Multiple dynamic regimes in polymer diffusion through cubic phases

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The diffusion of polymers is a fascinating topic involving different mechanisms such as random-coil conformations and hydrodynamic interactions [1]. A single polymer in a solvent diffuses according to the Zimm model, which depicts it as a sphere of size equal to its radius of gyration based on the effect of hydrodynamic interactions between distant monomers along the chain. In situations in which the hydrodynamic interactions can be neglected, it is instead more appropriate to depict the polymer according to the Rouse model, which describes it as a collection of non-interacting beads. A third typical framework for diffusion is the so-called reptation model, according to which the diffusion of the polymer happens only by sliding and reorientation of the two ends, similar to the movement of a snake. Such model is the most appropriate approach in e.g. polymer melts, where the presence of a high concentration of polymers impedes the other rearrangement modes of the chain conformation [1].

Cubic phases are interesting objects obtained by mixing water and certain lipids in suitable proportions, where the lipid bilayer self-organizes according to minimal surfaces creating labyrinthine water channels (Fig. 1). These objects form spontaneously e.g. during milk digestion, and are being widely studied due to their potential employment for drug-delivery purposes, for which it is paramount to fully understand the molecular transport within the network of water channels therein [2].

In a previous experimental study, we investigated how the size of a polymer affects its transport within the water channels of cubic phases [3]. The experimental data were rationalized by scaling arguments based on polymer physics, which predicted three different regimes, where according to size the diffusion coefficient should follow the Zimm, the Rouse or the reptation model, appointing this system as the only known case in which the three models are applicable at the same time. Experimental data supported the existence of the Zimm and Rouse regime, but practical limits prevented the study of the reptation regime.

In this project, we will perform a simulation study to be used as a virtual laboratory to test the theoretical predictions on the transport of polymers within cubic phases. The inclusion of hydrodynamic interactions and the effect of confinement will be implemented by considering particles located along the geometrical surface representing the interface between the lipid bilayer and the water phase, which will act as an environment for the diffusing polymer. Given the large

expected computational cost, the simulations will be performed on the GPU-based software UAMMD, developed in the Delgado group [4].
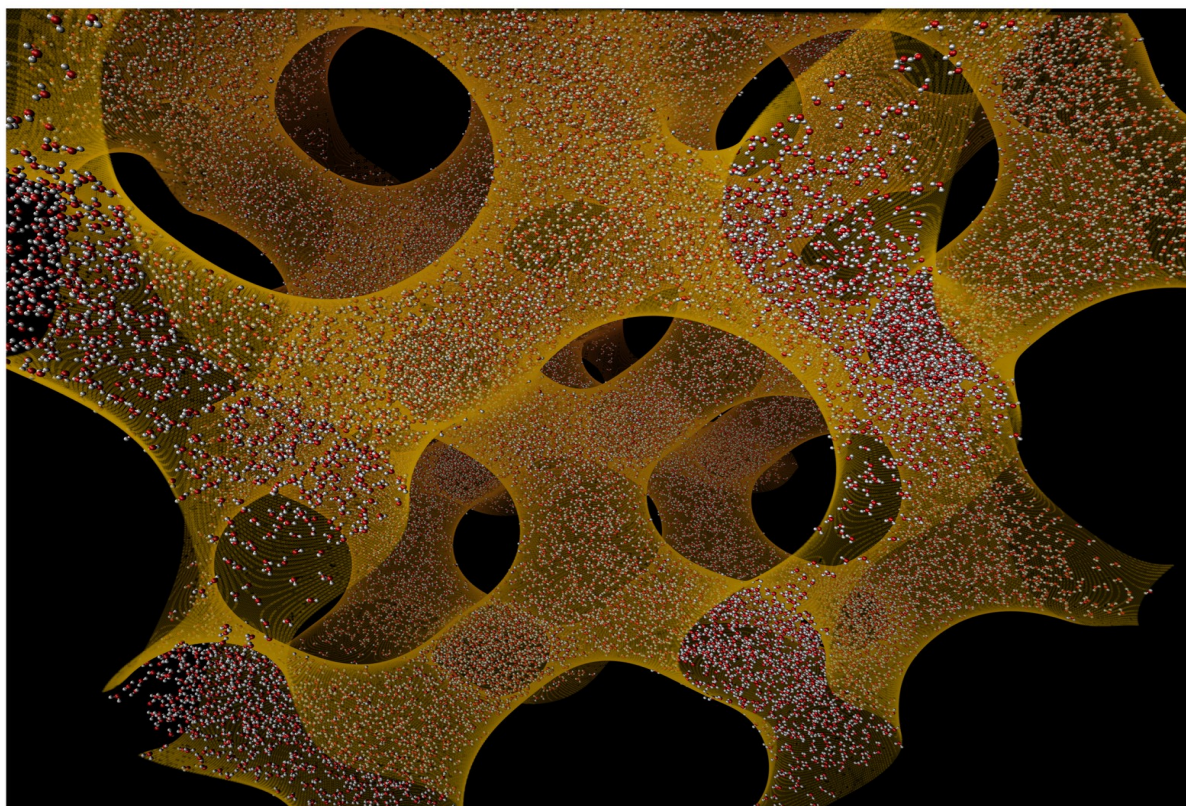

Figure 1: *Representative image of the geometry of a cubic phase (Pn3m symmetry). The lipid-water interface is depicted in orange, while representative water molecules (density not in scale) in the water channels are depicted as white and red beads.*

[1] M. Doi and S. F. Edwards, "The theory of polymer dynamics", Oxford Science Publications (1988).

[2] S. Assenza and R. Mezzenga, "Soft condensed matter physics of foods and macronutrients", *Nature Reviews Phys.* **1**:551 (2019).

[3] R. Ghanbari, S. Assenza, A. Saha and R. Mezzenga, "Diffusion of Polymers through Periodic Networks of Lipid-Based Nanochannels", *Langmuir* **33**:3491 (2017)

[4] https://github.com/RaulPPelaez/UAMMD