Germain **Salvato Vallverdu**

Associate Professor - Chemical physics and numerical simulations

10 août 1983, France
Maried, 2 children

Contact

germain.vallverdu@univ-pau.fr
(33) 5 59 40 78 51
(33) 6 88 59 08 87

IPREM
Technopôle Hélioparc
2 ave du Président P. Angot
FR-64053 Pau cedex 9
http://iprem.univ-pau.fr

Theoretical Chemistry

Computational strategy
Development
Complex matrices
Surfaces, interfaces
VASP, CRYSTAL (solid)
Gaussian, Orca (molecule)
Gromacs, Lammps (MD)

Programming

Python
Fortran, C
LaTeX, HTML/CSS

Languages

French
English

Bibliometry

18 articles
13 conferences
h-index: 8
12.5 citations per item
199 citations (181 w/o self-citations)

On the web

publons 2764008
GitHub GitLab: gvallverdu
gsalvatovallverdu.gitlab.io

Abstract

Associate professor at the University of Pau & Pays Adour, I am a specialist in theoretical chemistry, molecular modeling and numerical simulations at IPREM institute. My research activities, in physical-chemistry, concern the understanding of macroscopic phenomena such as reactivity, thermochemistry or spectroscopy from a microscopic description of matter. The implementation and combination of relevant computational strategies allows for the investigation of complex systems in various field among petroleum-chemistry, biological systems or energy storage materials.

Professional Experiences

since 2010 **Université de Pau et des Pays de l'Adour** — Pau, France
Associate professor
Theoretical chemistry and computational approaches. Surfaces, interfaces, reactivity and molecular interactions.

2009–2010 **CEA - DAM** — Bruyères le châtel, France
Postdoctoral position
Development and implementation of a mesoscopic model for reactive shock waves propagation in heterogeneous systems.

2006–2009 **Université Paris-Sud 11** — Orsay, France
PhD Student
Theoretical study of photophysical processes in fluorescent proteins.

Education

2006-2009 **PhD in chemistry** speciality theoretical chemistry — Université Paris-Sud 11
Mention très honorable

2004-2006 **Master degree of physical-chemistry** — Université Paris-Sud 11
speciality Physico-Chimie Moléculaire
Mention TB

2003-2004 **Bachelor Degree of physical-chemistry** — Université Paris-Sud 11
Mention TB

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

2001-2003 **Undergraduate** physics and chemistry — Lycée François Arago, Perpignan

Main publications

Munoz, G. et al. Redox activity of nickel and vanadium porphyrins: a possible mechanism behind petroleum genesis and maturation? RSC Advances **2019**, 9, 9509–9516.

Santos Silva, H. et al. Impact of H-Bonds and Porphyrins on Asphaltene Aggregation As Revealed by Molecular Dynamics Simulations. Energy & Fuels **2018**, 32, 11153–11164.

Quesne-Turin, A. et al. Morphology and Surface Reactivity Relationship in the Li1+xMn2–xO4 Spinel with x = 0.05 and 0.10: A Combined First-Principle and Experimental Study. ACS Applied Materials & Interfaces **2017**,

Santos Silva, H. et al. The role of metalloporphyrins on the physical-chemical properties of petroleum fluids. Fuel **2017**, 188, 374–381.

Vallverdu, G. et al. First principle study of the surface reactivity of layered lithium oxides LiMO2 (M = Ni, Mn, Co). Surf. Sci. **2016**,

Maillet, J. B. et al. Mesoscopic simulations of shock-to-detonation transition in reactive liquid high explosive. EPL **2011**, 96, 68007.

Vallverdu, G. et al. Relation between pH, structure, and absorption spectrum of Cerulean: A study by molecular dynamics and TD DFT calculations. Proteins: Struct., Funct., Bioinf. **2010**, 78, 1040–1054.

Teaching

- Lectures in chemical-physics, theoretical chemistry and programming languages.
- Strong involvement in new information and communication technologies for education
- Science popularization: Quantum mechanics and workshops for school students