Master 2 internship available

Machine learning and molecular dynamics for chemical reactivity: Application to electrocatalytic reduction of CO_2

Theoretical chemistry group (CPCV Laboratory, Ecole Normale Supérieure, Paris)

A Master 2 internship is available in the theoretical chemistry group at the Chimie Physique et Chimie du Vivant (CPCV) laboratory, located at École Normale Supérieure (ENS) in Paris.

The theoretical chemistry group at ENS develops machine learning interatomic potentials designed for accurate and efficient simulations of reactive chemical processes. Our group has introduced several advances for the optimized training of these potentials and their combination with advanced path-sampling methods. Our methods have successfully elucidated diverse aspects of key chemical mechanisms, including proton transport (Grotthuss mechanism), acid-base reactions relevant for atmospheric chemistry, and reactions of importance to prebiotic chemistry and origins of life scenarios.

This internship will apply these developments to the design of optimized catalysts for CO_2 reduction. Molecular metal-ligand complexes are promising catalysts but the elusive nature of the rate-limiting step hinders their optimization. Using a combination of machine learning simulations with fine-tuned foundation models and enhanced sampling, this project will identify the reaction mechanism for Co-phthalocyanine catalysts, determine the rate-limiting step and guide the design of improved catalysts.

This internship is part of an ANR project, and funding for its continuation as a PhD is secured.

Candidate Profile: We invite applications from master students in theoretical chemistry, condensed matter or statistical physics. Prior experience in machine learning and coding is advantageous but not mandatory.

Host laboratory: Chimie Physique et Chimie du Vivant (CPCV), ENS|PSL – Sorbonne Univ. – CNRS, Department of Chemistry, Ecole Normale Supérieure, 24 rue Lhomond, Paris, France.

Supervision: Damien Laage (DR CNRS) and Guillaume Stirnemann (DR CNRS).

Working environment: The theoretical chemistry group at ENS is internationally recognized for its multidisciplinary research, combining theoretical and computational methods (machine learning, density functional theory simulations, classical molecular dynamics), experimental collaborations (nonlinear vibrational spectroscopy, intense-field spectroscopy, chiral spectroscopy), and practical applications in environmental chemistry, catalysis, and drug design. Situated within the CPCV laboratory on the campus of Ecole Normale Supérieure, the group offers a stimulating research environment in the vibrant Latin Quarter of Paris.

Start Date: February 2026.

Application Process: Interested candidates should send a detailed CV, a motivation letter describing their research interests and in which aspects they feel most interested, and contact information for at least two references.

Contact: damien.laage@ens.psl.eu and guillaume.stirnemann@ens.psl.eu