Fanny Vazart
Female, 26, married
Nationality: French
Driving license

fanny.vazart@sns.it

PhD Student, 3rd year

Education:

2014 - present **PhD - Effective anharmonic models for the computation of spectroscopic, thermodynamic and kinetic properties of complex molecules**
Supervisor: Prof. Vincenzo Barone
Scuola Normale Superiore di Pisa (Italy)

2012 - 2014 **Master's Degree in Molecular Chemistry**
with a Theoretical Chemistry label from the French theoretical chemistry network
University of Rennes 1 (France)

2012 **Bachelor's Degree in Chemistry**
University of Rennes 1 (France)

Studied disciplines:
Atomic structure, thermodynamics, solid-state chemistry, organic and organometallic chemistry, analysis technics, biochemistry, kinetics, electrochemistry, quantum chemistry, magnetism, polymers, spectroscopies.
Advanced course in theoretical chemistry:
Extended Huckel Theory, introduction to ab initio calculations, Hartree-Fock theory, correlation treatments, post-HF calculations,
O. Delalande *Multi-scale simulation of bio-molecular systems*
J.-Y. Le Questel *Quantic methods application to the study of interactions by hydrogen bond*
R. Gautier *Quantum calculations of RMN properties*
A. Laurent *Quantum simulation of organic molecules' excited states*
F. Boucher *DFT applied to the study of solid-states*
A. Boucekkine *Dirac equation and relativistic quantum chemistry*
B. Le Guennic *Magnetic exchange calculations: the different quantic approaches*
C. Katan *Beyond the study of ground state in gaseous phase (excitation and environment)*
S. Di Matteo *Tight binding and LDA+U in solid-state chemistry*
T. Cauchy *Atoms and molecules, back to some concepts (AIM, ELF, conceptual DFT...)*

Work Experience:

February 2014 – June 2014 **2nd year of Master's Degree Intership – Phosphorus and iron based π –conjugated materials for electronic communication: a theoretical approach (DFT)**
Supervisor: Prof. J-F. Halet
Inorganic theoretical chemistry laboratory, CNRS, Rennes (France)
• Structural, electronic, optic and magnetic theoretical studies of bimetallic iron complexes. Application for electronic communication.

April 2013 - July 2013

1st year of Master's Degree Internship – Interplay between experiment and computation: a case study on caged-compounds
Supervisor: Prof. M. Abe
Research group of reaction organic chemistry, Hiroshima University, Hiroshima (Japan)
• Ascertainment and synthesis of an appropriate cage for the glutamate, with proper optical properties (two photon absorption)

May 2012 - June2012

Technician Assistant – Theoretical study of platinum(II) complexes' structural and spectroscopic properties (DFT)
Supervisor: Prof. A. Boucekkine
Inorganic theoretical chemistry laboratory, CNRS, Rennes (France)
• Application for OLED screens, medical imaging

June 2011 - July 2011

Technician Assistant – Analysis and quantification of organic products by gaseous chromatography
Supervisor: Dr N. Blin-Simiand
Gases and plasmas physics laboratory, CNRS, Orsay (France)
• Analysis and quantification of products obtained from an electric shock on toxic organic gases. Application for pollution issues.

Mathematics, Chemistry, Physics private lessons.
References available on request.

Skills:

Chemistry: Synthesis in organic chemistry (with procedure optimization), theoretical calculations and analysis (DFT, TD-DFT).
IT-knowledge: Origin, Regressi, Gaussian, Gabedit, SWizard, Gaussview, Chemdraw, Molden, Mercury.
French: Native speaker level.
English: Spoken and written.
Italian: Spoken.
Spanish: Basic.

Personal interests and activities:

Reading, music, cinema, travels

Travel experiences

Europe: England, Spain, The Netherlands, Belgium, Germany, Italy, Ireland.
America: Colombia, USA, Canada.
Asia: Japan.
Africa: Egypt, Tunisia.

Publications:

(1) Vazart, F.: Calderini, D.; Puzzarini, C.; Skouteris, D.; Barone, V. *J. Chem. Theory Comput.* State-of-the-art thermochemical and kinetic computations for astrochemical complex organic molecules: formamide formation in cold interstellar clouds as a case study, **2016**, DOI: 10.1021/acs.jctc.6b00379;
(2) Vazart, F.; Savel, P.; Latouche, C.; Barone, V.; Camerel, F.; Roisnel, T.; Fillaut, J.-L., Akdas-Kilig, H.; Achard, M. *Dalton Trans.* Neutral Copper(I) Complexes Featuring Phosphinesulfonate Chelates, **2016**, *45*, 6566-6573;
(3) Vazart, F.; Latouche, C.; Cimino, P., Barone, V. *J. Chem. Theory Comput.* Accurate Infrared (IR) Spectra for Molecules Containing the C≡N Moiety by Anharmonic Computations with the Double Hybrid B2PLYP Density Functional, **2015**, *11 (9)*, 4364-4369;
(4) Barone, V.; Latouche, C.; Skouteris, D.; Vazart, F.; Balucani, N.; Ceccarelli, C.; Lefloch, B. *Mon. Not. R. Astron. Soc.* Gas-phase Formation of the Prebiotic Molecule Formamide: Insights from new Quantum Computations, **2015**, *453*, L31-L35;
(5) Vazart, F.; Latouche, C.; Skouteris, D.; Balucani, N.; Barone, V. *Astrophys. J.* Cyanomethanimine Isomers in Cold Interstellar Clouds: Insights from Electronic Structure and Kinetic Calculations, **2015**, *810 (2)*, 111;
(6) Vazart, F.; Latouche, C. *Theor. Chem. Acc.* Validation of a Computational Protocol to Simulate near IR Phosphorescence Spectra for Ru(II) and Ir(III) Metal Complexes, **2015**, *134 (12)*, 144;
(7) Vazart, F.; Latouche, C.; Bloino, J.; Barone, V. *Inorg. Chem.* Vibronic Coupling Investigation to Compute Phosphorescence Spectra of Pt(II) Complexes, **2015**, *54 (11)*, 5588-5595;
(8) Vazart, F.; Calderini, D.; Skouteris, D.; Latouche, C.; Barone, V. *J. Chem. Theory Comput.* Re-assessment of the Thermodynamic, Kinetic, and Spectroscopic Features of Cyanomethanimine Derivatives: a Full Anharmonic Perturbative Treatment, **2015**, *11 (3)*, 1165-1171.

Oral communications:

- *Luminescent investigation of Pt(II) derivatives: computed vs. experimental phosphorescence*,

Fanny Vazart, Camille Latouche, Julien Bloino, Vincenzo Barone
Groupe d'études en Chimie Organométallique & Concertation en Chimie de Coordination (Gecom Concoord), Lyon (France), May 26th-29th **2015**

- *Cyanomethanimine isomers in cold interstellar clouds: insights from electronic structure and kinetic calculations,*

Fanny Vazart, Camille Latouche, Dimitrios Skouteris, Nadia Balucani, Vincenzo Barone
Life in a cosmic context, Trieste (Italy), September 15th-17th **2015**

- *Cyanomethanimine isomers in cold interstellar clouds: insights from electronic structure and kinetic calculations,*

Fanny Vazart, Camille Latouche, Dimitrios Skouteris, Nadia Balucani, Vincenzo Barone
COST meeting, Pisa (Italy), March 7th-8th **2016**

- *Feasible reaction mechanisms for formamide formation in cold interstellar clouds*, Fanny Vazart, Danilo Calderini, Cristina Puzzarini, Dimitrios Skouteris, Vincenzo Barone
Astronomical Complex Organic Molecules in different environments, Florence (Italy), March 10th-11th **2016**
- *Feasible reaction mechanisms for formamide formation in cold interstellar clouds*, Fanny Vazart, Danilo Calderini, Cristina Puzzarini, Dimitrios Skouteris, Vincenzo Barone
International Meeting on Atomic and Molecular Physics and Chemistry, Le Havre (France), June 27th-30th **2016**

Written communications:

- *Luminescent investigation of Pt(II) derivatives: computed vs. experimental phosphorescence*,

Fanny Vazart, Camille Latouche, Julien Bloino, Vincenzo Barone
Modelling Photoactive Molecules (MPM), Nantes (France), April 21st-24th **2015**

Summer school:

Astrochemistry: from Space to Earth,
IPAG Grenoble (France), August 28th-September 9th **2016**

References:

Prof. V. Barone
vincenzo.barone@sns.it

Prof. J.-F. Halet
halet@univ-rennes1.fr

Prof. M. Abe
mabe@hiroshima-u.ac.jp

Prof. A. Boucekkine
abdou.boucekkine@univ-rennes1.fr