



PhD Student in Computational Chemistry

IFP Energies Nouvelles, Solaize FRANCE

PROFESSIONAL EXPERIENCES

Since 11/2024 _ **PhD Student** directed by Dr. Céline Chizallet
IFP Energies Nouvelles, Solaize France

Topic: Contribution of machine learning in atomic-scale simulations of the dehydration of Butanols catalyzed by acidic zeolites

(Funded by MAMABIO Project within PEPR B-BEST)

- o **Ferrierite catalyst** for dehydration of isobutanol (last step of biomass conversion to valuable chemical intermediates)
- o Construction of external surface models of zeolite
- o **DFT, AIMD** and **ML** force field for the computation of chemical reactions with VASP and MACE
- o Collaboration with Dr. M. Badawi (Univ Lorraine) & Dr. T. Bučko (Univ Bratislava)

02/2024 - 07/2024 _ **Intern** with Dr. Evelyne Martin
CNRS, Laboratoire ICube - UMR 7357- équipe MaCEPV, Strasbourg France

6-month internship on atomic scale simulation of exciton dynamics in organic materials for photovoltaic applications - *DFT* (ROKS) and *Car-Parinello Molecular Dynamics*

04/2023 - 08/2023 _ **Intern** in the AI & Quantum Lab team
Merck KGaA, Darmstadt Germany, Allemagne

4-month internship. Bibliographic study on the implementation of *Transfer Learning* in the tool BayBE designed by Merck to perform *Bayesian Optimization* for chemical reaction optimization. Collaborative coding with *git*.

EDUCATION

Since 11/2024 _ **PhD ED Chimie Lyon - ENS Lyon**

2021-2024 _ **Ingénieure Chimiste** (Master's Degree in Chemistry)
ECPM : Ecole européenne d'ingénieurs en Chimie, Polymères et Matériaux, Strasbourg France

- o Studied organic chemistry, analytical chemistry, materials and polymers
- o Group projects in close contact with industry (PRYSMIAN Group and TotalEnergies)
- o Specialization in the use of **AI in chemistry**
- o Specialization in chemistry of **functional materials** and **nanoscience**

2019-2021 _ **CPGE PC*** (pre-engineering undergraduate studies)
Lycée St-Louis, Paris 6ème France

- o Preparation for entrance exams to French engineering school
- o Acquired extensive knowledge in physics, chemistry and mathematics

Skills

Materials Chemistry

- * Quantum mechanics and statistical physics for electronic structure calculation
- * Studied innovative materials used in healthcare, energy solutions and environment
- * Properties, synthesis and characterization of (nano)materials, thin layers and semi-conductors (organic and inorganic)

AI and Computational tools

- * Ab Initio Molecular Dynamics and DFT using VASP, ASE or CPMD
- * High Performance Computing with supercomputers
- * Python programming
- * Basis of data science and machine learning

EMELINE SOLA

Contact

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Languages

🇫🇷 **French**

Native language

🇬🇧 **English**

C1 level

TOEIC: 985/990

🇩🇪 **German**

B1 level

🇪🇸 **Spanish**

B1 level

Interests

Mountain

Rock-climbing, Bouldering
Hiking and Ski

Environment

Contributing to the transition
towards sustainability

Reading Novels

Musique