



Post-doctoral position available

Rational Design of Framework Materials with Tailored Mechanical and Thermal Properties: A Combined Physics/Chemistry Approach

Project

Crystalline materials with anomalous mechanical and thermal properties, such as negative linear compressibility, negative Poisson's ratio, or negative thermal expansion, are highly desirable for applications but relatively rare. They are more common among nanoporous framework materials (metal-organic frameworks, molecular frameworks, and others) than in dense inorganic materials, yet the relative roles of chemistry, geometry and topology on these properties have not been fully understood.

The project of the post-doc will be to develop and use simulation techniques from the fields of computational chemistry and physics to guide the design of new framework materials with tailored mechanical and thermal properties. This will combine at multiple scales of modeling: quantum chemistry calculations (typically Density Functional Theory) of structures and their elastic behavior, classical force field-based molecular dynamics simulations at varying temperature/pressure, and finite element-based mechanical models of the frameworks. These modeling approaches, along with statistical physics models of the (pressure, temperature) phase diagrams of the materials, will allow us to understand and predict the occurrence of anomalous mechanical and thermal behavior in framework materials.

Location

PSL Research 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. The project is part of a collaboration between Chimie ParisTech, a major French and internationally recognized college of Chemical Engineering, and the Physics Department of the École Normale Supérieure (ENS).

Candidates

Applicants should have a PhD in Physics, Chemistry, or Materials Science with experience in molecular modeling or numerical statistical physics. A passion for statistical physics will be a serious asset!

Position details

The position is part of a collaboration between **François-Xavier Coudert** and **Lydéric Bocquet**. The post-doctoral researcher will work at Chimie ParisTech, in the Theoretical Chemistry and Modeling group. The position is for 12 months, with a possibility to continue in the group on related projects. The monthly net salary is 1800–2000 € (depending on experience).

Contact

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Please provide a CV, list of publications, and the name of two referees you worked with.