Role of particle shape and membrane spontaneous curvature for nano-particle wrapping

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Abstract

Budding of cell membranes initiates intracellular vesicle transport and has been studied for a variety of soft matter systems. Uptake of nano-particles by cells is possible via two pathways: for small nano-particles with sizes that are comparable to the membrane thickness, the preferred mode of entry into the cell is translocation through the lipid bilayer; for larger particles, the preferred pathway is particle wrapping. Using a continuum model, we study wrapping of a single nano-particle as an interplay of the membrane deformation energy and the adhesion energy of the particle to the membrane. With the help of numerical energy minimization using triangulated surfaces, we investigate the role of shape and size of the particle as well as of the membrane's elastic parameters on nano-particle wrapping. Bending energy and surface tension oppose wrapping, while a spontaneous curvature and a line tension of a membrane domain can assist wrapping.

Particle wrapping can be described using wrapping diagrams that show unwrapped, partially wrapped and completely wrapped states that are separated by (i) a continuous binding transition between a non-wrapped and a partially-wrapped state and (ii) a discontinuous envelopment transition between a partially-wrapped and a completely-wrapped state. Curved membrane proteins or a lipid asymmetry can impose a preferred curvature on the membrane. Such a spontaneous curvature of the membrane can facilitate budding if it conforms with the particle's curvature and can change energy barriers that occur during the wrapping process for non-spherical particles. We find that a preferable spontaneous curvature shifts both transitions, the transition between the non-wrapped and the partially-wrapped as well as the transition between the partially-wrapped state and the completely-wrapped state, to smaller adhesion strengths.

For non-spherical (rod like or disc like) particles compared with spherical particles, we find a higher binding affinity to the membrane. Because of the energy barrier between the partially-wrapped state and the completely-wrapped state, such particles have a lower uptake to cells, as confirmed by experiments. More complex particle shapes, such as a Hauser's cube and supereggs, have partially-wrapped states with high wrapping fractions for sufficiently high adhesion strengths. The partially-wrapped state can be advantageous both from an application point of view as well as from a biological point of view. For example, elongated particles can be used as markers for imaging the membrane and for drug delivery. Furthermore, Ebola and Marburg viruses are not easily taken up by macrophages, which may explain their high virulence.