Molecular modeling of dendrimers, liposomes, and nanotubes grafted with polymers

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Multiscale molecular dynamics simulations of dendrimers, liposomes, and single-walled carbon nanotubes (SWNT) grafted with polyethylene glycols and polypeptides will be presented: (1) the effects of the polymer conjugation on the size, shape, and internal structure of PAMAM dendrimers; (2) self-assembly and phase behavior of PEGylated liposomes, bicelles, and micelles; (3) interparticle dispertion, membrane curvature, and penetration induced by SWNTs wrapped with lipids and PEGylated lipids. This work aids in the rational design of drug and nanoparticle complexes for drug delivery, and development of accurate nanopores for biosensor applications.