Eddy BARRAUD
PhD. Student

Modeling Chemist

I am specialized in molecular modelling using MD, DPD, DFT and Python post-processing. I have experience in modeling proteins, complex polymers, reticulations, and characterizing soft matter, as well as determining reaction energy profiles.

Work experience

2022

Quality Engineer Internship
March –September 2022, Dassault Systèmes
6-month internship in the BIOVIA quality assessment team. Application of a generic reaction definition, originally developed for battery materials, in the simulation of polymer network formation. In collaboration with the R&D team at Cambridge.
Keywords: reactive molecular dynamics, quantum mechanics (DFT), pipeline protocols

2021

Molecular Dynamics Internship
May – August 2021, University of Namur - Belgium
4-month internship in the Structural Biological Chemistry laboratory (unamur.be/en/sci/chemistry/cbs).
Subject: Modeling the dynamics of phosphoserine phosphatase and studying the influence of the level of representation of the solvent.
Keywords: molecular dynamics, simulations, GROMACS software, Python coding, ionic interactions

Education

2025 2022

IFP Energies Nouvelles
PhD. Student
Mesoscopic modeling of ion exchange membranes for energy conversion applications.
Keywords: semi-crystalline polymers, DPD, PFAS, Python coding

2022 2020

Rennes Graduate School of Chemistry - ENSCR
Master of engineering degree in chemistry
Major: biotechnologies, specialty: numerical chemistry

2019 2017

Rennes Graduate School of Chemistry - ENSCR
Undergraduate program for specific admission to French schools of Chemistry

Volunteering

ADIFP

President of ADIFP
PhD. Sutdents association at IFPEN – Mandate 2023-2024
Events organization: professional, integration, and networking.
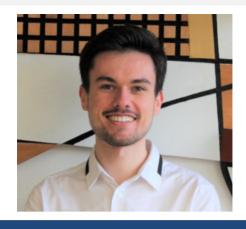
CRIPSE

Business development manager
Junior Business of ENSCR – Mandate 2020-2021
Project leadership, experiment design, team coordination.

2020

Contest CNP-CNJE
Avril 2020
National competition. Development of a chatbot on COVID-19.

Contact

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92140 Clamart, France

08/03/1999, 25 years old

Skills

Dynamic, committed, voluntary, team spirit

English : good working knowledge TOIEC : 935/990

Software : Microsoft Office, Mnova, PyMOL, VMD, Materials Studio, Pipeline Pilot

Molecular Modeling: GROMACS, SIRAH, MARTINI, CHARMM-GUI, MDTraj, Forcite, Gaussian, DMOL3, LAMMPS, DL_MESO, NEWTON

Coding: Python, Swift, PERL, R, C++

Hobbies

Swimming ● New Tech ● Video Games