Guillaume **Chevrot**

Computational scientist - Data analyst

contact

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@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
LaTeX

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 Hinsen, 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 Hinsen, 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][PF6] 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