MOLECULAR DYNAMICS SIMULATIONS OF SUPPORTED LIPID MEMBRANES

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Charles Sadron (Strasbourg)

LEVEL : M1
TEAM(S) : MMCI
THEOCHEM

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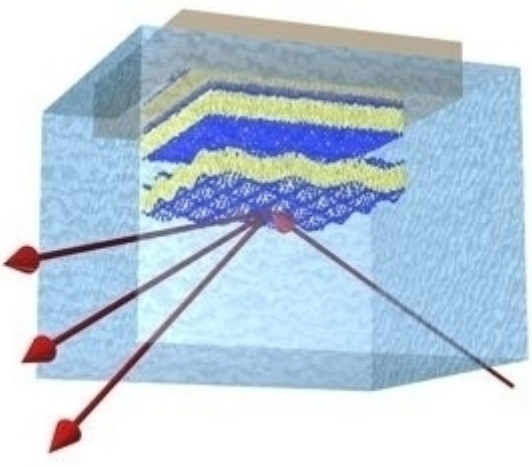
KEYWORD(S) : Nanofluidics / Numerical Modeling / Soft Matter

SCIENTIFIC CONTEXT :

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



Schematic view of off-specular reflectivity experiments on floating bilayers [2]

The internship is part of the BANANA-SLIP ANR project, which aims at **studying the mechanical properties of stacks of lipid membranes**. These play a major role in **reducing friction in living bodies [1]**. The understanding of the microscopic mechanisms involved in biolubrication remains very phenomenological, mainly due to the structural complexity of these systems. Moreover, the hydrodynamics of the complex lipidic fluid confined by the substrate is not yet fully understood.

Experimental partners [2] are going to investigate highly controlled supported lipidic layers 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, as in Ref. [3]. The aim of the internship is to perform molecular dynamics simulations of supported lipid layers [4], and to compare the simulated structures to recent experimental data.

MISSIONS :

After a literature study on supported lipid bilayers and on numerical simulations, the student is going to perform numerical modeling of lipid layers using all-atom molecular dynamics simulations, using existing, standard molecular dynamics packages. A PhD student has already developed the workflow. The system will be build using all-atom models and the simulations run on computing centers using linux operating systems. Finally, the simulations are going to be analyzed using scripts based on shell and python languages. The student will acquire some practical knowledge on **numerical tools** and **programming**. Interest for **biophysics** and **soft matter** are important. In particular, we are interested on the impact of electrostatic effects on the mechanical properties of lipidic bilayers.

OUTLOOKS :

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BIBLIOGRAPHY :

[1] https://arxiv.org/pdf/2305.12382.pdf

[2] https://doi.org/10.1073/pnas.1211669109

[3] "Coarse-Grain Simulations of Solid Supported Lipid Bilayers with Varying Hydration Levels". F. Benetti et al. J. Phys.Chem. B 2020 124 (38), 8287. https://pubs.acs.org/doi/10.1021/acs.jpcb.0c03913

[4] "Mixed Mechanism of Lubrication by Lipid Bilayer Stacks" A. Boţan, L. Joly, N. Fillot, and C. Loison Langmuir 2015 31 (44), 12197. https://pubs.acs.org/doi/10.1021/acs.langmuir.5b02786

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