

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)
Interaction of heavy ions with biomolecules: A multiscale microscopic dynamical approach
- 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