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Modeling the effect of dynamic surfaces on membrane penetration REID VAN LEHN, ALFREDO ALEXANDER-KATZ, MIT — The development of nanoscale materials for targeted drug delivery is an important current pursuit in materials science. One task of drug carriers is to release therapeutic agents within cells by bypassing the cell membrane to maximize the effectiveness of their payload and minimize bodily exposure. In this work, we use coarse-grained simulations to study nanoparticles (NPs) grafted with hydrophobic and hydrophilic ligands that rearrange in response to the amphiphilic lipid bilayer. We demonstrate that this dynamic surface permits the NP to spontaneously penetrate to the bilayer midplane when the surface ligands are near an order-disorder transition. We believe that this work will lead to the design of new drug carriers capable of non-specifically accessing cell interiors based solely on their dynamic surface properties. Our work is motivated by existing nanoscale systems such as micelles, or NPs grafted with highly mobile ligands or polymer brushes.

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