

# Guillaume Chevrot

## Computational scientist - Data analyst

### contact



gchevrot@protonmail.com  
@gchevrot

### languages

french mother tongue  
english fluent  
german & danish notions

### skills

data analysis  
programming  
simulation  
modeling  
technology monitoring  
project management  
oral presentation  
research report

### informatics

Python, C, R  
Mathematica  
MongoDB  
Shell scripting  
Git  
Django  
CSS & HTML  
Drupal  
HDF5  
HPC  
Unix, Linux, OS X  
L<sup>A</sup>T<sub>E</sub>X

### experience

2015–Now

#### Complex Systems Institute - University of Orléans

Orléans, France

*Research associate – computational/data science*

Collaborating with several teams to manage and analyze data.

Achievements – goals:

- Creation of a database from a corpus and statistical analysis
- Statistical analysis of neural data
- Reproducible research: combining ActivePapers and Exec&Share
- Classification of intrinsically disordered proteins
- Deployment of Mathematica applications
- Webmaster

2014–2015

#### MEMPHYS - University of Southern Denmark

Odense, Denmark

*Research associate – computational biophysics*

Multi-scale simulations to understand the behavior of proteins.

Achievements – research:

- Enhanced stability of proteins in 3rd generation ionic liquids
- Behavior of the motor-protein Kinesin-5 with an inhibitor
- Coarse-grained and atomistic simulations of lipid droplet genesis
- 2 publications

2011–2014

#### CNRS / SOLEIL synchrotron

Paris-Saclay, France

*Research associate – computational biophysics*

Simulations and dynamics of proteins.

Achievements – research:

- Extraction of internal motions from molecular dynamics simulations
- Impact of anisotropic atomic motions on incoherent neutron scattering intensities
- Author of one of the first ActivePapers
- 3 publications

2008–2010

#### CEA

Bruyères-le-Châtel - Paris area, France

*Research associate – computational chemistry*

Thermodynamics and kinetics properties of carbon nanoparticles under extreme conditions.

Achievements:

- Model used in another simulation program
- Programs to analyze the data
- 3 publications

### education

2004–2008

#### Ph.D. in computational chemistry

University of Strasbourg

*Extraction of ions at the liquid-liquid interface – 4 publications.*

2003–2004

#### Master in computational chemistry

University of Strasbourg

2002–2003

#### Master in chemistry

University of Dijon

07/2009

#### Summer school - methods in molecular simulation

University of Sheffield

## publications

### article in peer-reviewed journal

Enhanced stability of the model mini-protein in amino acid ionic liquids and their aqueous solutions

Guillaume Chevrot, Eudes Eterno Fileti, Vitaly V. Chaban  
*Journal of Computational Chemistry* 36, 2044 (2015)

Model-free simulation approach to molecular diffusion tensors

Guillaume Chevrot, Konrad Hinsén, Gerald R. Kneller  
*The Journal of Chemical Physics* 139, 154110 (2013)

Molecular dynamics and kinetic study of carbon coagulation in the release wave of detonation products

Guillaume Chevrot, Arnaud Sollier, Nicolas Pineau  
*The Journal of Chemical Physics* 136, 084506 (2012)

Impact of anisotropic atomic motions in proteins on powder-averaged incoherent neutron scattering intensities

Gerald R. Kneller, Guillaume Chevrot  
*The Journal of Chemical Physics* 137, 225101 (2012)

Least constraint approach to the extraction of internal motions from molecular dynamics trajectories of flexible macromolecules

Guillaume Chevrot, Paolo Calligari, Konrad Hinsén, Gerald R. Kneller  
*The Journal of Chemical Physics* 135, 084110 (2011)

Molecular dynamics simulations of nanocarbons at high pressure and temperature

G. Chevrot, E. Bourasseau, N. Pineau, J.-B. Maillet  
*Carbon* 47, 3392 (2009)

Formation of multiwall fullerenes from nanodiamonds studied by atomistic simulations

Jan H. Los, Nicolas Pineau, Guillaume Chevrot, Gérard Vignoles, Jean-Marc Leyssale  
*Phys. Rev. B* 80, 155420 (2009)

Molecular dynamics study of dicarbollide anions in nitrobenzene solution and at its aqueous interface. Synergistic effect in the Eu(III) assisted extraction

G. Chevrot, R. Schurhammer, G. Wipff  
*Phys. Chem. Chem. Phys.* 9, 5928 (2007)

Synergistic effect of dicarbollide anions in liquid-liquid extraction: a molecular dynamics study at the octanol-water interface

G. Chevrot, R. Schurhammer, G. Wipff  
*Phys. Chem. Chem. Phys.* 9, 1991 (2007)

Molecular dynamics simulations of the aqueous interface with the [BMi][PF<sub>6</sub>] ionic liquid: comparison of different solvent models

G. Chevrot, R. Schurhammer, G. Wipff  
*Phys. Chem. Chem. Phys.* 8, 4166 (2006)

Surfactant Behavior of “Ellipsoidal” Dicarbollide Anions: A Molecular Dynamics Study

G. Chevrot, R. Schurhammer, G. Wipff\*  
*The Journal of Physical Chemistry B* 110, 9488 (2006)

## interests

MOOC, technology, philosophy, cycling, running