Proposition de stage M2 2024/2025 au CBPsmn/LBMC à l'ENS-Lyon

Numerical simulations of polluted cell membrane models under extreme conditions

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Molecular pollution that can change the basic driving forces of cell membrane metabolism [1], has reached most corners of our planet, including those where the physical and physico-chemical parameters of the environment deviate significantly from their average on Earth. Pollution and polluted organisms are found everywhere in the ocean, potentially impacting life under a large range of pressures, from one bar at the surface up to the extreme of a thousand bar in the depths of the Mariana Trench. They are also found in other extreme conditions where life strives, as for instance in the high salinities of the Dead Sea. In this project we analyze by numerical simulations [2] how extreme conditions impact the structure and the functioning of polluted cell membrane models.

Results of the simulations will be compared to experiments being currently performed, bringing crucial insight into the structural impact of extreme conditions on polluted cell membrane models. This master project will thus contribute to the pathway for a better understanding of the molecular effects of plastic nanopollution.

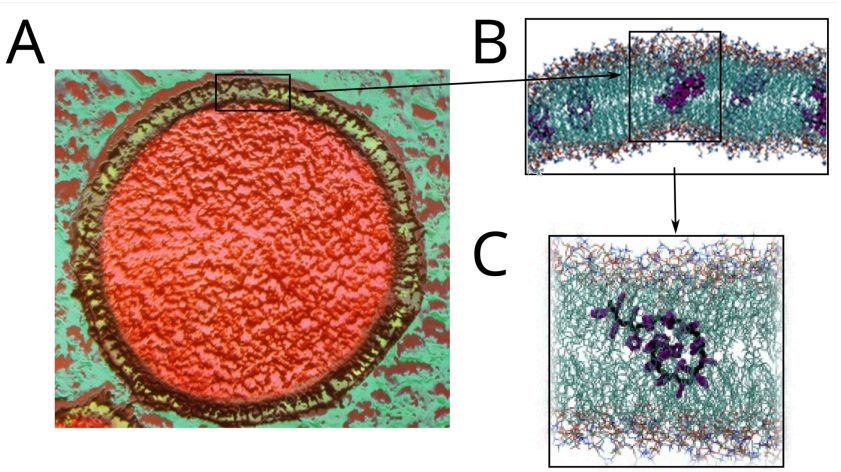

Figure 1: A. Colored TEM image of the micron-sized archaea *Staphylothermus marinus* that lives in deep ocean hydrothermal vents. B. Martini [2] coarse-grained MD simulations, showing the membrane of the microorganism in the presence of nanoplastics. C. Styrene Oligomers in an atomistic simulation.

The Master intern should have a keen interest in molecular dynamic simulations and towards work at the crossroads of Biology, Chemistry and Physics. She (he) will develop his work in the team of Paulo C. T. Souza at the Centre Blaise Pascal de Simulation et de Modélisation Numérique (CBPsmn) and Laboratoire de Biologie et Modélisation de la Cellule (LBMC) at ENS de Lyon close collaboration with the team of Carlos M. Marques (website) at the Laboratoire de Chimie of ENS de Lyon.

[1] Morandi, M.I.; Kluzek M.; Wolff, J.; Schroder, A.; Thalmann, F. and Marques, C.M., 2021. Accumulation of styrene oligomers alters lipid membrane phase order and miscibility. *Proceedings of the National Academy of Sciences*, *118*(4), p.e2016037118.

[2] Marrink, S. J.; Monticelli, L.; Melo, M.N.; Alessandri, R.; Tieleman, D.P and Souza, P.C.T. 2022. Two decades of Martini: better beads, broader scope, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 12, e1620