Sujet de stage de Master 2 (2023) proposé par l'équipe PMMD du LMGC

Molecular Simulations of super-capacitor electrodes

Context

The increasing energy demand in today's society is one of the most challenging problem. Due to population growth, the world will need significantly increased energy supply in the future, especially clean electricity generated from renewable sources. The intermittent nature of solar and wind require efficient and sustainable energy storage. Most electrochemical energy storage devices such as suparcapacitors and batteries utilise porous carbon based electrodes. A limiting factor of the long-term performance of carbon electrodes is ageing due to physical or chemical process. Insufficient knowledge on the charging and discharging mechanism at the atomistic scale hinders the design of efficient devices.

This project aims to study the *relationship between the microstructure of carbon electrodes and the adsorption of electrolyte under polarization* by molecular dynamics. The starting point of this work is a recently simulation study [Dupuis et al, PNAS 2022], proposing a charging scheme for carbon electrodes based on the topological defects of the carbon texture. We will develop and use codes to analyse water and ion dynamics near and within carbon electrodes to explore and understand the sorption mechanisms.

Methodology

The study of electrodes will be based in Molecular Dynamics simulations. The simulations will be performed using the LAMMPS code in the cluster of UM.

Host laboratory

This Master internship will take place at the Laboratoire de Mécanique et Génie Civil (LMGC) in Montpellier. It may be followed by a PhD thesis.

Contact

Please send your CV and your motivation letter to:
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Research profile

Master of physics, physical chemistry or mechanics, and strong interest in numerical simulations. The successful candidate for this project must have knowledge in Statistical Physics of Condensed Matter and be familiar with related numerical methods (Molecular Dynamics and Monte-Carlo techniques). Ability in coding will be strong advantage and a sufficient command of English will be a plus.