PhD Position, start Oct. 2026

Chair "Artificial Intelligence for chemistry and by chemistry"

Automated Discovery of Homogeneous Catalysts: Automation, Active Learning, and Generative AI

CONTEXT

The AI revolution is transforming molecular sciences. An upcoming research Chair at ENS-PSL is established to accelerate the discovery of molecules, materials, and processes through modern generative and agentic AI. A central bottleneck remains the low-data regime and the poor integration of theory, simulation, and experiment. Closing this loop through automated experimentation coupled with ML represents a frontier in modern chemistry.

GOAL

This PhD project aims to develop a fully integrated, automated workflow for the optimization of a homogeneous catalyst, serving as a proof-of-concept for closed-loop, AI-guided chemical discovery for new materials design (precursors, biodegradable membranes, etc.). The project will deliver: (i) a medium-throughput experimental platform, (ii) methodology for data acquisition and standardization, and (iii) an active learning pipeline capable of guiding synthesis and testing toward optimal catalytic performance.

STRATEGY

The project is organized around three tightly coupled axes. First, it will leverage the standardization of data acquisition in the experimental groups of L. Grimaud (ENS-PSL) and C. Serre (ENS-PSL / ESPCI-PSL) to automate reaction setup, execution, and characterization. Second, it will establish standardized digital data pipelines (electronic lab notebooks, structured databases) to produce high-quality training sets. Third, it will build new methods based on data augmentation, curriculum learning, active learning or similar approaches that integrate property prediction models, diffusion-based generative models, and quantum-chemical calculations to iteratively propose and prioritize new catalyst candidates.

APPROACHES

- **Medium-throughput platform:** automation of reaction setups, inline monitoring, and product characterization for homogeneous catalysis in the Grimaud and Serre groups.
- **Data standardization:** implementation of electronic lab notebooks and structured databases to ensure FAIR data acquisition across all experiments.
- **Property prediction:** training and fine-tuning graph neural networks and transformer-based models on experimental and computational catalysis data. Use curriculum learning and data augmentation strategies to reinforce the property prediction in a low data regime.
- **Generative modelling:** use of diffusion models to propose novel catalyst structures in under-explored chemical spaces.
- **Active learning pipeline:** iterative closed-loop integration of experimental results with model predictions and DFT calculations to steer catalyst optimization.

CANDIDATE PROFILE

We are looking for a highly motivated candidate holding a Master's degree (or equivalent) in chemistry, chemical engineering, or a closely related field. A background in the field of metal complexes, coordination chemistry, and, if possible, homogenous catalysis, is an advantage. Experience with programming (Python), or machine learning is a significant asset. The candidate should have excellent communication skills in English and a genuine enthusiasm for interdisciplinary research at the interface of chemistry and AI.

RESEARCH ENVIRONMENT

The PhD student will be integrated within the Chemistry Department of ENS-PSL, one of France's leading research institutions in AI for chemistry, co-supervised by Laurence Grimaud (DR CNRS, ENS-PSL) and Christian Serre (DR CNRS, ENS-PSL, ESPCI-PSL). They will benefit from the unique ecosystem of the department and of the Chair (including a dedicated research engineer), with access to state-of-the-art synthesis and characterization platforms, characterization platforms, computational resources, and close interactions with the chair's theory and ML teams (D. Laage, G. Stirnemann, R. Vuilleumier). The position is fully funded for 3 years, starting Oct. 2026.

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