Laboratoire PPSM – UMR CNRS 8531

Photochimie et Photophysique Supramoléculaires et Macromoléculaires

Séminaire PPSM

Lundi 5 Octobre 2015 - 11h00

Auditorium D. Chemla - Bâtiment IDA

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Invité par : Fabien Miomandre

«Molecular Quantum Dynamics or The quantum effects in Chemistry»

Many molecular processes, ranging from fundamental to applied problems, are known today to be impacted by strong nuclear quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Recent success in helping to understand experimental observations in fields like heterogeneous catalysis, photochemistry, reactive scattering, optical spectroscopy, or femto- and attosecond chemistry and spectroscopy underlines that nuclear quantum mechanical effects affect many areas of chemical and physical research. The correct theory to describe the corresponding dynamics is Molecular Quantum Dynamics [1,2]. In contrast to standard quantum chemistry calculations, where the nuclei are treated classically, molecular quantum dynamics can cover quantum mechanical effects in their motion. Although the calculation of large systems still presents a challenge - despite the considerable power of modern computers - new strategies have been developed to extend the studies to systems of increasing size. In particular, we present here several applications of the Multi-Configuration Time-Dependent Hartree method (MCTDH) [3,4,5] to the understanding and the control of molecular processes involving quantum effects. MCTDH can be seen as a time-dependent MCSCF approach for the nuclei where wavepackets are propagated on one or several potential energy surfaces. We focus on Infrared and UV spectroscopy, diffusion rates of molecules on metal surfaces and proesses guided by laser pulses, involving or not non-adiabatic transitions, at the femto and sub-femto/atto timescales.

[1] *Molecular Quantum Dynamics, From Theory to Applications*, Ed. F. Gatti, Springer, (2014) Heidelberg.
[2] *Quantum Physics, Applications to Chemistry*, F. Gatti, B. Lasorne, H.-D. Meyer and A. Nauts, Lectures Notes in Chemistry, Springer, in preparation.
[3] H.-D. Meyer, U. Manthe, and L.S. Cederbaum, *The multi-configurational time-dependent Hartree approach.* Chem. Phys. Lett. **165** (1990), 73.
[4] M. H. Beck, A. Jäckle, G. A. Worth and H.-D. Meyer, *The multiconfiguration time-dependent Hartree method: A highly efficient algorithm for propagating wavepackets,* Physics Reports **324** (2000), 1.
[5] H.-D. Meyer, F. Gatti, and G. A. Worth, editors, *Multidimensional Quantum Dynamics: MCTDH Theory and Applications,* Wiley-VCH (2009), Weinheim.

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