GERMAIN SALVATO VALLVERDU

Researcher in molecular simulations

1983 August 10 – Married, 2 children

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github.com/gvallverdu

Inquisitive, exigent physical chemistry specialist with 10+ years experience in numerical simulations and scientific programming. Seeking to leverage skills in communication, management and computer science as HPC engineer.

EXPERIENCE

Associate Professor in numerical simulations

University of Pau & Pays Adour

2010 – Ongoing Pau, France

- Develop original multi-scale computational strategies adapted to chemical systems in multi-disciplinary teams
- Develop and distribute data analyses libraries with Python
- Supervise research projects with Ph.D. and Master students
- Train UPPA users to HPC and programming languages using active learning

18 peer-reviewed articles, h-*index* 8, 200 citationsorcid.org/0000-0003-1116-8776

Research Engineer

CEA DAM

2009 – 2010 Bruyères le châtel, France

- Developed parallel, MPI-based, C rouines to extend HPC code
- Accomplished the parametrization of coarse grain models 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 adapted to biological systems
- Elaborated Fortran routines to produce and analyze hugh throughput simulations

SCIENTIFIC PROJECTS

Energy storage materials – Li-ion batteries

- Surface reactivity of cathode materials
- Coupled studies between quantum chemistry and experimental surface characterization
- Interfaces: structure, electronic properties and thermochemistry

Petroleum chemistry and complex matrices

- Physico-chemical properties of asphaltenes: solubility, aggregation
- Molecular modelling and molecular dynamics simulations
- Molecular characterization of complex matrices (heavy crude oil)

Python Scientific Libraries

- `Pymatgen`: Python Materials Genomics (`http://pymatgen.org/team.html`)
- LA-ICP MS: Chemical mapping analysis (`https://pychemapps.univ-pau.fr/icpms`)
- Mammoth: a molecular force field optimizer (`https://mammoth_uppa.gitlab.io/`)
- Mosaïca: A generator and analyzer of nano-materials based on their intrinsec geometry (`https://pychemapps.univ-pau.fr/mosaica/`)

SKILLS

Physical chemistry simulations ●●●●●

Molecular Modelling ●●●●●

Computer science ●●●●○

Data Visualization ●●●○○

Simulation codes

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