Interaction of nanoparticles with lipid membranes

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Abstract

Membrane budding initiates intracellular vesicle transport and has been studied for a variety of soft matter systems. Bud formation can be induced by a spontaneous membrane curvature and by line tension at a domain boundary[1] [2], as well as by conical inclusions[3] [4] such as partially attached viruses. We investigate wrapping of nanoparticles using the Helfrich model for lipid-bilayer membranes. With our theoretical calculations for a mathematical surface with appropriate curvature-elastic constants, we calculate deformation and adhesion energies to predict membrane budding. The aim of our calculations is to find nanoparticle shapes and values for the membrane spontaneous curvature that facilitate wrapping. Using analytical models, we study wrapping of spherical and infinitely long cylindrical nanoparticles. We complement our analytical results by numerical calculations for triangulated membranes that allow us to investigate several particle shapes such as ellipsoids and cylinders and go beyond existing calculations for spheres[5].

We model ellipsoidal gold particles and carbon nanotubes to obtain wrapping diagrams. We find parameter regimes for unbound, partially-wrapped, and fully-wrapped particles. The partially-wrapped state can be metastable and the energy barrier is determined by the energy for membrane deformation around the particle. A spontaneous curvature of the membrane can facilitate budding that preferentially occurs if spontaneous curvature of membrane and particle curvature conform. Our calculations allow to accurately determine the height of the energy barrier between a metastable partially-wrapped and a fully-wrapped state. We find that wrapping of finite-length cylindrical nanoparticles occurs already for lower adhesion strengths than for spherical nanoparticles with equal curvature radii.

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