

Guillaume Chevrot

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Computational chemist**Skills**

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| <ul style="list-style-type: none"> - 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. | <ul style="list-style-type: none"> - 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. |
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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) 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 dicarbolides anions, BTP and 18C6 in pure liquids and at liquid-liquid interfaces. Study at classical interfaces and at [BMI][PF₆] 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 dicarbolides 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. Hinsén, and G.R. Kneller. *Model-free simulation approach to molecular diffusion tensors*. J. Chem. Phys., **2013** (*accepted*).

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. Calligaris, K. Hinsén, 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