Master 2 internship; Net salary: ~ 450 euros/months

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Achieving very large slip at solid / supercooled water interfaces

Understanding the hydrodynamics of water at the nanoscale is important for many applications including lubrication, transport of biomolecules and energy harvesting devices. A quantity of prime importance in nanoscale friction is the so-called slip length (see Fig. 1), which depends on the wetting properties of the interface, and which together with water viscosity controls the flow rate of nanoconfined water. While the slip length has been characterized both experimentally and in molecular dynamics simulations at room temperature, less is known when liquid water becomes supercooled. Indeed, water may be maintained in a metastable liquid state down to 30 K below its melting point. Very recently, experimentalists at the ILM have measured the shear viscosity of supercooled water down to 240 K, and molecular dynamics simulations performed in our group have shown good agreement with the experimental results [1]. The goal of this internship is to extend these calculations to probe friction and the slip length for supercooled water.

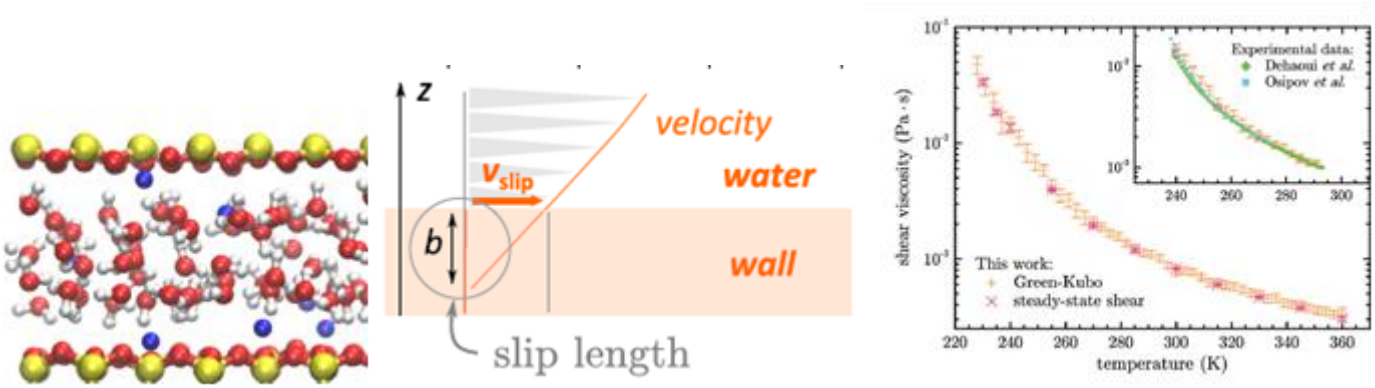

Fig. 1: Ilustration of nanoconfined water dynamics; slip length; shear viscosity of supercooled water compared to experimental data (@ILM), from [1].

The student will employ molecular dynamics (MD) simulations to probe the friction coefficient and slip length of supercooled water/solid interfaces. Depending on the student taste, the interfaces between water and carbon nanotubes or graphene may be considered as well. Additional local structural information will be computed to interpret the MD results.

The successful candidate should hold a Master degree in Physics, Chemistry or Material Science. He/she should have a taste for theoretical modelling, good knowledge of basic programming. The successful candidate will work at the Institute Lumière Matière (ILM) in Lyon, in the group “Modélisation de la matière Condensée et Interfaces”, and may benefit from interactions with experimentalists at the ILM, group “Liquides @ Interfaces”. This internship can be followed by PhD thesis, possibly purely numerical or combining modeling and experiments.

Interest candidates should send an email along with a resume to Laurent Joly (laurent.joly@univ-lyon1.fr) and Samy Merabia (samy.merabia@univ-lyon1.fr). Informal enquiries are always welcome.

References

[1] E. Guillaud, S. Merabia, D. De Ligny and L. Joly, Decoupling of viscosity and relaxation processes in supercooled water : a molecular dynamics study with the TIP4P/2005 f model, Phys. Chem. Chem. Phys. (2017)