Modeling the Thermodynamics of the Interaction of Nanoparticles with Cell Membranes\textsuperscript{1} VALERIY GINZBURG, SUDHAKAR BALKI-JEPALLI, The Dow Chemical Company — Interactions between nanoparticles and cell membranes may play a crucial role in determining the cytotoxicity of nanoparticles as well as their potential application as drug delivery vehicles or therapeutic agents. It has been shown that such interactions are often determined not by biochemical but by physico-chemical factors (e.g., nanoparticle size, hydrophobicity, and surface charge density). Here, we propose a mesoscale thermodynamic model describing the transitions in membrane morphology observed after exposure to various types of nanoparticles. Our simulations demonstrate under which conditions (determined by particle size and hydrophilic/hydrophobic interactions) the particles can adsorb into the membrane or compromise the membrane integrity to result in the formation of nano-sized holes. The model could be refined to include a more accurate description of various phospholipid membranes, and its results could be applied in the design of specific nanoparticles for various biomedical applications.

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