

# Loris GELIN

Nationality : French

Born in 19/07/1995

Address : 8 rue Callisto, 25300 Doubs

Driving Licence : Category B

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With a PhD in molecular modeling, I have transitioned to the field of data science and machine learning algorithms.

## Competency

### Molecular Modelling software:

Linux, Python  
Gaussian16 (DFT),  
ChemCraft,  
ChemDraw, COPASI  
MestreNova

### Data Scientist / ML software :

PyTorch,  
Scikit-Learn, Numpy,  
Pandas, Spark,  
Matplotlib, Seaborn  
RDkit, Git, GitHub  
SQL, Power BI,  
SAP ERP

## Languages

English : Fluent

Spanish : Intermediate

French : Native

## Work Experiences

- **Doctorat (2020-2023)** Burgundy Institute of molecular chemistry (ICMUB - UMR6302) – Pr P. FLEURAT-LESSARD et Dr J. ROGER.

### Skill acquired :

- Total autonomy in my research work (DFT calculations, organic and inorganic synthesis, characterisation)
- Project Management, Communication, Adaptability
- Proficient in High Performance Computing (Python, Linux)

- **Student employee** Temporary assignments, Construction industry, Food delivery

## Formation - Data Scientist / Machine Learning Engineer

- **Python for Data Analysis** : Analyzing of various Datasets
- **Machine Learning** : Implementing machine learning algorithms in various fields
- **Deep Learning** : Implementing deep learning algorithms (GNN networks) in the field of chemistry
- **Data Visualization** : Proficient in using visualization libraries to graphically represent data (Matplotlib, Seaborn). Experienced in using business intelligence tools to create interactive dashboards (Power BI)
- **Database with SQL** : Manipulating relational databases containing several million records (Leash competition)

## Education - Chemistry

### University of Burgundy

#### Master of molecular chemistry, T2MC : Transition Metals in Molecular Chemistry

M2 (2018-2019) : 13,9/20 – (Grading : 2<sup>nd</sup>/15)

M1 (2017-2018) : 13,6/20 – (Grading : 1<sup>st</sup>/11)

### University of Burgundy

#### 3<sup>rd</sup> bachelor degree of Science, Technology and Health degree in Chemistry

L3 (2016-2018) : 11,7/20

### University of Burgundy

#### 1<sup>st</sup> and 2<sup>nd</sup> bachelor degree of Life, Earth and Environmental Sciences Parcours

#### Chemistry-Biochemistry

L2 (2015-2016) : 10,4/20

L1 (2014-2015) : 10,3/20

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## Publications

1. Experimental and theoretical study of s-tetrazine mono-ortho-metallation catalyzed by iridium and rhodium. O. Adibi, L. Gelin, G. Divoux, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard, J. Roger, in preparation.
2. Theoretical and experimental comparison of s-tetrazine mono and di-ortho-metallation catalyzed by iridium and rhodium. L. Gelin, O. Adibi, H. Cattey, J.-C. Hierso, J. Roger, P. Fleurat-Lessard, in preparation.
3. Palladium catalyzed C5-arylation of 1,3,4-oxadiazole derivated. L. Gelin, H. Sabadin, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard, J. Roger.
4. Experimental and theoretical study of Palladacycle of s-tetrazine and oxadiazole. L. Gelin, O. Aroule, I. Tolbatov, C. Testa, F. Akhssas, P. Ghesquierre, M. Ponce Vargas, H. Cattey, J.-C. Hierso, J. Roger, P. Fleurat-Lessard, in preparation.

## Communication

- 1) **C.O.** Meeting of theoretical chemists from the Grand-Est region (RCTGE) – Dijon, 2-3 Juin, 2022
- 2) **C.A.** GreenCat 2020 –Rennes, March 30-April 2 , 2020

## Teaching and Supervision

- 20 hours, student's professional project, 2022, 1<sup>st</sup> bachelor degree level, University of Burgundy
- Supervision of two students on work experience. (15 days), Licence 3<sup>rd</sup> bachelor degree of chemistry, University of Burgundy.