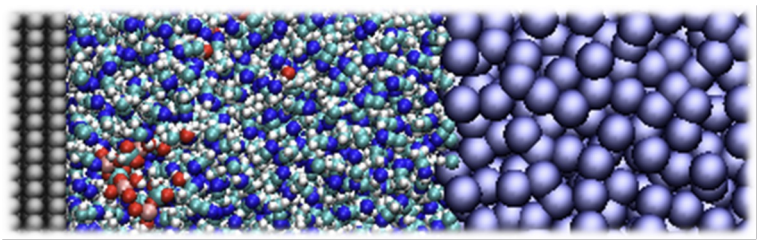
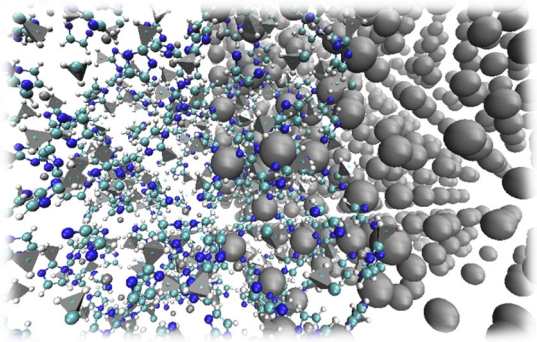
FULLY FUNDED PHD POSITION

Development and implementation of hybrid atomistic/coarse grained modelling applied to the interfaces

Understanding interfaces at the molecular scale is fundamental for the development and optimisation of the performance of composite materials used for energy storage and CO_2 capture. However, the experimental study of processes at interfaces remains a challenge to date. To study the structure and dynamics at the interfaces of these complex materials, it is necessary to be able to simulate longer time and space scales than those accessible to classical atomistic modelling techniques. The objective of this thesis is to develop and implement dual resolution classical methods to enable such simulations. In this family of methods,[1] all-atom and coarse grained (atoms grouped into superatoms) modelling are combined in the same simulation box as shown in the figure. The interface is treated with atomistic resolution, while the rest of the system is described by coarse grained models. This method will be applied to study the interfaces between an electrolyte and a solid electrode in the case of electrochemical systems, and those present in systems formed by the association of nanoparticles of porous hybrid materials and a polymer matrix.

The PhD candidate recruited will work as part of a team of researchers in the development and application of simulation methods applied to modelling interfaces. He or she will gain expertise in multi-scale molecular dynamics simulations, interface modelling and code development.





[1] M. Praprotnik, R. Cortes-Huerto, R. Potestio and L. Delle Site, Adaptive Resolution Molecular Dynamics Technique, Springer International Publishing, 2020, pp. 1443-1457

Candidate profile: We are looking for a motivated candidate with programming skills (c/c++, FORTRAN or python) and/or knowledge in the field of molecular modelling (molecular dynamics). He or she must have a master degree in Chemistry, Physics or Materials Science or an engineering degree in these disciplines. A good level of English, spoken and written, is also required.

How to apply: 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 May 10th 2023.

Period: October 2023 – September 2026. The PhD will take place in the PHENIX laboratory, located on the Pierre et Marie Curie Campus of Sorbonne Université.

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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.