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Thermodynamics of ligand-coated nanoparticle complexation with lipid bilayers REID VAN LEHN, Massachusetts Institute of Technology, RANDY CARNEY, KISLON VOITCHOVSKY, FRANCESCO STELLACCI, MARIA RICCI, Ecole Polytechnique Federale de Lausanne, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Recently, nanoparticles (NPs) coated with a mixed alkanethiol surface monolayer were observed to spontaneously penetrate cell membranes via a non-endocytotic mechanism. Penetration seems to depend on the structure of the ligand monolayer; particle uptake was greatest when the surface self-assembled into a striped morphology consisting of alternating domains of hydrophilic and hydrophobic ligands. Furthermore, these 'striped' particles form stable complexes with single component lipid bilayers, implying that cellular penetration may be related to bilayer interactions. Bilayer complexation is surprising, however, because the width of the striped domains is less than the thickness of the bilayer core, implying that charged ligands are exposed to hydrophobic lipid tails. In this work, we provide a thermodynamic analysis of NP-bilayer complexation supported by implicit bilayer simulations. Our results show that complexation is related to the deformation of both the ligand monolayer and the bilayer to maximize favorable hydrophobic interactions while minimizing unfavorable insertion of charges into the bilayer core. This study will improve our understanding of bilayer interactions and enable the design of ligand-coated nanoparticles for drug delivery and biosensing applications.

Reid Van Lehn
Massachusetts Institute of Technology

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