Phase diagram of Pluronics monolayer

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Pluronics are a class of amphiphilic linear triblock copolymers consisting of two hydrophilic polyethylene oxide poly(ethylene oxide) (PEO) blocks connected to a central hydrophobic polypropylene oxide poly(propylene oxide) (PPO) block. These copolymers have a wide range of application in numerous industrial sectors ranging from cosmetics to more recently in medical and pharmaceutical products. For example, they are used on nanoparticles as surface coatings and even as drug/gene nanocarriers exploiting their ability to self-assemble in polar solvents. Due to their potential biological activity, the toxicity of Pluronics of different monomer ratios has been studied recently.[1, 2]

We developed a MARTINI coarse-grain (CG) model for Pluronics. Existing MARTINI bead types are used to model the non-bonded part of the potential while single chain properties for both homopolymers, PEO and PPO, are used to develop the bonded interactions. The CG model developed overcomes the time and length scale limitations typical of the atomistic simulations.

Here, we show that the new set of force field parameters reproduces structural and dynamical properties of high molecular weight homo- and copolymers. Furthermore, the CG model preforms in solvents of different polarity and concentration, and in predicting the structure and the area-pressure isotherm of monolayer. For example, the surface tension at which the MARTINI model predicts the monolayer to be stable was in agreement with experimental data, 37 dyn/cm reproducing the area per polymer.[3]

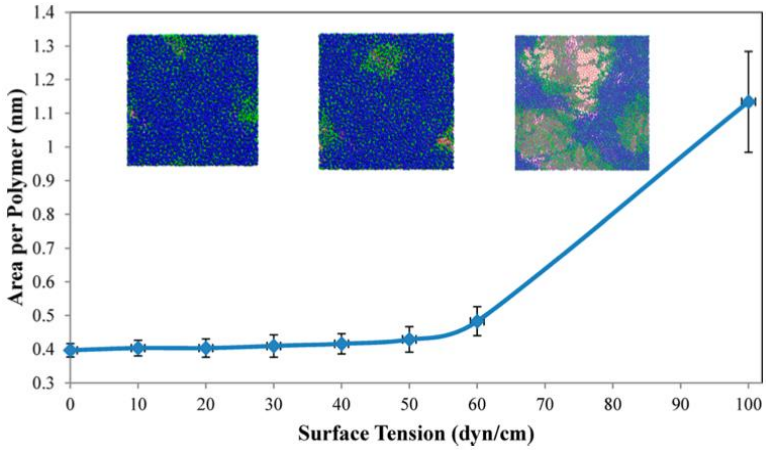

Figure 1. Area per polymer for the L44 (PEO_{10} PPO_{23} PEO_{10}) block copolymer monolayer at different surface tension values with snapshots of the monolayer taken perpendicular to the membrane normal at the three high surface tension values (50, 60, and 100 dyn/cm) illustrating the membrane rupture and high area per polymer as the surface tension increases.[3]

1. Redhead, M.; Mantovani, G.; Nawaz, S.; Carbone, P.; Gorecki, D.; Alexander, C.; Bosquillon, C. *Pharm. Res.* **2012**, 29, 1908−1918.
2. Nawaz, S.; Redhead, M.; Mantovani, G.; Alexander, C.; Bosquillon, C.; Carbone, P *Soft Matter*, **2012**, 8, 6744-6754
3. Selina Nawaz and Paola Carbone *J. Phys. Chem.*, **2014**, 118 (6), pp 1648–1659