

Germain Vallverdu

Associate Professor -- PhD in Chemical Physics



10 août 1983, France
Married, 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

Theoretical Chemistry

Computational strategy
Development
Surfaces, interfaces
VASP, CRYSTAL (solid)
Gaussian, Orca (molecule)
Gromacs, AMBER (dynamic)

Programming

Fortran, C
Python
L^AT_EX, HTML/CSS




Languages

French
English (Professional)

Bibliometry

15 articles
11 conferences
h-index: 7
12.5 citations per item
150 citations (142 w/o
self-citations)

On the web

 orcid.org/0000-0003-1116-8776
 [gVallverdu](https://github.com/gVallverdu)
 gvallver.perso.univ-pau.fr

Abstract

Associate professor at the Université de Pau et des Pays de l'Adour, I am a theoretical chemist at IPREM institute (Institute for Analytical sciences and chemical physics applied to environment and materials). My research activities concern the development of new methods in theoretical chemistry and new computational strategies at different time or space scales, applied to the investigations of complex systems. I teach mainly chemical-physics subjects and programming languages at the university of Pau.

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 château, 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 chemistry** Université Paris-Sud 11
speciality molecular chemical-physics
Mention TB
- 2003-2004 **Bachelor Degree of chemical-physics** 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

- Quesne-Turin, A. et al. Morphology and Surface Reactivity Relationship in the Li_{1+x}Mn_{2-x}O₄ 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**,
- Guille, E. et al. Possible Existence of a Monovalent Coordination for Nitrogen Atoms in Li_xPO_yN_z Solid Electrolyte: Modeling of X-ray Photoelectron Spectroscopy and Raman Spectra. *J. Phys. Chem. C* **2015**, 119, 23379–23387.
- Martin, L. et al. First principles calculations of solid–solid interfaces: an application to conversion materials for lithium-ion batteries. *J. Mater. Chem.* **2012**, 22, 22063–22071.
- 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 student