Nanoparticle-vesicle interactions

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Abstract

Engineered nanoparticles with tuned biophysical properties are fabricated for different diagnostic and therapeutic applications; biological analogues for engineered nanoparticles are viruses and parasites [1-3]. Furthermore, nanoparticles have applications in food and cosmetics industries. However, not much is known about their interaction with biological cells, organelles, and intra- and extracellular vesicles. For wrapping of particles with sizes above 20nm by model lipid-bilayer membranes, relevant energy contributions include the deformation energy cost for the membrane and the adhesion energy gain between particle and membrane. The wrapping state of the particle, determined by the competition of deformation and adhesion energies, can be non-wrapped, partial-wrapped, and complete-wrapped. Several partial-wrapped nanoparticles may aggregate due to membrane-mediated interactions [4].

Small biological vesicles, intracellular vesicles such as autophagosomes and lysosomes, and extracellular vesicles such as exosomes, have received increased attention in recent years. For instance, exosomes have been shown to contribute to tumor metastasis [5]. Nanoparticle-vesicle interactions depend on particle and vesicle sizes and shapes, nanoparticle surface chemistry and membrane composition, and membrane curvature [1]. For vesicles, also the osmotic pressure difference between the interior and exterior solutions, separated by the semi-permeable lipid bilayer, is key for deformation energy and vesicle shape calculations. At high osmolarities of the solutions, the osmotic pressure fixes the vesicle volume.

We systematically investigate nanoparticle-vesicle systems and calculate wrapping diagrams for various particle-to-vesicle size ratios, vesicle reduced volumes, membrane spontaneous curvatures, and osmotic conditions. A rich wrapping behavior with non-wrapped, partial-wrapped, and complete-wrapped states is found. For non-spherical vesicles, nanoparticle wrapping transitions can be coupled to vesicle shape transitions. The transitions are either continuous without an energy barrier or discontinuous with an energy barrier. Furthermore, partial-wrapped nanoparticles provide boundary conditions for the free membrane that stabilize prolates for particles that exit vesicles and oblates and stomatocytes for particles that enter vesicles. In agreement with Ref. [6], we find partial-wrapped states for particles that exit vesicles and energy barriers for particles that enter vesicles. Furthermore, high osmotic pressure induces energy barriers. Our calculations systematically characterize the interaction of nanoparticles with both (i) vesicles with various reduced volumes and (ii) vesicles in solutions that can lead to osmotic pressure differences upon vesicle deformation. Our results may help to understand the interaction of intra- and extracellular vesicles with nanoparticles and protein aggregates.

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