





JULES SCHLEINITZ







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I am a chemistry Ph.D. student spending my time between research and teaching college students. I plan to complete my doctorate during the second semester of 2022. My work focuses on the oxidative addition of nitroarenes and carbon-oxygen aromatic compounds on nickel and palladium complexes. I perform mechanistic investigation with theoretical and experimental means as well as investigate the potential of machine learning applications for synthetic chemists using nickel coupling reactions and literature data.

Education

2019 - present	Ph.D. student , in the Methods and Mechanisms team under the supervision of Dr. Laurence Grimaud .	
2019	Master of Physical and Theoretical Chemistry, highest honors Sorbonne Université , Paris	
2017	Admission to Agrégation de Chimie : nation-wide competitive examination for the recruitment of chemistry teachers for high school and preparatory classes (rank : 8/240)	
2014 - 2016	Chemistry and Physics at Ecole Normale Supérieure (Bachelor: Chemistry and Physics, first year of Master: Chemistry, highest honors), Paris	
2012 - 2014	Preparatory class (Math, Physics and Chemistry) admission to the most competitive research-engineer «Grandes Ecoles» (Universities) in France : Ecole Normale Supérieure (Ulm) (rank : 27/1200), Ecole Polytechnique (rank : 24/1400), Centrale Paris (rank : 38/2500), Lycée Thiers, Marseille.	

Research Experience

August 2020	Aqemia , Paris Dr. Maximilien Levesque Implemented a scoring function for the synthetizability of drug-like molecules.	
February - June 2019	LBM, Ecole Normale Supérieure, Paris Dr. Laurence Grimaud and Dr. Ilaria Ciofini Studied the mechanism of the deoxygenation of amine <i>N</i>-oxides by DFT and experimental means.	
February - June 2018	LCM, Ecole Polytechnique - CNRS, Palaiseau Dr. Mathieu Xémard and Dr. Gregory Nocton Synthesized and characterized divalent lanthanides dimers and sandwich single-molecule magnets.	
March - July 2016	Theoretical and Quantum Chemistry Group, Technische Universität Berlin, Berlin Dr. Anja H. Greif and Pr. Martin Kaupp. Analyzed the inverse trans influence on ¹H NMR hydride shifts in pseudo-octahedral U^{VI} complexes with relativistic DFT.	
May - June 2015	LCM, Ecole Polytechnique - CNRS, Palaiseau Dr. Gilles Frison. Described the coordination properties of <i>N</i>-heterocyclic mesoionic carbens with quantum-chemical tools.	
January 2015	Ultrafast Photochemistry Group, Ecole Normale Supérieure, Paris. Purified photoswitchable protein Padron and performed spectroscopic characterization. Under the supervision of Dr. Agathe Espagne.	

Publications

5. Can Organic Chemistry Literature Enable Machine Learning Yield Prediction ?
J. Schleinitz, M. Langevin, Y. Smail, B. Wehnert, L. Grimaud and R. Vuilleumier
(Writing)
4. A Single Bioinspired Hexameric Nickel Catechol-alloxazine Catalyst Combines Metal and Radical Mechanisms for Alkene Hydrosilylation.
A. Das, **J. Schleinitz**, L. Karmazin, B. Vincent, N. Le Breton, A. Guenet, S. Choua, L. Grimaud, M. Desage El Murr
(Submitted)
3. A Hybrid Bioinspired Catechol-alloxazine Triangular Nickel Complex Stabilizing Protons and Electrons.
A. Das, H. Jobelius, **J. Schleinitz**, S. Gamboa-Ramirez, G. Creste, G. Kervern, J. Raya, N. Le Breton, A. Guénet, Z. Boubegtiten-Fezoua, L. Grimaud, M. Orio, G. Rogez, P. Hellwig, S. Choua, S. Ferlaye and M. Desage-El Murr
Inorganic Chemistry Frontiers, **2021**, 8, 5286-5298, DOI: [10.1039/D1QI01131F](https://doi.org/10.1039/D1QI01131F)
2. Metal-Free Deoxygenation of Amine N-Oxides: Synthetic and Mechanistic Studies
J. Schleinitz, W. Lecroq, M. Billoue, A. Perfetto, A-C. Gaumont, J. Lalevée, I. Ciofini, L. Grimaud, S. Lakhdar
ChemPhysChem, **2021**, 22, 1237. DOI: [10.1002/cphc.202100108](https://doi.org/10.1002/cphc.202100108), PDF
1. Bis-Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Single-Molecule Magnets.
J. Moutet, **J. Schleinitz**, L. La Droitte, M. Tricoire, F. Pointillart, F. Gendron, T. Simler, C. Clavaguéra, B. Le Guennic, O. Cador, G. Nocton
Angewandte Chemie International Edition, **2021**, 60 (11), 6042-6046. DOI: [10.1002/anie.202015428](https://doi.org/10.1002/anie.202015428), PDF

Current Collaborations

Dr. Ilaria Ciofini	DFT studies of organic and inorganic mechanism pathways. I-CLeHS, Chimie-Paris Tech, Paris, France
Pr. Marine Desage - El Murr	Electrochemical and DFT study of Nickel multimers for catalysis applications. Institut de Chimie, Strasbourg, France
Pr. Pietrick Hudhomme	Experimental and theoretical mechanistic investigations on an unusual oxydative addition of nitroperylene-diimide with palladium tetrakis phosphine. Université d'Angers, Angers, France
Pr. Rodolphe Vuilleumier	Machine learning for reaction yield prediction with literature extracted data. Ecole Normale Supérieure, Paris, France



Teaching Experiences

2020 - present	Supervision of exploratory projects conducted by students for the TFChim national contest. \simeq 10h/year
2019 - present	<ul style="list-style-type: none">○ Recrutement of the ENS chemistry students : 4h experimental evaluation sessions, written exam conception and corrections, \simeq 3 weeks/year.○ Organic Chemistry Lessons for students applying for Agregation competitive exam.<ul style="list-style-type: none">• \simeq 25 students. Mostly graduate physicist students, \simeq 40h/year• More details on the lessons here.○ Teaching assistant in Electrochemistry, theoretical tutorials and experimental session.<ul style="list-style-type: none">• \simeq 20 students. First year chemistry ENS students (third year university equivalent), \simeq 25h/year• More details on the lessons here.○ Preparation of graduate students for the Agregation competitive examination.<ul style="list-style-type: none">• 15 graduated students. the teaching consist in the evaluation of diverse chemical subjects presented by the students. The presentations can take place in the laboratory as practical work sessions or in a classroom. \simeq 60h/year○ Teaching practical chemistry<ul style="list-style-type: none">• \simeq 20 students. First year chemistry ENS students (third year university equivalent), \simeq 20h/year
2018 - 2019	Oral examinations in Physics for first and second year undergraduate students («Colles» for French preparatory classes)

Skills

Languages	French (native speaker), English (fluent), Spanish (conversant)
Experimental	NMR techniques for characterization and kinetic studies, EPR, UV-Vis Spectroscopy, Fluorimetry, Infrared spectroscopy, Electrochemistry : Stationary (RDE, UME techniques) and Non Stationary Voltammetry (CV, SWV, DPV, Chronamperometry) for compound characterization and mechanistic studies. Inorganic synthesis, XRD : crystallization of inorganic complexes. Inert atmosphere synthesis : glovebox and Schlenk line techniques.
Computational	DFT/TD-DFT: Gaussian, Orca and ADF. Ground state/excited states optimization, Transition state optimization. Single electron transfer barrier modeling (Marcus Theory). RDKit toolkit, sklearn: machine learning basics, github. Data Analysis.
Supervision	<ul style="list-style-type: none">• bachelor student week to month internships: electrochemistry and inorganic synthesis 6 students (2019 to present)• master 1 student, semester internship: python and machine learning for reaction prediction 2 students (April - August 2021)• master 2 student, semester internship: DFT and experimental mechanistic studies 1 student (February - July 2021)• master 2 student, semester internship: goal directed molecule optimization (DFT and ML) 1 student (February - July 2022)

References

PhD supervisor and Team leader : Dr. Laurence Grimaud : laurence.grimaud@ens.psl.eu
Team leader : Dr. Maxime Vitale : maxime.vitale@ens.psl.eu
Former PhD supervisor : Dr. Maximilien Levesque, CEO at Aqemia : maximilien.levesque@aqemia.com
Former internship supervisor : Dr. Grégory Nocton : gregory.nocton@polytechnique.edu