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Strategies for optimal control in complex systems

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We present strategies for the optimal control of the ground and excited state dynamics in complex systems, based on the combination of the quantum chemical molecular dynamics "on the fly" with the semiclassical Wigner distribution approach [1]. We first demonstrate our strategy for the optimal control of the ground state dynamics based on the MD "on the fly" with explicit treatment of the interaction with the laser field which is optimized using a genetic algorithm [2]. This approach will be illustrated on two prototype systems representing rigid symmetrical molecules and floppy biomolecules with low frequency modes. Our results show that the ground state isomerization process can be selectively driven by ultrashort laser pulses with different shapes which are characteristic for the prototype systems. Furthermore, for the optimal pump-dump control involving ground and excited electronic states we have developed a new "field induced surface hopping" method in which the nuclear dynamics is treated classically while the laser induced electronic transitions are treated fully quantum mechanically. We illustrate our approach on the optimal control of cis-trans isomerization in prototype Schiff base molecular switches. Our theoretical approach allows us to explore the controllability of dynamics in complex systems and to unravel the mechanisms underlying the control of molecular processes. Furthermore, the outlook for laser selective photochemistry of nanoparticles and nanoparticle-biomolecule hybrid systems will be given.

[1] V. Bonačić-Koutecký, R. Mitrić , Chem. Rev. 105, 11 (2005).
[2] R. Mitrić, V. Bonačić-Koutecký, Phys. Rev. A, 76, 031405 (2007).