Jules Schleinitz

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I am a **third year PhD Student**, working on the **oxydative addition** of nitroarenes and carbon-oxygen aromatic compounds with Nickel and Palladium. I perform **mechanistic investigation** with **theoretical** and **experimental** means. I am also interested in the potential of **machine learning** applications for synthetist chemists.

Education

2019 - present	PhD student, in the Methods and Mechanims team under the supervision of Laurence Grimaud. I study coupling reactions of nitroarene and C-O aromatic compounds on Pd and Ni complexes using experimental and therotetical tools.
2019	Master Chimie Analytique Physique et Théorique, Sorbonne Université, Paris
2017	Admission to Agrégation de Chimie : competitive examination for future chemistry teachers for high school and preparatory classes.
2014 - 2019	Chemistry and Physics at Ecole Normale Supérieure, Paris
2012 - 2014	Preparatory class : Math, Physics and Chemistry, Lycée Thiers, Marseille

Research Experiences

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.
Stage supervisé par Dr. Agathe Espagne.

Publications

2. Metal-Free Deoxygenation of Amine N-Oxides : Synthetic and Mechanistic Studies
W. Lecroq, **J. Schleinitz**, 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

Collaborations

Ilaria Ciofini
DFT studies of organic and inorganic mechanisms.
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
Reaction yield prediction with litterature 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 writing 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, EPR, XRD, UV-Vis Spectroscopy, Electrochemistry, Inorganic synthesis, Inert atmosphere : glovebox and schlenk line techniques.

Computational: DFT tools (Gaussian, Orca and ADF), Python (rdkit, sklearn, git)...

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

Laurence Grimaud : laurence.grimaud@ens.psl.eu
Maxime Vitale : maxime.vitale@ens.psl.eu
Maximilien Levesque : maximilien.levesque@aqemia.com
Grégory Nocton : gregory.nocton@polytechnique.edu