

MARIO BURBANO

Cloud Data Engineer and Scientist

14 November 1984 – Cohabitation

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Antony, FRANCE

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PhD in Computational Chemistry with extensive experience in cloud computing, task automation and data analysis.

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 château, 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

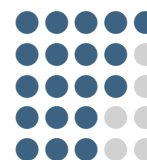
Python

Linux/Unix/Bash

Fortran

Machine Learning

git



AWS

GCP

Plotly/Dash

scikit-learn

Flask

pandas

Visual Studio Code

Simulations code

Lammps

VASP

Gromacs

Amber

Gaussian

Orca

VMD

LANGUAGES

English



Spanish



French



EDUCATION

Ph.D. in Computational 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