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Influence of chain rigidity on the conformation of model lipid membranes in the presence of cylindrical nanoparticle inclusions CHRIS DILORETO, ROBERT WICKHAM, Department of Physics, University of Guelph — We employ real-space self-consistent field theory to study the conformation of model lipid membranes in the presence of solvent and cylindrical nanoparticle inclusions ("peptides"). Whereas it is common to employ a polymeric Gaussian chain model for the lipids, here we model the lipids as persistent, worm-like chains. Our motivation is to develop a more realistic field theory to describe the action of pore-forming anti-microbial peptides that disrupt the bacterial cell membrane. We employ operator-splitting and a pseudo-spectral algorithm, using SpharmonicKit for the chain tangent degrees of freedom, to solve for the worm-like chain propagator. The peptides, modelled using a mask function, have a surface patterned with hydrophobic and hydrophillic patches, but no charge. We examine the role chain rigidity plays in the hydrophobic mismatch, the membrane-mediated interaction between two peptides, the size and structure of pores formed by peptide aggregates, and the free-energy barrier for peptide insertion into the membrane. Our results suggest that chain rigidity influences both the pore structure and the mechanism of pore formation.

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