Molecular Simulation Methods to Advance Micellar Drug Delivery

Sharon Loverde, University of Pennsylvania

Molecular simulation is an emerging tool to bridge relevant time and length scales in self-assembly and interfacial processes in soft matter and biological systems. Utilizing a range of techniques, such as Dissipative Particle Dynamics and coarse-grained molecular dynamics, I have examined phenomena ranging from the break-up of mixed worm like micelles to the solubility of the anti-cancer drug paclitaxel in different micellar morphologies. For example, worm micelles have been shown to be stable over a narrow range of micellar core volume to interfacial area. Utilizing DPD, it is shown that that copolymer bidispersity can induce budding and breakup of a worm-like micelle into spherical micelles. Next, atomistically accurate, coarse-grained polymer models have been developed and studied for poly(ethylene oxide) -poly(caprolactone) (PEO-PCL), with molecular dynamics simulations comparing well with solution phase behavior and expected interfacial properties of the copolymer. The anti-cancer drug paclitaxel is also coarse-grained with intramolecular interactions again obtained from all-atomistic molecular dynamics. Utilizing free energy techniques, it is found that the hydrophobic drug possesses a greater partitioning in a worm micelle morphology of the same diblock weight than a spherical micelle morphology, consistent with previous results found by the Discher laboratory.