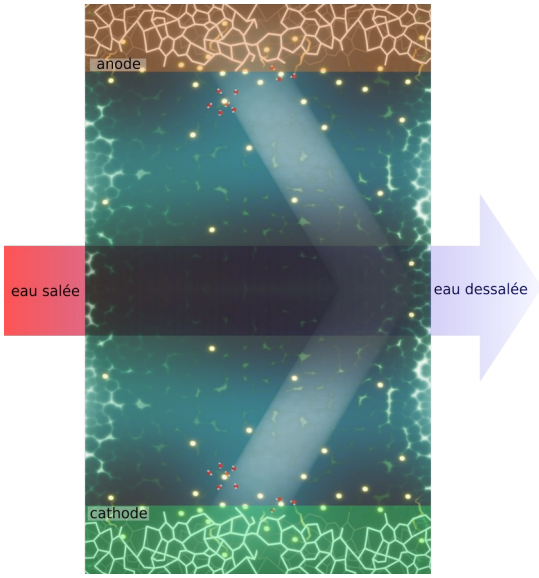
18 months Postdoctoral Position in Statistical Physics and Molecular Dynamics Simulations in France

Are you a highly motivated and talented young researcher with a strong background in statistical physics and molecular dynamics simulations? Join our international research team at the Laboratory of Mechanics and Civil Engineering (LMGC) at the University of Montpellier, France.

The successful candidate will work in a group with highly prolific environment on an exciting project that aims to advance our understanding of capacitive systems for water desalination using atomistic simulations. Capacitive systems are an essential component of modern water treatment technology, and their performance relies on a fundamental understanding of the mechanisms that govern the adsorption of ions at the electrode-electrolyte interface.



The project is based on our recent paper published in PNAS (doi.org/10.1073/pnas.2121945119) in which we developed an approach to simulate the adsorption of ions in carbon electrodes by considering the effect of defects. Ions adsorbed during desalination can also be considered as defects and we need to understand how they will affect the adsorption of other salt ions. The project will involve the simulation of the dynamics of ionic adsorption and desorption in capacitive electrodes under various conditions (pH, ionic concentration, water flux, cycling, etc.) using classical molecular dynamics under voltage. The successful candidate will work closely with our collaborators at INRAE, who will perform complementary experiments to validate and compare our simulation results.

The ideal candidate should have a Ph.D. in physics, chemistry, or a related field, with a strong background in statistical physics and molecular dynamics simulations. Experience with classical force-fields or *ab-initio* approaches for simulating diffusion processes, or electrochemical systems and/or adsorption phenomena is highly desirable. Strong programming skills in C++, Fortran, or Python, knowledge on parallel computing and communication skills are also desirable.

Our research team PMMD is highly international and has collaborations with multiple groups (EPIDAPO, INRAE, CEA, IEM, etc.), including on the simulation of ionic transport. The successful candidate will have the opportunity to participate in these collaborative projects and contribute to the development of cutting-edge simulation tools for studying complex systems. She/He will have the opportunity to work closely and develop her/his management skills with a newly hired Ph.D. student that will join our group this year and work on the same materials.

This is a full-time position for 18 months, the position is available immediately. To apply, please submit a cover letter, CV, and contact information for references to Dr. Romain Dupuis at romain.dupuis@umontpellier.fr. Applications will be reviewed on a rolling basis until the position is filled.