Guillaume Chevrot
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Computational chemist

Professional background

04/2014 – Present Postdoctoral Research Associate
MEMPHYS, Center for Biomembrane Physics
University of Southern Denmark (SDU)
Campusvej 55, 5230 Odense M, Denmark
Khandelia group
• Molecular dynamics simulations of the Na+/K+-ATPase membrane protein.
• Adaptation of a new molecular dynamics method for the simulation of proteins.

01/2011 – 02/2014 Postdoctoral Research Associate
CBM-CNRS / SOLEIL synchrotron
Paris Area, France
Kneller group
• 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.

02/2008 – 08/2010 Postdoctoral Research Associate
CEA-DAM Ile de France
Paris Area, France
Soulard group
• 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
Wipff group
• Molecular dynamics simulations of dicarbollides anions, BTP and 18C6 extractants.
• Simulations 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
Wipff group
• Surfactant behavior of dicarbollides anions at interfaces: a molecular dynamics study.

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

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.

Publications

G. Chevrot, K. Hinsen, and G.R. Kneller. *Model-free simulation approach to molecular diffusion tensors*. J. Chem. Phys., **2013**, *139*, 154110.

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.