Multiscale simulations of nanoparticles, polymers, and membranes for drug delivery and nanopore applications

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Interactions of peptides, nanoparticles, polymers, and membranes have been studied using all-atom and coarse-grained molecular dynamics simulations. The following topics will be presented: (1) structure of peptides interacting with monolayers and micelles; (2) membrane curvature and pore formation induced by differently sized, charged, shaped, and concentrated nanoparticle (dendrimer) and linear polymer; (3) conformation and hydrodynamics of polyethylene glycol (PEG) in water and on surface; (4) self-assembly and phase behavior of PEG-conjugated liposomes, bicelles, and micelles; (5) parameterization of all-atom and coarse-grained models for simulations described above. This work aids in the rational design of synthetic peptides, nanoparticles, and drug complexes for drug delivery, and development of accurate nanopores for biosensor applications.