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 synthetist chemists using Nickel coupling reactions and literature data.

Education

2019 - present	PhD student, in the Methods and Mechanisms team under the supervision of Dr. Laurence Grimaud. I study coupling reactions of nitroarene and C-O aromatic compounds on Pd and Ni complexes using experimental and theoretical tools.
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 Ecole Normale Supérieure (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	Aqemia, Paris **Implemented a scoring function for the synthetisability of drug-like molecules.** Under the supervision of Dr. Maximilien Levesque
February - June 2019	LBM, Ecole Normale Supérieure, Paris **Studied the mechanism of the deoxygenation of amine $N-$oxides by DFT and experimental means.** Under the supervision of Dr. Laurence Grimaud and Dr. Ilaria Ciofini
February - June 2018	LCM, Ecole Polytechnique - CNRS, Palaiseau. **Synthetized and characterized divalent lanthanides dimers and sandwich single-molecule magnets.** Under the supervision of Dr. Mathieu Xémard and Dr. Gregory Nocton.

March - July 2016
Theoretical and Quantum Chemistry Group, Technische Universität Berlin, Berlin.
Analyzed the inverse trans influence on ^{1}H NMR hydride shifts in pseudo-octahedral U^{VI} complexes with relativistic DFT.
Under the supervision of Dr. Anja H. Greif and Pr. Martin Kaupp.

May - June 2015
LCM, Ecole Polytechnique - CNRS, Palaiseau.
Described the coordination properties of $N-$heterocyclic mesoionic carbens with quantum-chemical tools.
Under the supervision of Dr. Gilles Frison.

January 2015
Ultrafast Photochemistry Group, Ecole Normale Supérieure, Paris.
Purified photoswitchable protein Padron and did it's 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. Wenhert, R. Vuilleumier and L. Grimaud
(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

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, 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, PDF

Current Collaborations

Ilaria Ciofini
DFT studies of organic and inorganic mechanism pathways.
I-CLeHS, Chimie-Paris Tech, Paris, France

Marine Desage - El Murr
Electrochemical and DFT study of Nickel multimers for catalysis applications.
Institut de Chimie, Strasbourg, France

Pietrick Hudhomme
Experimental and theoretical mechanistic investigations on an unusual oxydative addition of nitroperylene-diimide with palladium tetrakis phosphine.
Université d'Angers, Angers, France

Rodolphe Vuilleumier
Maxime Langevin
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 — ⬡ Recruitement 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.
- — $\simeq$ 25 students. Mostly graduate physicist students, $\simeq$ 40h/year
- — More details on the lessons here.

⬡ Teaching assistant in Electrochemistry, theoretical tutorials and experimental session.
- — $\simeq$ 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.
- — 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
- — $\simeq$ 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 characterisation and kinetic studies, EPR, UV-Vis Spectroscopy, Fluorimetry, Infrared spectroscopy, Electrochemistry : Stationnary (RDE, UME techniques) and Non Stationnary Votalmmetry (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
- — bachelor student week to month interships : electrochemistry and inorganic synthesis several students (2019 to present)
- — master 1 student, semester internship : python and machine learning for reaction prediction 2 students (April - August 2020)
- — master 2 student, semester internship : dft and experimental mechanistic studies 1 student (February - July 2020)

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