may be used to excite the internal rotation ω around the chiral axis, thereby selectively changing the chirality of the fully oriented molecule, e.g. "switch on" its chirality [1]. For an ensemble of surface mounted switches with multiple defined orientations *stochastic pulse optimization* allows to control the handedness of the molecules independent of their orientation [2]. Non-linear polarized laser pulses are employed for highly stereoselective switching for each orientation [3]. For two coupled torsional degrees of freedom around the chiral axis, ω and φ (see Fig. 1), laser control becomes very challenging, but is still possible [4].

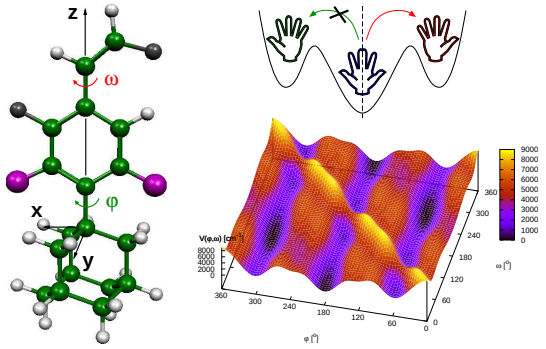

Figure 1: 1-(2-cis-Fluoroethenyl)-2-fluorobenzene with sterically demanding Br-substituents chemisorbed to adamantane and its potential energy surface along ω and φ, which describe the torison of the ethenyl- and phenyl group around the z-axis. Stochastically optimized non-linearly polarized laser pulses allow to selectively change the handedness of the molecular model system, see sketch.

[1] D. Kröner, B. Klaumünzer, *Phys. Chem. Chem. Phys.* 9 (2007) 5009.
[2] T. Klamroth, D. Kröner, *J. Chem. Phys.* 129 (2008) 234701.
[3] D. Kröner, B. Klaumünzer, T. Klamroth, *J. Phys. Chem. A* 112 (2008) 9924.
[4] D. Kröner, Ch. Hensel, T. Klamroth, *in preparation.*