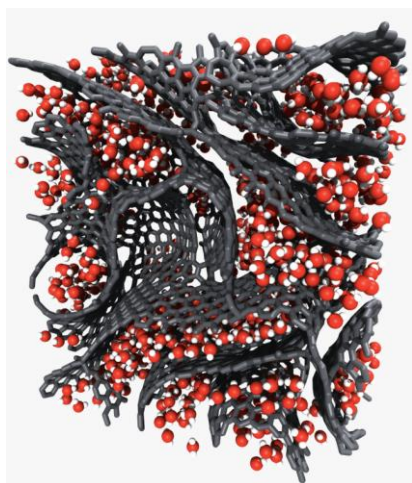


Title: Machine-learning-enabled quantum friction of water: from carbon nanotubes to nanoporous disordered carbons

Keywords: Machine learning, nanofluidics, quantum friction, nanoporous carbons, molecular dynamics (MD), interfacial transport, statistical mechanics, structure–property relationships

Scientific description: Water transport through carbon nanochannels can exhibit exceptionally low friction, yet experiments reveal strong dependences on nanotube radius, confinement and electronic properties that are not reproduced by conventional molecular dynamics. A promising explanation is quantum friction, where charge fluctuations in water exchange momentum with electronic excitations in the carbon surface.



Recent classical models using polarizable Drude oscillators have reproduced key signatures of this mechanism, suggesting that the dynamical response of the solid plays an important role in nanoscale friction.

This Master project will extend this framework from graphene to carbon nanotubes and realistic nanoporous carbons. Using molecular dynamics, the student will compare non-polarizable, metallic constant-potential and Drude-polarizable descriptions of the carbon wall to disentangle the effects of roughness, curvature, confinement and electronic response. Simulations of nanotubes with different radii will establish how confinement modifies the coupling between water dynamics and the carbon substrate.

The approach will then be transferred to realistic templated nanoporous carbons with controlled pore size and disorder, designed in our group in a previous thesis [1]. Friction and permeability will be related to structural descriptors such as pore size, curvature and defect density, as well as to the electronic response of the carbon framework. Machine-learning analysis of the simulation database will identify the descriptors that best predict nanofluidic transport, providing a route toward AI-assisted design of carbon materials with optimized water-transport properties.

Techniques/methods in use: Ab initio and classical MD, Green–Kubo and non-equilibrium transport calculations; constant-potential and Drude-polarizable models, statistical mechanics

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

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

Internship supervisor(s): A. Marco SAITTA, marco.saitta@phys.ens.fr, 06.66.04.14.16

Internship location: LPENS – Campus Ulm – Ecole Normale Supérieure – 24 rue Lhomond Paris

Possibility for a Doctoral thesis: Y

[1] Z. Waysenson, A. France-Lanord, P. Simon, M. Salanne, A. M. Saitta, “Soft-Templated Carbon Models Elucidate the Anomalous Increase of Capacitance in Nanopores,” ACS Nano (2026). DOI: 10.1021/acsnano.6c11953.