

Line MOUAFFAC

PHD STUDENT, PHYSICIST

69 Rue de la Tour, 75116 Paris

☎ (+33) 6-76551720 | ✉ linemouaffac28@gmail.com

Experience

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC) - SU

Paris, France

PHD STUDENT

Oct. 2022 - PRESENT

- Thesis topic consists of modeling the dynamics of complex systems using stochastic processes and machine-learned coordinates
- Designed and applied computational models to complex systems such as protein-protein interaction and nucleation
- Generated molecular dynamics simulations for barnase-barstar system

Sorbonne Université - Université Pierre et Marie Curie

Paris, France

TEACHER

Oct. 2022 - PRESENT

- Taught a programming course in C and Python for computer science bachelor students
- Administered a thermodynamics lab (TP) to physics bachelor students
- Supervised numerical physics projects of bachelor students

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M2 INTERN

Feb. 2022 - Jul. 2022

- Applied a Langevin equation framework on a benchmark system: the 2-D double potential well
- Studied the dependence of the reaction coordinate on the kinetic barrier and rate
- Developed a model that optimises the reaction coordinate-based kinetic rates using a Monte Carlo Algorithm

Education

Sorbonne Université - Université Pierre et Marie Curie

Paris, France

MASTER 2 IN MATERIALS SCIENCE AND NANO-OBJECTS - SMNO

Sep. 2021 - Sep. 2022

- High-level training on the structural and electronic properties of condensed matter and nanostructures
- 15/20 average, mention bien

Sorbonne Université - Université Pierre et Marie Curie

Paris, France

MASTER 1 IN FUNDAMENTAL PHYSICS, PARIS PHYSICS MASTER

Sep. 2020 - Sep. 2021

- Program jointly run by Sorbonne Université and Université de Paris that focuses on advanced fundamental, experimental and numerical physics

American University of Beirut (AUB)

Beirut, Lebanon

BACHELOR'S OF ENGINEERING IN MECHANICAL ENGINEERING WITH DISTINCTION

Aug. 2016 - Jun. 2020

- Graduating GPA 3.63/4, Cum Laude Distinction

Publications

2023

Line Mouaffac, Karen Palacio-Rodriguez, and Fabio Pietrucci. "Optimal reaction coordinates and kinetic rates from the projected dynamics of transition paths"

Journal of Chemical Theory and Computation

Technical Skills

Programming

C, C++, Python (PyTorch & TensorFlow), Fortran, LaTeX, MATLAB/Simulink

Computational tools

GROMACS, LAMMPS, PLUMED

High-Performance Computing

SLURM, PBS, MPI basics

Languages

English, French, Arabic

Contributions at conferences

2024

PEPR Diadem, NumPex and AI, When AI and HPC, meet Material Sciences (poster)

Paris

2024

CECAM workshop, From methods to applications: challenges and opportunities in contemporary simulations (poster)

Paris

2023

CECAM school, Enhanced sampling methods with PLUMED (flash talk)

Lausanne

2023

GDR IAMAT, Thematic school on artificial intelligence (poster)

Roscoff

2022

CECAM workshop, Chasing CVs using Machine Learning: from methods development to biophysical applications (poster)

Paris