Germain **Salvato Vallverdu**

Associate Professor - Chemical physics and numerical simulations

10 août 1983, France
Maried, 2 children

Contact

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IPREM
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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

28 articles
21 conferences
h-index: 11
13.8 citations per item
385 citations (340 w/o self-citations)

On the web

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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

Sabalot-Cuzzubbo, J. et al. Relating the molecular topology and local geometry: Haddon's pyramidalization angle and the Gaussian curvature. The Journal of Chemical Physics **2020**, 152, 244310, Publisher: American Institute of Physics.

Villegas, O. et al. Molecular Cartography of A1 and A2 Asphaltene Subfractions from Classical Molecular Dynamics Simulations. Energy & Fuels **2020**, 34, 13954–13965, Publisher: American Chemical Society.

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**,

Guille, E. et al. Possible Existence of a Monovalent Coordination for Nitrogen Atoms in LixPOyNz 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.

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