FULLY FUNDED POSTDOC 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 postdoctoral researcher recruited will work as part of a team of researchers in the development 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 analyze simulation data, all applied to a challenging and exciting fundamental chemistry problem.


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 strong background in chemical physics, statistical mechanics and skills in programming and molecular modelling (atomistic molecular dynamics). Preference will be given to candidates with experience in enhanced sampling methods (metadynamics ideally) or coarse graining method development, hybrid atomistic / coarse graining approaches and/or modelling self-assembly phenomena or reactive processes in solution. A good level of English is also required. To apply, please send us a CV including the names and emails of two referees that we can contact and a short letter explaining why you would like to join us. The starting date can be negotiated from October 2024 onward (2025 is also possible). The contract will be for 18 months with possibility to extend it upon mutual agreement.

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.