Aria Gheeraert

89 rue Sommeiller
73000, Chambéry, France
+33 (0) 6 04 03 15 96
aria.gheeraert@ens-lyon.fr

Education

September 2019 – Current **PhD in Applied Mathematics**, *Université Savoie-Mont Blanc*, Le Bourget-du-Lac, France.
under the supervisition of Laurent Vuillon
"A multidisciplinary approach to study protein dynamics and signaling." Application of graph theory and machine learning to the study of biological systems.

2018 – 2019 **Long Research Plan**, *École normale supérieure de Lyon*, Lyon, France.
1 year of research internships and 200 hours of courses to prepare to the academic world.
Courses : History of Sciences, Scientific Integrity

2017 – 2018 **Master 2 *Computational Sciences* – Chemistry major**, *École normale supérieure de Lyon*, Lyon, France.
MSc in Chemistry.
1st semester : Computational statistical physics, Density Functional Theory, Quantum approach to catalytic reactivity (with practical coursework on modeling)

2016 – 2017 **Master 1 *Sciences de la Matière* – Chemistry major**, *École normale supérieure de Lyon*, Lyon, France.
1st semester : Orbital Chemistry (with practical coursework on modeling), Spectroscopies
2nd semester : Theoretical Chemistry, Theoretical Photochemistry (with practical coursework on modeling)

2015 – 2016 **Licence *Sciences de la Matière* – Chemistry major**, *École normale supérieure de Lyon*, Lyon, France.
Three-year university degree in science.
1st semester : Mathematical tools, Computational tools and programming, Mathematical methods
2nd semester : First statistical approach to physics and chemistry, Mathematical methods, Introduction to digital methods, Group theory and spectroscopies

2013 – 2015 **Classe préparatoire aux grandes écoles**, *Lycée Montaigne*, Bordeaux, France.
Two-year undergraduate courses to prepare for nationwide competitive exams in sciences.
Ranked 121th in the École normale supérieure de Lyon's entrance exam

2013 **Baccalauréat scientifique**, *Lycée Gustave Courbet*, Belfort, France.
High-school degree.

Experience

March 2019 – July 2019 **22-week research internship**, *Université de Nantes*, Nantes, France.
under the supervisition of Denis Jacquemin and Adèle Laurent
"Characterization and design of Donor Acceptor Stenhouse Adducts."
Bibliographic study of the subject, study of the systems using gaussian and turbomole.

September 2018 – February 2019 **22-week research internship**, *E.N.S de Lyon*, Lyon, France.
under the supervisition of Ivan Rivalta and Claire Lesieur
"Graph theory and machine learning approaches to the study of allosteric mechanisms."
Bibliographic study of the subject, developed graph theory analysis algorithms using the package networkx, developed machine learning algorithms using scikit learn, wrote shell scripts in bash.

February 2018 – July 2018 **22-week research internship**, *Concordia University*, Montreal, Canada.
under the supervisition of Guillaume Lamoureux
"Application of deep learning techniques to the modeling of biomolecular interactions"
Bibliographic study of the subject, drafted a 20-page bibliographic report, developed deep-learning algorithms using the Pytorch framework, wrote shell scripts in bash, used the frequency analysis softwares hhmer and hh-suite, and drafted a 30-page internship report.

Summer 2017 **12-week research internship**, *ENS de Lyon*, Lyon, France.
under the supervisition of Tangui le Bahers
"Modeling the photochromism of S-Doped sodalites using DFT, TD-DFT methods"
Bibliographic study of the subject, study of the systems using Gaussian and Crystal14, analysis of data, wrote shell scripts in bash, and drafted a 20-page internship report.

Summer 2016 **7-week research internship**, *IRCELyon (Institut de Recherches sur la Catalyse et l'Environement), Université Claude Bernard Lyon 1*, Lyon, France.
under the supervisition of Stéphane Loridant
"Synthesis of gold nanoparticles"
Bibliographic study of the subject, synthesis of nanoparticles, analysis of data, Raman spectrometry, and drafted a 20-page internship report.

Scientific Activities

Talks

January 2019 **Graph theory approaches to the study of an allosteric mechanism**, *E.N.S de Lyon*, Lyon, France.
Group talk

December 2018 **Allosteric pathways in imidazole glycerol phosphate synthase**, *Université Lyon 1*, Lyon, France.
Group talk

Publications

31 March 2020 Pauline Colinet, Aria Gheeraert, Antton Curutchet et Tangui Le Bahers. « On the Spectroscopic Modelling of Localized Defects in Sodalites by TD-DFT ». In : *J. Phys. Chem. C* (2020)

3 April 2019 Aria Gheeraert, Lorenza Pacini, Victor Batista, Laurent Vuillon, Claire Lesieur et Ivan Rivalta. « Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks ». In : *J. Phys. Chem. B* (2019)

Fellowships

December 2019 **Federation of European Biochemical Societies Short-Term Fellowship**, Competitive European fellowship awarded for a 2-month stay in Italy.

Technical skills

OS Debian-based Linux, macOS.
Text editors Proficient with vi, VSCode.
Typesetting Proficient with LaTeX and HTML.
Programming Proficient with Python and Bash.

Languages

French Native speaker.
English Advanced level – *Cambridge English Advanced : CAE* C1 level certificate.
German Intermediate level.
Italian Beginner level.

Interests and activities

- Treasurer of the E.N.S de Lyon queer association.

- Technical director of the Kantor theater in Lyon.
- Martial arts (judo, budo, taijutsu, ninjutsu) and greco-roman wrestling.