Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Analysis of Striped Nanoparticle Complexation with Lipid Bilayers REID VAN LEHN, ALFREDO ALEXANDER-KATZ, MIT — A recent study has shown that a new class of synthetic ligand-protected gold nanoparticles is able to penetrate the cell membrane without inducing poration or endocytosis. Furthermore, these nanoparticles fuse with pure lipid bilayers while retaining high solubility in biological conditions. This complexation behavior is related to the morphology of the ligand shell, which is composed of alternating ribbon-like domains of linear alkanes with either hydrophobic or charged end-groups. Spontaneous complexation is surprising given the large free energy barrier for moving charges through the hydrophobic bilayer core. In this work, we provide a thermodynamic analysis of bilayer complexation supported by multiscale simulations. We show that the key to bilayer complexation is the rearrangement of ligands by bending to maximize hydrophobic matching and minimize charge exposure. We believe this result will improve our understanding of transmembrane proteins and enable the design of nanoparticles for drug delivery and biosensing applications.

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Date submitted: 27 Nov 2010 Electronic form version 1.4