





# 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 by the end 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	PhD student, in the <a href="#">Methods and Mechanisms</a> team under the supervision of <a href="#">Dr. Laurence Grimaud</a> .	
2019	Master of Physical and Theoretical Chemistry, highest honors Sorbonne Université, Paris	
2017	Admission to Agrégation de Chimie : high-level competitive examination for future chemistry teachers for high school and preparatory classes (rank : 8/240)	
2014 - 2016	Chemistry and Physics at <a href="#">Ecole Normale Supérieure</a> (Bachelor in Chemistry and Physics and first year of Master in 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	<a href="#">Aqemia</a> , Paris <b>Implemented a scoring function for the synthetisability of drug-like molecules.</b> Under the supervision of Dr. Maximilien Levesque	
February - June 2019	LBM, Ecole Normale Supérieure, Paris <b>Studied the mechanism of the deoxygenation of amine <math>N</math>-oxides by DFT and experimental means.</b> Under the supervision of Dr. Laurence Grimaud and Dr. Ilaria Ciofini	
February - June 2018	<a href="#">LCM</a> , Ecole Polytechnique - CNRS, Palaiseau. <b>Synthesized and characterized divalent lanthanides dimers and sandwich single-molecule magnets.</b> Under the supervision of Dr. Mathieu Xémard and Dr. <a href="#">Gregory Nocton</a> .	

March - July 2016	Theoretical and Quantum Chemistry Group, Technische Universität Berlin, Berlin. <b>Analyzed the inverse trans influence on <math>^1\text{H}</math> NMR hydride shifts in pseudo-octahedral <math>\text{U}^{\text{VI}}</math> complexes with relativistic DFT.</b> Under the supervision of Dr. Anja H. Greif and Pr. Martin Kaupp.	
May - June 2015	LCM, Ecole Polytechnique - CNRS, Palaiseau. <b>Described the coordination properties of <math>N</math>-heterocyclic mesoionic carbens with quantum-chemical tools.</b> Under the supervision of Dr. Gilles Frison.	
January 2015	Ultrafast Photochemistry Group, Ecole Normale Supérieure, Paris. <b>Purified photoswitchable protein Padron and performed spectroscopic characterization.</b> 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. Wenhert, L. Grimaud and R. Vuilleumier an  
(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 Droite, 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

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 oxidative 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 <a href="#">TFChim</a> national contest. $\simeq$ 10h/year
2019 - present	<ul style="list-style-type: none"><li>○ Recrutement of the ENS chemistry students : 4h experimental evaluation sessions, written exam conception and corrections, <math>\simeq</math> 3 weeks/year.</li><li>○ Organic Chemistry Lessons for students applying for Agregation competitive exam.<ul style="list-style-type: none"><li>— <math>\simeq</math> 25 students. Mostly graduate physicist students, <math>\simeq</math> 40h/year</li><li>— More details on the lessons <a href="#">here</a>.</li></ul></li><li>○ Teaching assistant in Electrochemistry, theoretical tutorials and experimental session.<ul style="list-style-type: none"><li>— <math>\simeq</math> 20 students. First year chemistry ENS students (third year university equivalent), <math>\simeq</math> 25h/year</li><li>— More details on the lessons <a href="#">here</a>.</li></ul></li><li>○ Preparation of graduate students for the Agregation competitive examination.<ul style="list-style-type: none"><li>— 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. <math>\simeq</math> 60h/year</li></ul></li><li>○ Teaching practical chemistry<ul style="list-style-type: none"><li>— <math>\simeq</math> 20 students. First year chemistry ENS students (third year university equivalent), <math>\simeq</math> 20h/year</li></ul></li></ul>
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 characterisation and kinetic studies, EPR, UV-Vis Spectroscopy, Fluorimetry, Infrared spectroscopy, Electrochemistry : Stationnary (RDE, UME techniques) and Non Stationnary Votallmetry (CV, SWV, DPV, Chronamperometry) for compound characterisation and mechanistic studies. Inorganic synthesis, XRD : cristallisation 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 modelisation (Marcus Theory). Rdkit toolkit, sklearn : machine learning basics, github. Data Analysis.
Supervision	<ul style="list-style-type: none"><li>— bachelor student week to month interships : electrochemistry and inorganic synthesis 6 students (2019 to present)</li><li>— master 1 student, semester internship : python and machine learning for reaction prediction 2 students (April - August 2021)</li><li>— master 2 student, semester internship : dft and experimental mechanistic studies 1 student (February - July 2021)</li><li>— master 2 student, semester intership : goal directed molecule optimization (dft and ML) 1 student (February - July 2022)</li></ul>

## References

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