PhD proposal
at Chimie ParisTech / PSL University
2025 call for PR[AI]RIE-PSAI funding

Discovery of novel mechanical metamaterials using generative methods

Position details.

Start date: 1st October 2025

Supervisor: François-Xavier Coudert fx.coudert@chimieparistech.psl.eu

Research group: This project will take place in the Coudert group at Institut de Recherche de Chimie Paris. Visit https://www.coudert.name to learn more about our research activities.

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

Candidate profile. We welcome candidates with a strong data science background, who want to learn materials chemistry, as well as candidates with a chemistry or materials sciences background, who want to learn data science skills. Applications will be judged based on scholarly excellence, and experience of international mobility will be considered.

Context. This project is within the framework of the PR[AI]RIE-PSAI program of PSL University. See more at https://prairie-institute.fr

How to apply? By email to François-Xavier Coudert fx.coudert@chimieparistech.psl.eu

Please provide the following:

- CV detailing your training, as well as previous research experience (internships, projects, etc.)
- One-page motivation letter, describing the applicant's ambitions for the subject described and the relevance of the application to the subject description
- A copy of your most recent diplomas

Deadline.

Applications should be sent before May 15. Funding decisions will be made by PR[AI]RIE-PSAI in a two-stage selection procedure: first stage May 30, second stage June 15.

Non-discrimination, openness and transparency.

All PR[AI]RIE-PSAI partners are committed to supporting and promoting equality, diversity and inclusion within our communities. We encourage applications from a wide range of profiles, which we will select through an open and transparent recruitment process.

Context of the proposal.

Theoretical chemistry and materials science have benefited in recent years from the rapid development of methodologies based on large-scale data and machine learning methods: this is linked both to the increase in the size of accessible databases and computing resources, and to the availability of software libraries enabling non-experts in learning methods to tame these tools. The combination of theoretical chemistry tools (notably Density Functional Theory, DFT) with

databases of experimental structures (CSD, ICSD, etc.) has enabled major high-throughput screening studies for physical or chemical properties of interest, as well as the production of "augmented" databases of properties derived from calculations. In the field of dense inorganic materials, the Materials Project database includes 169,385 structures and their electronic properties, 13,094 material elastic tensors, and 3,322 piezoelectric property data.[1]

The Coudert group is at the forefront of this research theme: we have already published several high-throughput screening studies on different families of materials, for their physical properties, such as adsorption, molecule diffusion, thermal or mechanical properties. We are developing our own methodologies in this field, combining atomistic molecular modeling, mesoscopic approaches and learning methods.

However, despite the volume of data available, **direct screening approaches are proving limited in describing certain rare properties**, for two reasons: (i) the number of known materials exhibiting these properties is small, (ii) due to the imbalance between positive and negative cases in these datasets, training reliable machine learning models for detection is very inefficient.[2] In order to overcome this current blockage in the methodology and propose new materials with rare elastic properties (mechanical metamaterials[3]), we propose to combine the high-throughput prediction approach with the creation of new material structures, hitherto unknown and therefore with unexplored properties, by evolutionary algorithms. The aim is therefore to **introduce generative AI methods into the "loop" of new mechanical metamaterials discovery**.[4]

Scientific objectives and strategy.

The main scientific objective of the project is to add a generative aspect to high-throughput screening methods for inorganic materials, generally applied to predetermined databases. Starting from the initial database drawn from the Materials Project, we will use evolutionary algorithms to extend the list of structures considered. These new structures will be characterized by a multi-scale workflow, including (i) a fast machine learning structure/property predictor,[5] and (ii) periodic DFT calculations for the best performing materials. These steps will first be validated independently, before being integrated into a single methodology, providing the evolutionary algorithm generating the new structures with a multi-objective score function, including both compound stability and mechanical properties.

The strategy proposed for this project combines 3 axes:

1. The generation of new structures from the Materials Project database by applying evolutionary algorithms. Several options will be tested and evaluated, including the USPEX[6] and XtalOpt codes[7] — first focused on subfamilies of materials, like aluminosilicates and oxides, then expanding them more widely. The objective function at this stage will be an existing, low-computational-cost predictor of mechanical properties: the first intention is to test an optimized MLIP force field on the Materials Project database, such as MACE-MP0 (or one of its later versions).
2. These new structures will be studied in detail from an energetic and mechanical point of view, with the aid of DFT calculations using the CP2K code.[8] The data thus generated will not only enable new structures of interest to be discovered, but will also improve the performance of the ML algorithm for structure/mechanical property prediction by means of a larger and, above all, more diverse training database.[9]
3. Instead of simply "closing the loop" by iterating the process, the aim of Part 3 is more ambitious: to integrate the two previous building blocks into a single on-the-fly workflow, enabling real multi-objective optimization of structures coupled directly to generative AI.

The expected results are both methodological and physico-chemical in nature. On the first front, the PhD student will produce a robust method for generating new crystalline inorganic structures, associating them with mechanical properties by DFT calculations, and training ML prediction algorithms to apply them on a larger scale. Secondly, the results obtained will enable the publication of an open-access materials database, so that their properties can be further explored by other teams, and potential candidates synthesized by experimental teams in the medium term.

The thesis program is scientifically ambitious, as it consists in developing a modeling methodology for crystalline inorganic materials, coupled and driven by the prediction of large-scale mechanical properties. While the first aspect (prediction of new materials) is well explored in the scientific literature, coupling with mechanical properties is a major development. However, the project benefits from the team's expertise in these modeling techniques, and from the skills of the planned collaborators in aspects relating to generative methods and multi-criteria optimization of materials. We will perform this work in collaboration with the groups of Prof. Gilles Frapper (Université de Poitiers; expert in the use of evolutionary algorithms for generation of novel materials phases) and Prof. Aron Walsh (Imperial College London; expert in exploration of chemical and topological space of inorganic materials).

References

1. Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, and Kristin A. Persson, APL Mater., 2013, 1, 011002.
2. “Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning”, R. Gaillac, S. Chibani and F.-X. Coudert, Chem. Mater., 2020, 32 (6), 2653–2663.
3. “Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior”, F.-X. Coudert and J. D. Evans, Coord. Chem. Rev., 2019, 388, 48-62.
4. “Scaling deep learning for materials discovery”, A. Merchant, S. Batzner, S. S. Schoenholz, M. Aykol, G. Cheon and E. D. Cubuk, Nature, 2023, 624, 80–85.
5. “Machine learning approaches for the prediction of materials properties”, S. Chibani and F.-X. Coudert, APL Mater., 2020, 8 (8), 080701.
6. “New developments in evolutionary structure prediction algorithm USPEX”, A. O. Lyakhov, A. R. Oganov, H. T. Stokes and Q. Zhu, Comp. Phys. Comm., 2013, 184, 1172-1182.
7. “XtalOpt Version 13: Multi-Objective Evolutionary Search for Novel Functional Materials”, S. Hajinazar, E. Zurek, Computer Physics Communications, 2024, 304, 109306
8. “Systematic exploration of the mechanical properties of 13 621 inorganic compounds”, S. Chibani and F.-X. Coudert, Chem. Sci., 2019, 10 (37), 8589–8599.
9. “Neural Network-Based Interatomic Potential for the Study of Thermal and Mechanical Properties of Siliceous Zeolites”, L. Brugnoli, M. Ducamp and F.-X. Coudert, J. Phys. Chem. C, 2024, 128 (47), 20512–20522.