MO 57: Poster: Quantum Control

Zeit: Donnerstag 16:30–18:30 Raum: Poster A

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Quantum dynamical simulations and control of light-induced molecular torsion — •Steffen Belz[1], Omar Deeb[2], Shireen Alfalah[2], and Monika Leibscher[1] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Germany — [2]Department of Chemistry and Chemical Technology, Al-Quds University, Jerusalem, Palestinian Authority

Photochemical isomerization reactions or molecular torsion as occurring e.g. in the process of vision are currently attaining increasing interest. These light induced isomerizations which usually proceed within very short time-scales of several hundred femtoseconds [1] are governed by conical intersections between different electronic states.

In this study, we investigate molecular torsion for model systems like fulvene by means of quantum dynamical simulations. Moreover, we present the transformation of the adiabatic potential energy surfaces obtained by quantum chemical ab initio calculations into a so called diabatic representation [2,3] and point out how the pathway of the photochemical reaction depends on the structure of the conical intersection. Another aim of our study is the control of the outcome of isomerization reactions by specially designed femtosecond laser pulses. Here we show how series of two UV-laser pulses can be applied in order to increase the efficiency of the cis-trans isomerization.

[1] J.E. Kim, D. W. McCamant, L. Zhu, R.A. Mathies, *J. Phys. Chem.* B **105**, 1240 [2001].

[2] A. Thiel, H. Köppel, *J. of Chem. Phys.* **110**, 9371 [1999].

[3] M. Baer, R. Englmann, *Mol. Phys.* **75**, 293 [1992].

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Quantum control in strong laser fields with SPODS — Tim Bayer, •Andrea Klumpp, Dirk Liese, Cristian Sarpe-Tudoran, Andreas Präkelt, Matthias Wollenhaupt, and Thomas Baumert — Experimentalphysik III, CINSaT, Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

An exciting new strong field control scenario which makes explicit use of the manipulation of the temporal phase of a pulse sequence with attosecond precision was demonstrated recently [1]. The physical mechanism of this strong field scheme is based on Selective Population of Dressed States (SPODS). Since switching between selective population of either dressed states occurs within a few femtoseconds, this technique is also interesting for applications in the presence of decoherence processes. Because SPODS combines high selectivity and tunability with efficient population transfer, relevant applications to chemistry - so far investigated theoretically [2] are within reach. In our future work we will perform experiments with shaped femtosecond laser pulses on different molecules to understand and manipulate the underlying processes of ionization and fragmentation in strong laser fields. The complex electronic structure of the molecules and the molecular dynamics are the challenges for this mechanism. First measurements will be presented.

[1] M. Wollenhaupt, V. Engel, T. Baumert, Annu. Rev. Phy. Chem. 56, 25 (2005)

[2] M. Wollenhaupt, T. Baumert, J. Photochem. Photobiol. A, 180, 248-255 (2006)

MO 57.3 Do 16:30 Poster A

Ultraschnelle Starkfeldkontrolle an K_2 durch selektive Bevölkerung bekleideter Zustände — •Tim Bayer, Matthias Wollenhaupt, Christian Sarpe-Tudoran und Thomas Baumert — Universität Kassel, Institut für Physik und CINSaT, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany

Die selektive Bevölkerung bekleideter Zustände (SPODS) ist ein elementarer und robuster Mechanismus der kohärenten Quantenkontrolle in intensiven Laserfeldern. In jüngster Vergangenheit wurden zwei Wege zur Realisierung von SPODS durch Pulssequenzen und gechirpte Pulse untersucht und an atomaren Systemen erfolgreich demonstriert. Ferner konnte das Potential dieses Kontrollmechanismus als Anwendung in der Steuerung chemischer Reaktionen anhand von Modellrechnungen am Kalium-Dimer aufgezeigt werden [1]. Nach dem theoretisch vorgeschlagenen Doppelpulsszenario ist es möglich, Populationstransfer via SPODS ultraschnell, selektiv und mit hoher Effizienz zwischen verschiedenen Endkanälen zu schalten.

Der experimentelle Nachweis dieses Szenarios befindet sich derzeit in Arbeit. Wir synchronisieren dazu einen geformten Femtosekundenlaserpuls zur Anregung der neutralen K_2-Dynamik mit einem Nanosekundenlaserpuls zur Endzustandsabfrage, und nutzen die energieaufgelöste Photoelektronenspektroskopie als Methode zum Nachweis der erzielten Endzustandsbesetzung. Es werden vorläufige Ergebnisse präsentiert.

[1] M. Wollenhaupt, T. Baumert, J. Photochem. Photobiol. A **180**, 2006

MO 57.4 Do 16:30 Poster A

Kontrolle der Ausrichtungsdynamik von N_2 — •Christian Horn[1], Rebeca de Nalda[2], Marc Krug[1], Matthias Wollenhaupt[1], Luis Bañares[2] und Thomas Baumert[1] — [1]Universität Kassel, Institut für Physik und CINSaT, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Dpto. Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Avda. Complutense s/n, 28040 Madrid, Spain

Mit Hilfe von ultrakurzen Laserpulsen kann eine transiente Ausrichtung von Molekülen in der Gasphase erzeugt werden [1]. Wir zeigen, dass die zeitliche Struktur der transienten Ausrichtung mit Hilfe von geformten Laserpulsen kontrolliert werden kann. Dies wird mit Hilfe von Experimenten an N_2 demonstriert. Sowohl die Ergebnisse von "closed-loop" Experimenten, bei denen ein computergesteuerter Algorithmus bestimmte Merkmale der Transiente optimiert, als auch die Ergebnisse von "open-loop" Experimenten werden gezeigt [2]. Der Effekt der Temperatur des Molekülensembles auf das Ausmaß der erzielten Ausrichtung und insbesondere auf die Kontrollmöglichkeiten wird durch numerische Simulationen untersucht [3].

[1] H. Stapelfeldt, T. Seideman, Rev. Mod. Phys. **75**, 543 (2003)

[2] C. Horn, M. Wollenhaupt, M. Krug, T. Baumert, R. de Nalda, L. Bañares, Phys. Rev. A **75**, 1(R) (2006)

[3] R. de Nalda, C. Horn, M. Wollenhaupt, M. Krug, L. Bañares, T. Baumert, J. Raman Spectrosc. (in print)

MO 57.5 Do 16:30 Poster A

Local control of the quantum dynamics in multiple potential wells. — •Volker Engel, Philipp Marquetand, Stefanie Gräfe, and Daniel Scheidel — Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

The driven wave-packet dynamics in potentials exhibiting several potential wells is investigated. Therefore, local control strategies are employed where the control field is constructed from the system's dynamics at any instant of time [1]. It is shown that particles can be moved successively between various potential minima. Furthermore, results are presented which indicate that the intuitive local control scheme allows for the initiation of a clockwise or counter-clockwise rotational motion of a model molecular motor [2]. [1] S. Gräfe, C. Meier, V. Engel, J. Chem. Phys. 122, 184103 (2005). [2] P. Marquetand, S. Gräfe, D. Scheidel, V. Engel, J. Chem. Phys. 124, 054325 (2006).

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Transfer of Vibrational Energy and Quantum Information through Molecular Chains — •Caroline Gollub, Markus Kowalewski, Ulrike Troppmann, and Regina de Vivie-Riedle — LMU Department Chemie, Butenandt-Str. 11, 81377 München, Germany

We are interested in the mechanisms of intramolecular vibrational energy transfer in the context of quantum information transfer and developed different approaches to describe one-dimensional chain molecules. The linear systems consisting of $(C{\equiv}C-)_n$ units are set up with a flexible, modular ansatz based on ab initio quantum chemical data and vibrational eigenfunctions. Additionally, octatetrayne, as a chain molecule, is treated explicitly in a local eigenstate representation. In the modular approach the propagation behavior of the linear, kinetic coupled quantum oscillators of the molecular chains could be studied and dynamical aspects of the vibrational energy transfer were clarified.

These molecular bridge systems offer an innovative possibility to construct quantum networks within our approach of molecular quantum computing [1]. The vibrational qubits are encoded in molecular subunits, linked by the molecular chains. The bridging molecules guarantee the communication between the subunits, which is realized by specially shaped laser pulses, calculated with Optimal Control Theory.

Selective quantum state transfer through different quantum channels of the bridging molecules, as well as the entanglement generation and the corresponding mechanisms of the processes are presented.

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