GERMAIN SALVATO VALLVERDU

Researcher in molecular simulations

1983 August 10 - Married, 2 children

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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

Pruyères 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

LammpsVASPGromacsAmberGaussianOrcaVMD

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

Q 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