1. Conférences invitées


[2] Sept. 2014 Coupled TDDFT-Ehrenfest simulations of the ultrafast dissociation of biomolecules PROGRESS IN NUMERICAL IMPLEMENTATIONS OF TDDFT (Le Mans, France)


[8] Juin 2012 First-principle simulations of silver in hydrothermal fluids GOLDSCHMIDT 2012 (Montréal, Canada)

[9] Sept. 2011 Speciation of silver in saline hydrothermal fluids from first-principle molecular dynamics ICSC 2011 (Montpellier, France)

[10] Août 2011 First-Principle Molecular Dynamics simulation of liquid CaCO₃ GOLDSCHMIDT 2011 (Prague, République Tchèque)


[13] Juin 2010 Fragmentation of small biomolecules in high LET ion tracks from first-principles WORKSHOP ELECTRON DYNAMICS IN LIFE SCIENCES (Belfast, UK)


[15] 2-4 Décembre 2009 Theoretical investigation of the ultrafast dissociation of ionized biomolecules immersed in water : Direct and indirect effects THEORY DAYS ON IRRADIATION OF BIOMOLECULES (Toulouse, France).

[16] 23-27 Novembre 2009 Theoretical investigation of the ultrafast dissociation of ionized biomolecules immersed in water : Direct and indirect effects INTERNATIONAL WORKSHOP ON ATOMIC PHYSICS (Dresden, Germany).


2-5 Juin 2009 Microscopic flow around a diffusing particle EPSRC Symposium Workshop on Molecular Dynamics (Warwick, UK).

2-5 Avril 2009 Microscopic flow around a diffusing particle Indo-French meeting on Diffusion in nanoporous and dense media (Bangalore, India).

2-4 Oct. 2008 Microscopic flow around a tagged diffusing particle : effects of fluctuations on the hydrodynamics description Workshop CECAM Common trends between Kinetic theory, Dynamical Density Functional methods and mesoscopic methods based on effective free energy models (Lausanne, Suisse).

7-10 Juil. 2008 Photo-dissociation et recombinaison de l'iode en solution observée par diffraction X résolue en temps AFC 2008 (Rennes, France).

Fev. 2008 Microscopic flow around a diffusing particle ESI program Metastability and Rare Events in Complex Systems (Vienna, Austria)

Juil. 2007 Extracting effective normal modes from molecular dynamics simulations Classical and Quantum Approaches in Molecular Modeling, Summer program of the Institute for Mathematics and its Applications (Minneapolis, Etats-Unis)

Juil. 2007 Microscopic flow around a diffusing particle Meeting in honour of Jean-Pierre Hansen (Cambridge, UK)

Avril. 2007 Vibrational spectroscopy of small molecules of biological interest in liquid water by Car-Parrinello simulations Workshop SIMBIOMA, Progress in ab initio modelling of biomolecules : towards computational spectroscopy (Rome, Italie)

Déc. 2006 Mean free path in a Lennard-Jones fluid Workshop SIMBIOMA, Sampling paths in molecular simulation : algorithms for phase transitions, reactivity and kinetics (Orsay)

Nov. 2006 Extracting information from molecular dynamics, Maxwell Institute Colloquium on Applications of Mathematics, (Edinburgh, UK)

Juin 2006 Infrared spectroscopy and atomic dynamical partial charges in liquid water Stockholm Discussion meeting – Structure and molecular scale properties of liquid water (Stockholm, Suede)

Juillet 2005 Vibrational spectroscopy and Born partial charges of liquid water keynote lecture de la session water, solutions and reaction dynamics, 6th Liquid Matter Conference (Utrecht, Pays-bas)

Mai 2005 Theoretical approach to time-resolved x-ray diffraction of chemical reactions in liquids : application to the photo-dissociation of iodine Symposium on the scientific potential of a short pulse option at Petra III (HAYSILAB, DESY), (Hamburg, Allemagne)

Mars 2005 Non-linear statistics and molecular dynamics simulations for the interpretation of time-resolved x-ray diffraction conference internationale Transient Chemical Structures in Dense Media (Paris)

Novembre 2004 Trajectories analysis from Molecular Dynamics simulations Workshop du COST D26 ‘Molecular Dynamics : Fundamentals and Recent Developments (Paris)

3-4 juin 2004 Analysis of time-dependent x-ray diffraction signals with the help of Molecular Dynamics simulations, Workshop on Ultrafast Structural Dynamics with Pulsed X-rays (ESRF, Grenoble)
2. Séminaires invités depuis 2010

[3] Mars 2012 First-Principle Molecular Dynamics simulation of liquid CaCO3 and CO2 in natural silicate melts (Univ. of Amsterdam, Pays-Bas)
[5] Fev. 2010 Microscopic flow around a diffusing tagged particle : effects of fluctuations on the hydrodynamics description (Univ. of Texas at Austin, USA)