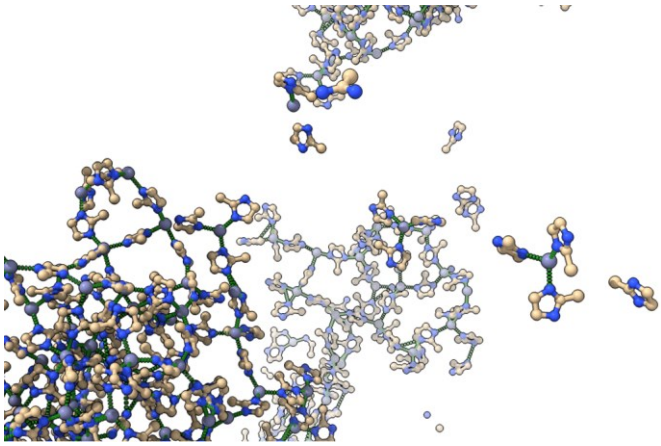
FULLY FUNDED PHD POSITION

Decoding the Mechanisms Underlying Metal-Organic Frameworks Self-Assembly

The Project: Metal-Organic Frameworks (MOFs) are porous materials with many societally relevant potential applications, such as carbon capture, removal of environmental toxins and drug-delivery. Despite the progress in the field, synthesizing a MOF currently requires tens to hundreds costly and time-consuming trial-and-error synthesis experiments because our ability to correlate the synthesis conditions with the desired MOF structure is very limited. To overcome this, we need to decode the mechanisms underlying MOF self-assembly, a highly complex non-equilibrium process covering a wide range of time- and length-scales, from the formation of the building units to nucleation and growth.

The PhD candidate recruited will work as part of a team of researchers in the development and application of a multi-scale computational methodology[1-3] to decode the mechanisms underlying MOF self-assembly and predict synthesis conditions-structure (topology, defects) relationships within the MAGNIFY project, funded by the European Research Council. He or she will gain expertise in multi-scale molecular dynamics simulations, enhanced sampling techniques and application of machine-learning techniques to analyse simulation data, all applied to a challenging and exciting fundamental chemistry problem.



[1] Computer Simulation of the Early Stages of Self-Assembly and Thermal Decomposition of ZIF-8; S. R. G. Balestra, R. Semino; J. Chem. Phys, 157, 184502 (2022)
[2] Force Matching and Iterative Boltzmann Inversion Coarse Grained Force Fields for ZIF-8, https://arxiv.org/abs/2312.05192
[3] Microscopic Mechanism of the Thermal Amorphization of ZIF-4 and Melting of ZIF-zni Revealed via Molecular Dynamics and Machine Learning Techniques, https://arxiv.org/abs/2311.16351

About us: the project will be carried out at Sorbonne Université, within the PHENIX laboratory. Many conferences and workshops are held on campus, as we are a CECAM node. We work in a supportive and vibrant environment, we value teamwork and diversity and we actively help promote the career of our PhDs and postdocs.

Candidate profile and application: We are looking for a motivated candidate with a degree in Chemistry, Physics or Materials Science or an engineer degree in these disciplines, programming skills (c/c++, FORTRAN or python) and/or knowledge in the field of molecular modelling (molecular dynamics). Experience in the use of enhanced sampling methods, coarse-graining methodologies or hybrid simulations would be considered a plus. A good level of English is also required. To apply, please send us a CV, a short letter explaining why you would like to join us, a document stating your master and licence qualifications and one or two reference persons (master professor or master supervisor) that we can contact. The initial deadline for the application is February 29th 2024.

Period: October 2024 – September 2027 (the duration of a PhD in France is 3 years). The starting date can be postponed for a few months if needed.

Contact & more information: rocio.semino@sorbonne-universite.fr, www.rociosemino.com

Sorbonne University is a world-class, research-intensive university bringing together a broad range of arts, humanities, social sciences, natural sciences, engineering and medicine. The scientific Pierre and Marie Curie campus was completely refurbished in 2016.

PHENIX is a laboratory at the interface between Chemistry, Physics and Materials Science with a long-standing expertise of colloidal systems, electrolytes and fluids under confinement. Its strength lies in a combination of experimental and modelling activities (numerical simulations). Several international projects and networks are in place in PHENIX, providing a rich and multinational environment.