Interaction of Polyethylene Oxide and Polypropylene Oxide with Biological Interfaces

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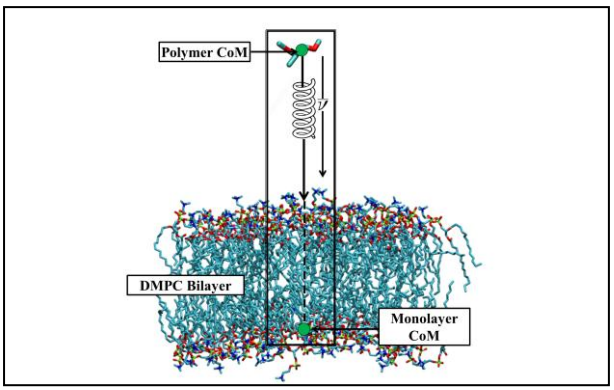

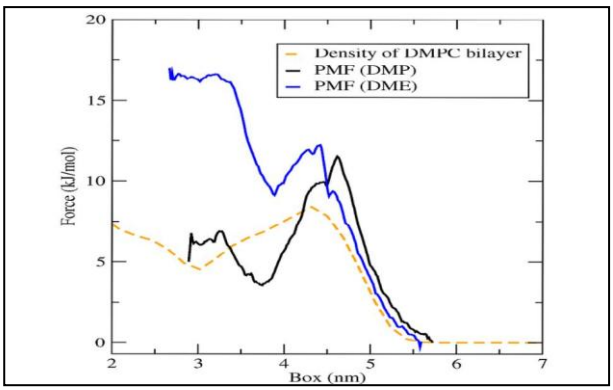

Polyethylene oxide (PEO) and polypropylene oxide (PPO) homopolymers as well as the block copolymers based on them (Pluronics® or Polaxamers®) are among the most versatile polymers used in new areas of nanotechnology connected to medicine and pharmacology as potential drug carriers. Despite of many experimental and theoretical studies on them, the actual mechanisms of their interactions with biosystems and drug molecules are still unknown. The main goal of this study is the understanding the behavior of these polymers with biological interfaces using molecular dynamics (MD) simulation methods. We wish to investigate on the thermodynamics and kinetics of percolation of Pluronics® through lipid bilayer. We also intend to study block copolymers (Pluronics®) in various non-aqueous solvents to have an insight on its thermodynamic and structural properties in these environments that can be considered simplified model for more complex systems like membranes or protein surfaces. Aiming at that, we have started our study with PEO and PPO in various non-aqueous solvents (e.g., methanol, CCl_4 and *n*-heptane) to understand their behavior in complex environments. Also, we have studied thermodynamics of the percolation process of 1,2-dimethoxyethane (DME) and 1,2-dimethoxypropane (DMP), which are the simplest oligomers of PEO and PPO respectively, through dimyristoylphosphatidylcholine (DMPC) lipid bilayer.

We expect that the findings of the study will help us to understand the interactions of block copolymers with biomembranes to a detailed level. Also, we will be able to have a better insight on the dynamic and thermodynamic process of the drug delivery process across cell membranes.

[1] S. Hezaveh, S. Samanta, G. Milano, D. Roccatano, *submitted*, **2011**.
[2] S. Pal, G. Milano, D. Roccatano, *J. Phys. Chem. B*, **2006**, *110*, 26170-27179.
[3] S. Samanta, S. Hezaveh, G. Milano, D. Roccatano, *manuscript under preparation.*