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**Mechanism of lipid bilayer penetration by mixed monolayer-protected gold nanoparticles** REID VAN LEHN, PRABHANI ATUKORALE, MIT, RANDY CARNEY, FRANCESCO STELLACCI, EPFL, DARRELL IRVINE, ALFREDO ALEXANDER-KATZ, MIT — Recently, gold nanoparticles (AuNPs) protected by a binary mixture of hydrophobic and hydrophilic alkanethiol ligands were observed to spontaneously penetrate cellular membranes via a non-specific mechanism. Penetration was observed even at low temperatures and in the presence of endocytotic inhibitors, implying that AuNPs crossed the membrane by a non-endocytotic process. Furthermore, penetration was shown to depend on the amphiphilicity and nanoscale morphology of the protecting monolayer. In this work, we use a variety of simulation techniques to elucidate the mechanism of lipid bilayer penetration and compare our results to experiments with lipid vesicles. We show that these AuNPs can stably embed within lipid bilayers by “snorkeling” charges out of the bilayer core; the stability of such a state is a function of particle size, the composition of the protecting monolayer, and other environmental conditions. We use detailed simulations to analyze structural changes in the surrounding lipids and show that the energy barrier for embedding is considerably reduced in the presence of bilayer defects. We expect that these results will enable the design of novel drug delivery carriers and biosensors.

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