# MARIO BURBANO

## Researcher in molecular simulations

**1983 August 10 – Married, 2 children**

@ **germain.vallverdu@gmail.com** **06 88 59 08 87** **gsalvatovallverdu.gitlab.io**
**github.com/gvallverdu** **orcid.org/0000-0003-1116-8776**

Inquisitive, exigent HPC specialist with 12+ years experience in numerical simulations and scientific programming. Seeking to leverage skills in communication, management and computer science as HPC engineer.

## EXPERIENCE

### Associate Professor

**University of Pau & Pays Adour**

2010 – Ongoing — Pau, France

- Develop multi-scale computational strategies adapted to complex systems
- 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 citations

### Research Engineer

**CEA DAM**

2009 – 2010 — Bruyères le châtel, France

- Used C and MPI to include Dissipative Particle Dynamics algorithms in a massively parallel program
- Parametrization of coarse grain models for molecular simulations

### Ph.D. in physical-chemistry

**Université Paris Sud 11**

2006 – 2009 — Orsay, France

Theoretical study of photophysics properties of fluorescent proteins

- Produced molecular simulations of biological systems
- Used Fortran to write simulations and data analysis programs

## PROJECTS

### Energy storage materials – Li-ion batteries

**University of Pau & Pays Adour / RS2E**

- 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

**University of Pau & Pays Adour / C2MC**

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

### Python Scientific Libraries

**University of Pau & Pays Adour**

- `Pymatgen`: Python Materials Genomics (`http://pymatgen.org/team.html`)
- Mammoth: a molecular force field optimizer (`https://mammoth_uppa.gitlab.io/`)
- Mosaïca: a generator of nano-materials based on their intrinsic geometry

## SKILLS

**High Performance Computing** ●●●●●

**Molecular Modelling** ●●●●●

**Mathematics / Statistics** ●●●○○

**Data Visualization** ●●●●○

### Computer science

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

Java | Plotly/Dash | HTML/CSS/PHP | Hugo/Jekyll | Django | Visual Studio Code

### Simulations code

Lammps | VASP | Gromacs | Amber | Gaussian | Orca | VMD

## 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