PhD Position in Molecular Dynamics for Materials Science available in France

We are seeking a highly motivated and talented PhD candidate with a strong background in computational materials science and molecular dynamics simulations to join our group Physique et Mécanique des Milieux Divisés at the Laboratory of Mechanics and Civil Engineering (LMGC) at the University of Montpellier in France.

The successful candidate will work in a highly prolific environment on an exciting project that aims to advance our understanding of the formation capacitive electrodes via pyrolysis of biomass and of the adsorption of ions in capacitive electrodes.
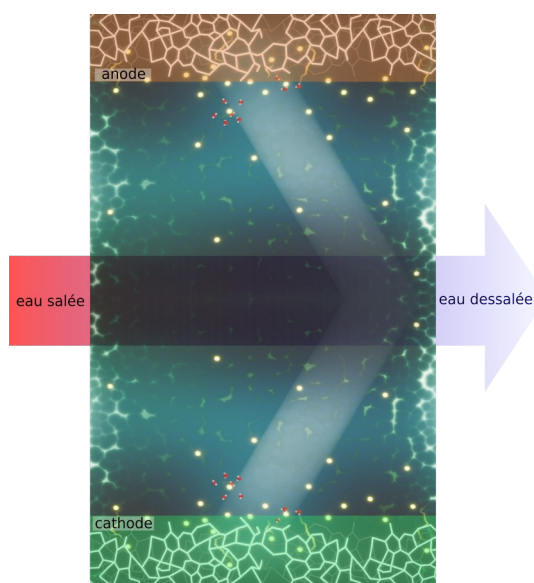
The PhD project will involve the development and implementation of new simulation algorithms to investigate various conditions (temperature, heating rate, microstructure, etc.) and study performance of carbon electrodes. The successful candidate will work closely with our postdoctoral researcher who is going to simulate the diffusion of ions in electrodes and compare with simulation results obtain with our experimental colleagues at INRAE.

The ideal candidate should be fluent in English, have a master's degree in materials science, statistical physics, or a related field, with a strong background in computational materials science and molecular dynamics simulations. Experience with classical force-fields or ab-initio approaches for simulating materials synthesis or processing is desirable. Programming skills in C++, Fortran, or Python, knowledge of parallel computing are also useful.

Our research team at the LMGC is highly international and has worked on different topics related to materials science, including the simulation of ionic transport in capacitive systems. 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.

This is a full-time PhD position for three years to start in October 2023. To apply, please submit a cover letter, CV, and contact information for references to Katerina Ioannidou at aikaterini.ioannidou@umontpellier.fr or Romain Dupuis at romain.dupuis@umontpellier.fr. Applications will be reviewed on a rolling basis until the position is filled.