

# Theory days

## Biomolecule irradiation

Dec 2, 3, 4, 2009

IRSAMC

Toulouse

Collisional/laser irradiation  
Ab initio methods  
Time dependent DFT  
Direct/indirect mechanisms  
Effects of solvent

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dépasser les frontières

GdR

DFT++



Université  
Paul Sabatier

TOULOUSE III

# THEORY DAYS ON BIOMOLECULE IRRADIATION

## Toulouse, Dec. 2–4, 2009

### Scientific program

December 2, 2009

- 14:00 - 15:00 : P. Moretto-Cappelle (Univ. Paul Sabatier, Toulouse) and A. Le Padellec (Univ. Paul Sabatier, Toulouse)  
*Irradiation of biomolecules: experimental investigations*
- 15:00 - 16:00 : D. Shemesh (Technical Univ. Munich, Garching)  
*Photoinduced dynamics in short peptides*
- 16:00 - 16:15 : Coffee break
- 16:15 - 17:15 : U. Saalman (MPIPKS, Dresden)  
*Core-shell systems in strong X-ray pulses*

December 3, 2009

- 09:00 - 10:00 : F. S. Zhang (Beijing Normal Univ., Beijing)  
*title to be announced*
- 10:00 - 11:00 : J. Kohanoff (Queen's Univ. Belfast, Belfast)  
*First-principles simulations of the interaction of ionic projectiles with liquid water and ice*
- 11:00 - 11:15 : Coffee break
- 11:15 - 12:15 : R. Vuilleumier (ENS, Paris)  
*Theoretical investigation of the ultrafast dissociation of ionised biomolecules immersed in water: Direct and indirect effects*
- 14:00 - 15:00 : E. Dumont (ENS, Lyon)  
*What can hybrid methods tell us about electron attachment to biomolecules?*
- 15:00 - 16:00 : F. Gatti (Univ. Montpellier II, Montpellier)  
*Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) Approach. Applications to spectroscopy and control of reactions*
- 16:00 - 16:15 : Coffee break
- 16:15 - 17:15 : General discussion

December 4, 2009

- 09:00 - 10:00 : A. Solov'yov (Goethe University, Frankfurt am Main)  
*Physics of ion beam cancer therapy: a multiscale approach*
- 10:00 - 11:00 : E. Cauët (Université Libre de Bruxelles, Bruxelles)  
*Ionization and charge transfer in DNA from Ab Initio and hybrid quantum mechanics/molecular mechanics (QM/MM) calculations*
- 11:00 - 11:15 : Coffee break
- 11:15 - 12:15 : P. M. Dinh (Univ. Paul Sabatier, Toulouse)  
*Dynamics of small organic molecules in strong electromagnetic fields*