GERMAIN SALVATO VALLVERDU

Researcher in molecular simulations and physical chemistry

1983 August 10 – Married, 2 children

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github.com/gvallverdu **0000-0003-1116-8776** in **g-salvato-vallverdu/**

Associate professor, specialist in molecular simulations, molecular modeling and theoretical chemistry applied to complex systems.

EXPERIENCE

Associate Professor in theoretical physical chemistry

University of Pau & Pays Adour

2010 – Ongoing — Pau, France

- Develop original computational strategies for the simulations of complex systems at the molecular scale.
- Develop and distribute data analyses libraries with Python
- Supervise research projects with Ph.D. and Master students
- Teaching from 1st year to doctoral students in chemistry and computer sciences

34 peer-reviewed articles, h-*index* 14, 534 citations 0000-0003-1116-8776

Research Engineer

CEA DAM

2009 – 2010 — Bruyères le châtel, France

- Developed parallel, MPI-based, C rouines to extend HPC code
- Parameterized a reactive coarse grain model for energetic materials

Ph.D. in physical-chemistry

Université Paris Sud 11

2006 – 2009 — Orsay, France

Theoretical study of photophysics properties of fluorescent proteins

- Developed novel numerical simulation strategies for biological systems
- Elaborated Fortran routines to produce and analyze high throughput simulations

SCIENTIFIC PROJECTS

Theroetical chemistry

- New strategies for joined experimental/theoretical approaches in chemistry
- Development of accurate force fields for bio-ionorganic compounds
- Development of computational tools for fast probing of molecular reactivity

Computational chemistry and HPC

- Surface reactivity and electronic properties of energy storage materials
- Molecular dynamics simulations for the characterization of complex matrices
- Reactive molecular simulations of complex systems (pyrolysiys, molecular degradation pathway)

Development of Scientific Libraries

- `Pymatgen`: Python Materials Genomics (`http://pymatgen.org/team.html`) — contributor
- `PyC2MC` Python Analysis of Complex Matrices (`https://gvallver.perso.univ-pau.fr/pyc2mc`) — project leader
- `pychemcurv`: local molecular curvature analyzes (`https://github.com/gVallverdu/pychemcurv`) — lead developer

SKILLS

Molecular Simulations HPC ●●●●●

Molecular Modelling ●●●●●

Computer science ●●●●○

Data Visualization ●●●○○

Molecular Simulation softwares

Lammps · VASP · Gromacs · Amber · Gaussian · Orca · VMD

Computer science

Python ●●●●●
Slurm ●●●○○
Linux/Unix/Bash ●●●●○
MPI ●●●○○
Fortran/C ●●●●○
git ●●●○○

Jupyter · Plotly/Dash · C++ · Java · HTML/CSS · Django

LANGUAGES

English ●●●●○

Spanish ●●○○○

EDUCATION

Ph.D. in physical-chemistry
2006 – 2009 — Université Paris-Sud 11

M.Sc. in Physical-Chemistry
2004 – 2006 — Université Paris-Sud 11

Magistère de Physico-Chimie Moléculaire
2003 – 2006 — Université Paris-Sud 11 ENS Cachan

CPGE in Physics & Chemistry
2001 – 2003 — Lycée F. Arago Perpignan