Guillaume Chevrot
14 rue du Docteur Charcot 91290 Arpajon (FRANCE)
(+33)1.78.65.52.43
(+33)6.25.42.76.56 (cell)
guillaume.chevrot@gmail.com
http://gchevrot.github.io/home/

Computational chemist

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 : advanced
  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.

Professional background

01/2011 – Present Postdoctoral Research Associate. 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) of 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_6] 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 - 14th july).
University of Sheffield, United Kingdom.

Publications

G. Chevrot, K. Hinsen, and G.R. Kneller. *Model-free simulation approach to molecular diffusion tensors*. J. Chem. Phys., **2013** (*submitted*).

G.R. Kneller and **G. Chevrot**. *Impact of anisotropic atomic motions in proteins on powder-averaged incoherent neutron scattering intensities.* J. Chem. Phys., **2012,** *137*, 225101.

G. Chevrot, A. Sollier, and N. Pineau. *Molecular dynamics and kinetic study of carbon coagulation in the release wave of detonation products.* J. Chem. Phys., **2012,** *136,* 084506.

G. Chevrot, P. Calligari, K. Hinsen, and G.R. Kneller. *Least constraint approach to the extraction of internal motions from molecular dynamics trajectories of flexible macromolecules.* J. Chem. Phys., **2011,** *135,* 084110.

J.H. Los, N. Pineau, **G. Chevrot**, G. Vignoles and J.-M. Leyssale. *Formation of multiwall fullerenes from nanodiamonds studied by atomistic simulations.* Phys. Rev. B, **2009,** 155420.

G. Chevrot, E. Bourasseau, N. Pineau and J.-B. Maillet. *Molecular dynamics simulations of nanocarbons at high pressure and temperature.* Carbon, **2009,** *47,* 3392-3402.

G. Chevrot, R. Schurhammer and G. Wipff. *Molecular dynamics study of dicarbollide anions in nitrobenzene solution and at its aqueous interface. Synergistic effect in the Eu(III) assisted extraction.* Phys. Chem. Chem. Phys., **2007,** *9,* 5928-5938.

G. Chevrot, R. Schurhammer and G. Wipff. *Synergistic effect of dicarbollide anions in liquid - liquid extraction: a molecular dynamics study at the octanol – water interface.* Phys. Chem. Chem. Phys., **2007,** *9,* 1991-2003.

G. Chevrot, R. Schurhammer and G. Wipff. *Molecular dynamics simulations of the aqueous interface with the [BMI][PF6] ionic liquid: comparison of different solvent models.* Phys. Chem. Chem. Phys., **2006,** *8,* 4166-4174.

G. Chevrot, R. Schurhammer and G. Wipff. *Surfactant behavior of 'ellipsoidal' dicarbollide anions: a molecular dynamics study.* J. Phys. Chem. B, **2006,** *110,* 9488-9498.

References are available upon request