#### **Guillaume Chevrot**

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# **Computational chemist**

## **Professional background**

01/2011 – Present Postdoctoral Research Associate. CBM-CNRS / SOLEIL synchrotron. Paris Area, France.

- Extraction of internal motions from molecular dynamics simulations.
- Impact of anisotropic atomic motions on incoherent neutron scattering intensities.
- New approach to molecular diffusion tensors.
- Scripting for simulations analysis.
- Performance tests (serial and parallel) on HDF5 files (in progress).

02/2008 – 08/2010 Postdoctoral Research Associate. CEA-DAM Ile de France. Paris Area, France.

- Molecular dynamics simulations of carbon nanoparticles under detonation conditions.
- Modeling the kinetics of carbon nanoparticles coalescence.
- Development of programs to analyze molecular dynamics simulations.

10/2004 – 01/2008 Ph.D. in computational chemistry. University of Strasbourg, France.

Modeling and Molecular Simulations laboratory. Director: Pr. Georges Wipff.

• Molecular dynamics simulations of dicarbollides anions, BTP and 18C6 in pure liquids and at liquid-liquid interfaces. Study at classical interfaces and at [BMI][PF<sub>6</sub>] ionic liquids interfaces.

01/2004 - 06/2004 Intern (M2 - computational chemistry). University of Strasbourg, France.

Modeling and Molecular Simulations laboratory. Director: Pr. Georges Wipff.

• Surfactant behavior of dicarbollides anions at interfaces: a molecular dynamics study.

04/2003 – 08/2003 Intern (M1 - chemistry). CEA Valduc. Dijon Area, France.

Director: Jean-Charles Hubinois.

• Gas analysis by mass spectrometry and gas chromatography.

06/2002 – 09/2002 Laboratory assistant. Dijon Area, France.

Sanofi pharmaceutical group.

• Water, drug and raw materials analysis.

#### **Educational background**

**2004 – 2008** Ph.D. in computational chemistry. University of Strasbourg, France.

**2003 – 2004** Master degree (M2) in computational chemistry.

University of Strasbourg, France.

**2002 – 2003** Master degree (M1) in chemistry.

University of Dijon, France.

**07/2009** Methods in molecular simulation summer school 2009 (5 - 14<sup>th</sup> july).

University of Sheffield, United Kingdom.

## **Skills**

- Extensive experience in molecular simulations.
- Programming experience in Python, C, Shell scripting, Mathematica, Django, HTML, CSS, Git.
- Experience working with large data sets (HDF5, NetCDF).
- HPC experience.
- English : full professional proficiency TOEIC test (11-28-06) : 885/990.
- 10 articles published in international peer-reviewed journals.
- Oral and poster communications in international and national congress.
- Contribution to the european project « europart ».
- Technological monitoring.
- Preparing and delivering reports, presentations.

G. Chevrot, Ph.D.