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Membrane deformation controlled by monolayer composition of embedded amphiphilic nanoparticles REID VAN LEHN, ALFREDO ALEXANDER-KATZ, MIT — In recent work, we have shown that charged, amphiphilic nanoparticles (NPs) can spontaneously insert into lipid bilayers, embedding the NP in a conformation resembling a transmembrane protein. Many embedded membrane proteins exert an influence on surrounding lipids that lead to deformation and membrane-mediated interactions that may be essential for function. Similarly, embedded NPs will also induce membrane deformations related to the same physicochemical forces. Unlike many transmembrane proteins, however, the highly charged NPs may exert preferential interactions on surrounding lipid head groups. In this work, we use atomistic molecular dynamics simulations to show that the membrane around embedded particles may experience local thinning, head group reorientation, and an increase in lipid density depending on the size and surface composition of the NP. We quantify the extent of these deformations and illustrate the complex interplay between lipid tail group and head group interactions that go beyond pure thickness deformations that may be expected from coarse-grained or continuum models. This work thus suggests guidelines for the design of particles that spontaneously partition into lipid bilayers and influence local membrane mechanical properties in a targeted manner.

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