

INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: **Institut Lumière Matière**

CNRS identification code: **UMR 5306**

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Internship location: institut Lumière Matière, 10 rue Ada Byron 69622 Villeurbanne, France

Thesis possibility after internship: **YES**

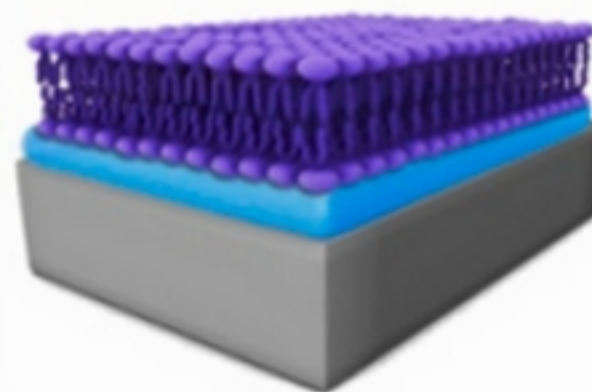
Funding: **YES**

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MOLECULAR DYNAMICS SIMULATIONS OF SUPPORTED LIPID MEMBRANES

Keywords : Nanofluidics / Numerical Modeling / Soft Matter

Supported lipid layers (SLL) are composed of ordered lipids covering the surface of a solid which are commonly used to study biomolecular phenomena, e.g. protein adsorption. One of the advantages of these model systems is that they can be synthesized with a precise control of composition.



The internship is part of the BANANA-SLIP ANR project, which aims at **studying the mechanical properties of stacks of lipid, which play a major role in reducing friction in living bodies.** The understanding of the microscopic mechanisms involved in biolubrication remains very phenomenological.

Experimental partners investigate highly controlled SSL under mechanical stress, using recent instrumental development allowing to study both the tribology and velocity profile of confined systems. One aim is to compare the microscopic quantities measured with numerical simulations. **The challenge is to develop the numerical simulations of the complete system : substrate, solvent, lipid layers.**

The student will perform **numerical modeling** of SSL using all-atom molecular dynamics simulations, using existing, standard molecular dynamics packages running on computing centers. Then, the results are going to be analyzed using scripts based on shell and python languages. The student will acquire some **practical knowledge on numerical modeling.** Understanding, and analyzing, the system will require some theoretical knowledge of **statistical physics** and **hydrodynamics.** Interest for **biophysics** and **soft matter** is important.

- *Coarse-Grain Simulations of Solid Supported Lipid Bilayers with Varying Hydration Levels* F. Benedetti et al. <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c03913>

- *Mixed Mechanism of Lubrication by Lipid Bilayer Stacks* A. Boğan, et al .
<https://pubs.acs.org/doi/10.1021/acs.langmuir.5b02786>