INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: LPENS
CNRS identification code: UMR8023
Internship director'surname: Saitta, A. Marco
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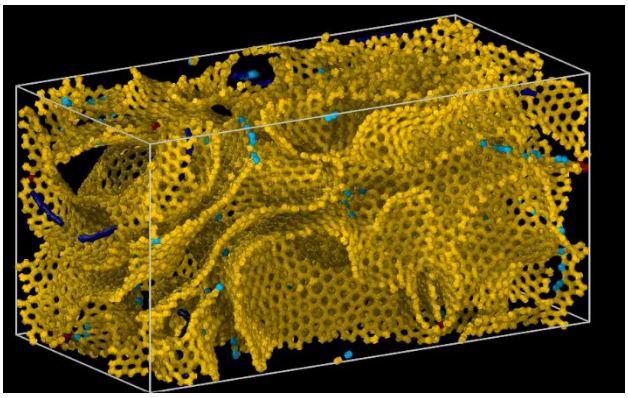
Web page:
Internship location: LPENS – 24 rue Lhomond 75005 Paris

Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: PEPR DIADEM/ED397/NTU Singapore

AI-driven electronic response of nanoporous carbon electrodes in molecular dynamics simulations of supercapacitors

The internship will focus on the AI-driven design of high-performance nanoporous carbon electrodes for supercapacitors, a central challenge for next-generation electrochemical energy storage. While state-of-the-art simulations typically treat electrodes as rigid, recent work has shown that electrode flexibility profoundly impacts charging kinetics and ion dynamics. However, this should impact the local electronic response by the carbon surface, which is accounted in a uniform way in current constant potential models. In this work we would like to leverage a new approach based on the machine learning of the electron density by applying it to realistic disordered carbons. This would enable large-scale molecular dynamics simulations with an electrode response to ion adsorption at near ab initio accuracy. By systematically exploring the role of pore size distribution, sp^2/sp^3 content, and mechanical compliance, the student will identify structural motifs that maximize both power and energy density. The work will be carried out in close collaboration with colleagues at NTU Singapore and CNRS@CREATE, within the framework of the PEPR DIADEM programme, ensuring strong international and national visibility. This internship is designed as the first stage of a PhD thesis, where the methodology will be extended to other electrode materials.



Techniques/methods in use: Ab initio/Density Functional Theory, Machine learning of the electronic density, molecular dynamics

Applicant skills: solid formation in quantum and statistical physics, familiarity with python and computer skills in general

Foreign partnership: Shuzhou LI (Materials Science), Mathieu SALANNE (CNRS@CREATE), NTU Singapore

Internship supervisor(s): A. Marco SAITTA, marco.saitta@sorbonne-universite.fr, Andrea GRISAFI (PHENIX), andrea.grisafi@sorbonne-universite.fr

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: YES
Quantum Physics: YES Theoretical Physics: YES