Conférences et séminaires invités par Rodolphe Vuilleumier

1. Conférences invitées

[1] **Mai 2015** *Microscopic flow around a diffusing particle* CECAM Workshop – Molecular hydrodynamics meets fluctuating hydrodynamics (Madrid, Espagne)

[2] **Sept. 2014** *Coupled TDDFT-Ehrenfest simulations of the ultrafast dissociation of biomolecules* Progress in Numerical Implementations of TDDFT (Le Mans, France)

[3] **Aout 2014** *Molten carbonates : from the Earth mantle to fuel cells* CECAM Workshop – Modelling ionic liquids at electrochemical interfaces (Paris, France)

[4] **Juin 2014** *Maximum probability domains for exploring the structure of liquid water* WaterEurope 2014 (Saragosse, Espagne)

[5] **Sept. 2013** *Liquids and solutions of geochemical interests studied by first-principle molecular dynamics* EMLG 2013 (Lille, France)

[6] **Sept. 2013** *Building Classical Force-Fields from Maximally Localized Wannier Orbitals* CPMD 2013 (Leipzig, Allemagne)

[7] **Août 2013** *CO_2 speciation and transport properties of CO_2-bearing silicate melts from First-Principle simulations* Goldschmidt 2013 (Florence, Italie)

[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 $CaCO_3$* Goldschmidt 2011 (Prague, République Tchèque)

[11] **Juillet 2011** *Infrared spectroscopy and atomic dynamical partial charges in liquid water* CECAM workshop - Spectroscopic characterisation of liquid water from the electronic structure (Lausanne, Suisse)

[12] **Novembre 2010** *Theoretical investigation of the ultrafast dissociation of ionized biomolecules immersed in water* Transient Chemical Structures in Dense Media (Paris, France)

[13] **Juin 2010** *Fragmentation of small biomolecules in high LET ion tracks from first-principles* Workshop Electron Dynamics in Life Sciences (Belfast, UK)

[14] **Juin 2010** *Use of maximally localized Wannier orbitals to build classical force fields from ab initio simulations* CECAM workshop - Advances in the Implementation of Polarizable Force Fields for Molecular Simulations (Lausanne, Suisse).

[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).

[17] **15-16 Octobre 2009** *Infrared spectra of small biomolecules from first ?principle molecular dynamics simulations and effective normal mode analysis* Fifth International meeting Workshop : Mathematical Methods for Ab Initio Quantum Chemistry (Nice, France).

[18] **Juillet 2009** *First-Principle Molecular Dynamics and its application to the estimation of redox potentials* Workshop on Density Functional Theory (Berlin, Allemagne).

[19] **2-5 Juin 2009** *Microscopic flow around a diffusing particle* EPSRC Symposium Workshop on Molecular Dynamics (Warwick, UK).

[20] **2-5 Avril 2009** *Microscopic flow around a diffusing particle* Indo-French meeting on Diffusion in nanoporous and dense media (Bangalore, India).

[21] **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).

[22] **7-10 Juil. 2008** *Photo-dissociation et recombinaison de l'iode en solution observée par diffraction X résolue en temps* AFC 2008 (Rennes, France).

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

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

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

[26] **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)

[27] **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)

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

[29] **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)

[30] **Juillet 2005** *Vibrational spectroscopy and Born partial charges of liquid water* **keynote lecture** de la session *water, solutions and reaction dynamics*, 6$^{\text{th}}$ Liquid Matter Conference (Utrecht, Pays-bas)

[31] **Mai 2005** *Theoretical approcah 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)

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

[33] **Novembre 2004** *Trajectories analysis from Molecular Dynamics simulations* Workshop du COST D26 'Molecular Dynamics : Fundamentals and Recent Developments (Paris)

[34] **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)

[35] **8-12 juillet 2003** *Theoretical analysis of time-resolved x-ray diffraction experiments on the photodissociation of iodine*, Femtochemistry 6 (Paris, France).

[36] **29 Sept.-3 Oct. 2001** *Comparison of the solvation of Ag+ and Na+ in water by an ab-initio Molecular Dynamics study of Pearson's hardness*, 6th International Conference on Molecular Spectroscopy (Lądek Zdrój, Poland).

[37] **6-11 Août 2000** *A molecular dynamics study of an excess proton in aqueous solution : Use of an extended empirical valence-bond approach*, Gordon Research Conference "Water and Aqueous Solutions" (Holderness school, Plymouth, USA).

[38] **Sept. 1999** *Quantum dynamics of an excess proton in liquid water*, XIIIth Conference-Workshop "Horizons in Hydrogen Bond Research" (Świeradów Zdrój, Poland).

2. Séminaires invités depuis 2010

[1] **Jan. 2015** *Molten carbonates : from the Earth mantle to fuel cells* (Univ. Bonn, Allemagne)

[2] **Juil. 2013** *Microscopic flow around a diffusing tagged particle : effects of fluctuations on the hydrodynamics description* (Univ. Rome 1 La Sapienza, Italie)

[3] **Mars 2012** *First-Principle Molecular Dynamics simulation of liquid CaCO3 and CO2 in natural silicate melts* (Univ. of Amsterdam, Pays-Bas)

[4] **Avril 2011** *First-Principle Molecular Dynamics simulation of liquid CaCO3* (IMPMC, UPMC)

[5] **Fev. 2010** *Microscopic flow around a diffusing tagged particle : effects of fluctuations on the hydrodynamics description* (Univ. of Texas at Austin, USA)