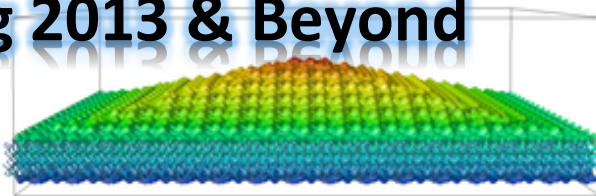


# Conquest Meeting 2013 & Beyond



Wednesday, June 12<sup>th</sup> to Friday 14<sup>th</sup> 2013

Place: Institut des Sciences moléculaires (ISM), CNRS/Université Bordeaux 1 (UB1)  
Bâtiment A12, 351 Cours de la Libération, 33405 TALENCE

Contact: Lionel Truflandier ([l.truflandier@ism.u-bordeaux1.fr](mailto:l.truflandier@ism.u-bordeaux1.fr))  
Alain Fritsch ([a.fritsch@ism.u-bordeaux1.fr](mailto:a.fritsch@ism.u-bordeaux1.fr))

## Conquest team:

- From London Centre for Nanotechnology (LCN) at UCL, London (UK)  
David Bowler  
Lianheng Tong  
Conn O'Rourke
- From National Institute for Materials Science (NIMS) at Tsukuba (Japan)  
Tsuyoshi Miyazaki  
Michiaki Arita  
Ayako Nakata
- From Biology Center (Qbic) RIKEN at Kobe (Japan)  
Takao Otsuka

## Local speakers:

Frédéric Castet  
Arnaud Desmedt  
Philippe Bopp  
Laure Lespade

## Invited speakers:

Benoit Champagne, Laboratoire de Chimie Théorique, Université de Namur (Belgium)  
Jean-Marc Leyssale, Laboratoire des Composites Thermostructuraux, UB1/CNRS/CEA/SAFRAN  
Olivier Aumage, INRIA Bordeaux

**Conferences take place in the room:**  
**Auguste Laurent, Chemistry Department (UFR), A11**

**Talks: approx. 30 min. (40 min. limit)**



ISM - Université Bordeaux 1 - CNRS UMR 5255 - F33405 Talence cedex  
Tél. : 33(0)5 4000 6282 - Fax : 33(0)5 4000 6994 - e-mail : [secretariat@ism.u-bordeaux1.fr](mailto:secretariat@ism.u-bordeaux1.fr) –  
[www.ism.u-bordeaux1.fr](http://www.ism.u-bordeaux1.fr)



---

## Developer's corner: Wednesday, June 12<sup>th</sup>

Time	Speaker	Title
10:00	David Bowler	Recent Developments and Plans for Blips in Conquest
10:40	Lianheng Tong	Flexible non-cubic Hilbert curve partitioning method for efficient load
11:20	Conn O'Rourke	Real-time TD-DFT in Conquest

12:00 *Lunch break "Carpe Diem"*

Time	Speaker	Title
14:00	Tsuyoshi Miyazaki	Applications of Conquest at NIMS
14:40	Michiaki Arita	Implementation of efficient Born-Oppenheimer dynamics in Conquest

*Coffee Break*

15:30	Ayako Nakata	Development of multisite local orbitals in Conquest
16:10	Takao Otsuka	Research plan for biomolecular simulations with the Conquest code

---

## Local & Invited speakers: Thursday, June 13<sup>th</sup>

Time	Speaker	Title
10:00	Philippe A. Bopp	Computer simulations of the thermocapillary effect at model liquid-liquid interfaces
10:40	Arnaud Desmedt	Dynamics of ionic clathrate hydrates
11:20	Jean-Marc Leyssale	Molecular dynamics simulation for disordered materials

12:00 *Lunch break "Carpe Diem"*

Time	Speaker	Title
14:00	Benoit Champagne	Simulating the second-order nonlinear optical properties: From molecules to functionalized surfaces and molecular crystals
14:40	Laure Lespade	Oxidative stress in theoretical chemistry

*Coffee Break*

15:30	Frédéric Castet	Simulating the charge transfer processes at organic heterojunctions: relevance for photovoltaic applications
16:10	Olivier Aumage	StarPU: An executive support for heterogeneous and parallel machines
17:30		Discussion & Beer Meeting

20:00 *Meeting diner chez "Fernand" (7 quai de la Douane, Bordeaux centre)*

---

## Friday, June 14<sup>th</sup>

Time	
14:00	Visit Tour of Bordeaux / Meeting spot Place de la Bourse / Organized by Delphine?

