Master's Thesis Physical Chemistry • From Jan/Feb 2023

Groups of Damien Laage and Guillaume Stirnemann, CNRS, École normale supérieure and Institut de Biologie Physico-Chimique, Paris, France

How does local dynamics at the interface influence transport properties in nanoconfined environments?

Subject Water flow in nanometer-size confinement occurs in a variety of biological, geological and technological contexts. As opposed to macroscopic hydrodynamic motions, which are mostly sensitive to the geometry of the confining medium and to the viscosity of the fluid, nanoscopic flows very much depend on the chemical nature of the confining interfaces. This is both because the surface:volume ratio increases significantly, and because the molecular interactions between the fluid molecules and the interface become important for the transport properties of the liquid. However, the link between these interactions (and how they influence the local reorientation and diffusion dynamics of water) and the more traditional hydrodynamic descriptions of the liquid flow remains unclear.

Building up on previous work in our groups focusing on the water local dynamics next to solutes and interfaces, the goal of this internship is to use a combination of equilibrium and non-equilibirum molecular dynamics simulations to understand the molecular origins for the water flow characteristics in nanotubes of varying size and chemistries. The candidate will first perform molecular dynamics simulations of liquid flow within channels of varying structure and chemical nature. He/she will then calculate both mesoscopic hydrodynamic quantities including the slip length, and molecular-level features of the interface, including the local arrangement of interfacial water molecules and their translation and reorientation dynamics. Finally, a physical model will be developed to connect these mesoscopic and microscopic descriptions, in order to relate the local dynamics to the flow properties, with predictive abilities regarding the dependence upon the chemical properties of the interface.

Techniques/Methods The candidate will gain strong experience in molecular dynamics simulations (no previous experience is required), using a well-employed and distributed code, as well as advanced techniques to generate non-equilibrium simulations under flow. In-house analysis codes will be adapted and then used. Tools: Molecular dynamics simulations; programming and simulation analysis tools.

Research environment Research will take place in the lab of Theoretical Biochemistry of the CNRS Institute of Physical and Chemical Biology with Guillaume Stirnemann, and in the Chemistry Department of the École Normale Supérieure. Both labs are located in the very stimulating research environment of the Latin Quarter, at the heart of Paris. Our groups have extensive experience in applying advanced simulation and theoretical tools to tackle a variety of questions, ranging from water ultrafast dynamics in aqueous solutions to reactivity in biomolecular environments. We have access to state-of-the-art computing facilities that include local mesoscale computer clusters. More information about the groups: www.chimie.ens.fr/recherche/laboratoire-pasteur/chimie-theorique/ www-lbt.ibpc.fr/people/stirnemann.

Extension into a PhD may be considered upon mutual agreement of the candidate and the supervisors and if funding can be secured.

Contact information Interested candidates should contact Damien Laage (damien.laage@ens.psl.eu) and Guillaume Stirnemann **as soon as possible** (stirnemann@ibpc.fr), together with a curriculum vitae and contact information for one or two references.