PhD position at PSL University

Active learning to accelerate discovery of multi-variate MOFs

Start date: 1st October 2025
Applications will be reviewed on a rolling basis

Project description

We propose a new data-driven approach for optimizing the synthesis of multivariate metal-organic frameworks (MOFs) using **active learning methods to drive high-throughput robotic synthesis**. Traditional MOF discovery methods rely on serendipity, with computational screening unable to predict synthesizability or control synthesis conditions. By integrating experimental data acquisition with machine learning, the project aims to systematically explore the effect of synthesis parameters and help shorten the MOF discovery loop. Bayesian optimization will guide experiment selection, minimizing costs and maximizing insights.

We will develop this methodology on a specific family of materials: multivariate MOFs. Mixed-ligand or mixed-metal MOFs can offer enhanced adsorption and catalytic activity over their parent compounds, but are difficult to characterize due to their structural complexity. The study is divided into three phases: (1) optimizing MOF synthesis on a single Zn-based MOF, (2) controlling polymorphism in mixed-linker Zn-based MOFs, and (3) extending methods to heterometallic MOFs for improved CO_2 adsorption.

Focusing on machine learning-driven optimization, this research will leverage existing infrastructure and collaboration, ensuring feasibility within a PhD timeline. This innovative integration of active learning and robotics offers a more systematic approach to materials discovery, focusing on efficiency in terms of both data and chemicals.

Previous publications from the group on this topic:

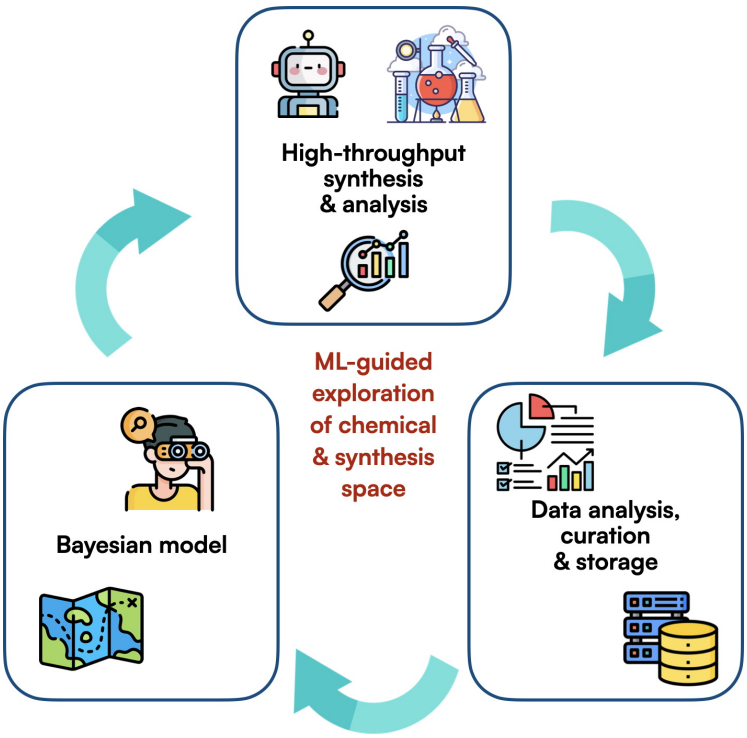
- "Multiscale Modeling of Physical Properties of Nanoporous Frameworks: Predicting Mechanical, Thermal, and Adsorption Behavior", A. Hardiagon and F.-X. Coudert, ***Acc. Chem. Res.*, 2024**, 57 (11), 1620–1632.
- "Best practices in machine learning for chemistry", N. Artrith, K. T. Butler, F.-X. Coudert, S. Han, O. Isayev, A. Jain and A. Walsh, ***Nature Chem.*, 2021**, 13 (6), 505–508
- "Machine learning approaches for the prediction of materials properties", S. Chibani and F.-X. Coudert, ***APL Mater.*, 2020**, 8 (8), 080701.
- … learn more about our research at www.coudert.name

Location. PSL University has a long tradition in teaching and research excellence. It is located in the center of Paris, at the heart of the "Quartier Latin", the lively and cultural university district.

Candidates. Applicants should have a MsC in Physics, Chemistry, or Materials Science, with an interest for computational methods. Experience with data science and/or learning methods, or molecular simulation, will be greatly appreciated.

Position details. This position will be funded jointly by the ChemAI "Grand Programme" of PSL University and the DIM MaTerRE (ongoing call). The PhD student will work at Chimie ParisTech, in the Institut de Recherche de Chimie Paris. The project is in collaboration with the group of Prof. Christian Serre (CNRS, ENS/ESPCI, PSL) for the high-throughput synthesis and characterization of materials.

Contact. **François-Xavier Coudert**, fx.coudert@chimieparistech.psl.eu
Please provide a CV detailing your training, as well as previous research experience (internships).


High-throughput synthesis & analysis
Data analysis, curation & storage
Bayesian model
ML-guided exploration of chemical & synthesis space