

Quantum analysis and design of laser pulses for control of chemical reactions

Jörn Manz

*Institut für Chemie – Physikalische und Theoretische Chemie,
Freie Universität Berlin, Takustr. 3, D-14195 Berlin, Germany*

An important topic in femtosecond chemistry is control of chemical reactions by means of laser pulses. I shall present recent progresses for the corresponding quantum analysis and design of efficient laser pulses applied to six model systems:

1. Optimal control of selective ionization versus bond breaking in an organometallic compound $\text{CpMn}(\text{CO})_3$ [1]
2. Selective preparation of pure enantiomers from an oriented racemate [2], see also [3]
3. Symmetry breaking in FHF^- with directed separation of products $\text{F}+\text{HF}$ [4]
4. Control of vibrational momenta for selective bond breaking in HOD [5]
5. Control of torsional angular momenta for quantum ignition of a molecular propeller [6]
6. Quantum ignition of uni-directional electron ring currents and cyclic electron transfer in Mg-porphyrin [7]

The laser driven molecular quantum dynamics will be demonstrated by films showing the time evolution of corresponding molecular nuclear (1-5) and electronic (6) wavepackets.

Acknowledgement: I would like to express my gratitude to distinguished international partners and young scientists in my group, for so pleasant and fruitful cooperations. Their names are listed as co-authors in references [1-7]. I am also grateful to Deutsche Forschungsgemeinschaft (DFG) and Fonds der Chemischen Industrie (FCI) for generous financial support.

References:

1. C. Daniel, J. Full, L. González, C. Lupulescu, J. Manz, A. Merli, S. Vajda, L. Wöste, Deciphering the reaction dynamics underlying optimal control laser fields, *Science* **299**, 536-539 (2003).

2. L. González, J. Manz, B. Schmidt, M. F. Shibl, Optical resolution of oriented enantiomers via photodissociation: Quantum model simulations for H₂POSD, submitted to J. Chem. Phys.
3. Y. Fujimura, L. González, K. Hoki, D. Kröner, J. Manz, Y. Ohtsuki, From a racemate to a pure enantiomer by laser pulses: Quantum model simulations for H₂POSH, *Angew. Chem. Intern. Ed.* **39**, 4586-4588 (2000).
4. N. Elghobashi, J. Manz, Separating the photofragments of randomly oriented symmetric reactants by IR+UV laser pulses: Quantum simulations for FHF → F+HF+e, *Israel J. Chem.* **43**, 293-303 (2003).
5. N. Elghobashi, P. Krause, J. Manz, M. Oppel, IR+UV laser pulse control of momenta directed to specific products: Quantum model simulations for HOD* → H+OD versus HO+D, *Phys. Chem. Chem. Phys.* **5**, 4806-4813 (2003).
6. Y. Fujimura, L. González, D. Kröner, J. Manz, I. Mehdaoui, B. Schmidt, Quantum ignition of intramolecular rotation by means of IR+UV laser pulses, *Chem. Phys. Lett.* **386**, 248-253 (2004).
7. I. Barth, J. Manz, Y. Shigeta, K. Yagi, Quantum ignition of uni-directional electronic ring currents in oriented Mg-porphyrin by few-cycle circular polarized laser pulses, to be submitted