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EINLADUNG

zum Vortrag
von

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über

Structure, dynamics and control of optical molecular switches

am

Dienstag, 28. April 2009, um 17 Uhr

Ort: Lise-Meitner Hörsaal, Fakultät für Physik, Universität Wien
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Abstract:
Fulgides are discussed as promising candidates for optical molecular switches. Prototype operations using fulgides as switchable bridge molecules in donor-bridge-acceptor systems [1, 2] or as ultrafast write-readout-units for binary encoding of information [3] have recently been reported. The basic mechanism is the switching of molecular structure between two thermally stable isomers. This process is induced by laser light and mediated via conical intersections. Our aim is to characterize the electronic structure of the selected fulgid (trifluoromethyl-pyrrolylfulgid) and to identify the conical intersection seam involved. Furthermore we investigate strategies to enhance the switching process using light fields modulated in phase and amplitude.

By linear interpolation methods and constrained gradient difference optimization, we were able to identify and characterize the low-lying conical intersection seam decisive for the switching process. From the topology of the optimized seam, we could distinguish different regions that significantly influence the course of the reaction. The temporal evolution of a wave packet generated by a femtosecond laser pulse is analyzed for adapted model potentials. The light field optimally driving the switching process is found by optimal control theory and is analyzed to enlighten the underlying control mechanism [2]. Our studies show that molecular switches can be tuned by molecular design as well as by shaped light fields.

[1] In: B.L. Feringa, Editor, Molecular Switches, Wiley, VCH (2001)
[2] D. Geppert and R. de Vivie-Riedle, J. Photochem. Photobiol. A 180 (2006) 282-288.
[3] Stephan Malkmus, Florian O. Koller, Simone Draxler, Tobias E. Schrader, Wolfgang J. Schreier, Thomas Brust, Jessica A. DiGirolamo, Watson J. Lees, Wolfgang Zinth, and Markus Braun, Adv. Funct. Mater. 17 (2007) 3657–3662.