

Guillaume Chevrot

Python developer & trainer

contact

NUMGRADE
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languages

french mother tongue
english fluent
german & danish notions

skills

data analysis
programming
simulation
modeling
oral presentation
research report

informatics

Python, C, R
Mathematica
MongoDB
Shell scripting
Git
Django
CSS & HTML
Drupal
HDF5
HPC computing
Unix, Linux, OS X
L^AT_EX

experience

- 2018– **Entrepreneur - NUMGRADE** Orléans, France
Training and development in Python
- 2016–2018 **Freelance** Orléans, France
Python trainer / developer
- Python training courses for several companies (TOTAL, Synchrotron SOLEIL, CEA, SNCF, 01-Technologies) : Introduction to Python, scientific Python, Python for data analysis, ...
 - Automating administrative tasks (Scoop communication), backend development in Python/Django
- 2015–2018 **Complex Systems Institute - University of Orléans** Orléans, France
Research associate – computational/data science
Collaborate with several teams to manage data and improve their analysis.
Achievements – goals:
- WebNmoldyn: interactive notebooks in the cloud.
 - Creation of a database from a corpus and statistical analysis
 - Statistical analysis of neural data
 - 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 - 3 publications.
Python programming for data analysis.
- 2011–2014 **CNRS / SOLEIL synchrotron** Paris-Saclay, France
Research associate – computational biophysics
Simulations and dynamics of proteins - 3 publications.
Python programming for data analysis.
- 2008–2010 **CEA** Bruyères-le-Châtel - Paris area, France
Research associate – computational chemistry
Thermodynamics and kinetics properties of carbon nanoparticles under extreme conditions - 3 publications.
C programming for modeling and data analysis.

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

interests

technology, science, philosophy, cycling, running

publications

article in peer-reviewed journal

The role of caveolin-1 in lipid droplets and their biogenesis

Weria Pezeshkian, Guillaume Chevrot, Himanshu Khandelia
Chemistry and Physics of Lipids 211 (2018) pp. 93–99

Protein remains stable at unusually high temperatures when solvated in aqueous mixtures of amino acid based ionic liquids

Guillaume Chevrot, Eudes Eterno Fileti, Vitaly V. Chaban
Journal of Molecular Modeling 22, 258 (2016)

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][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)