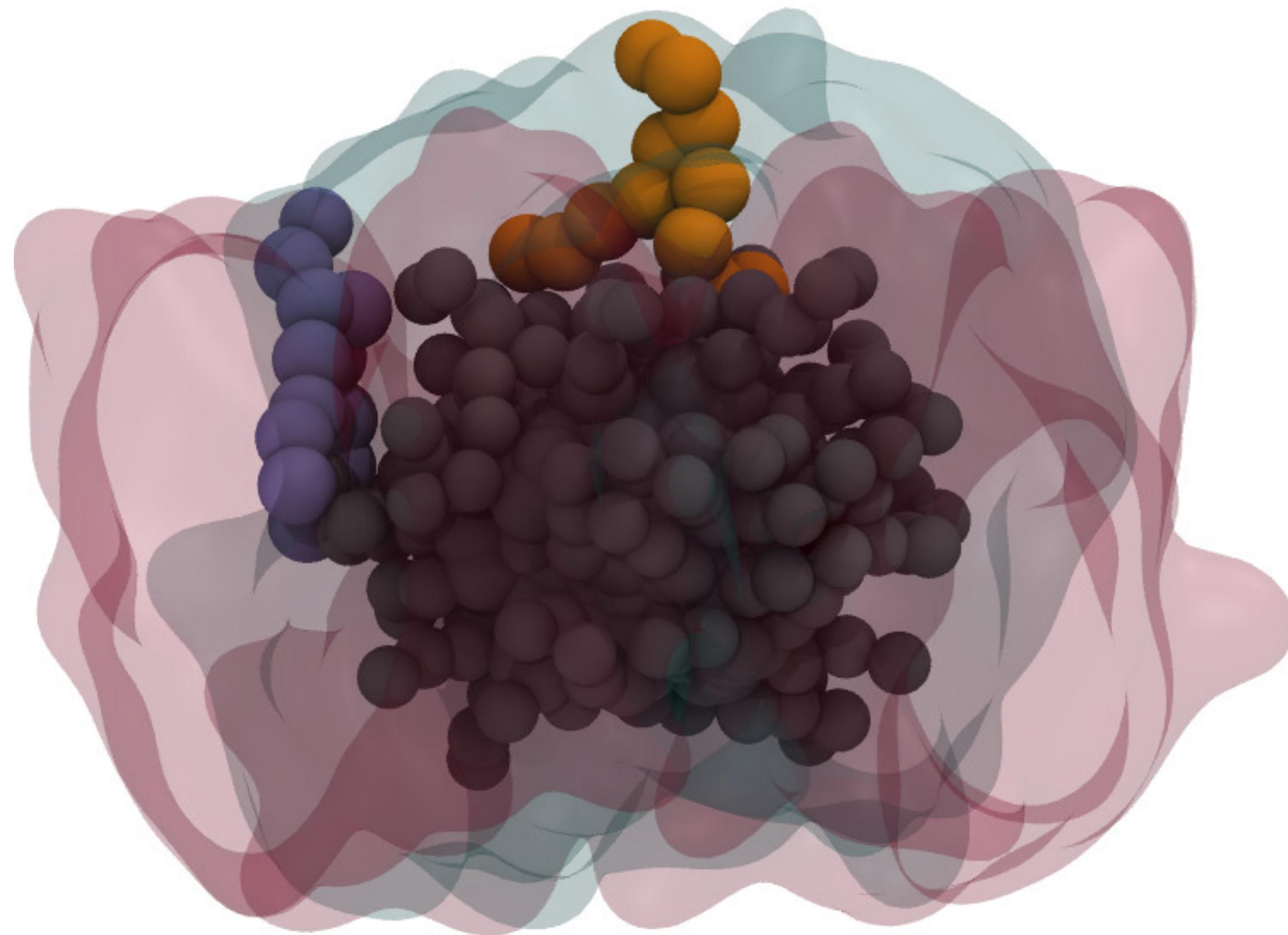


# Membrane Consortium Update

Jahmal Ennis



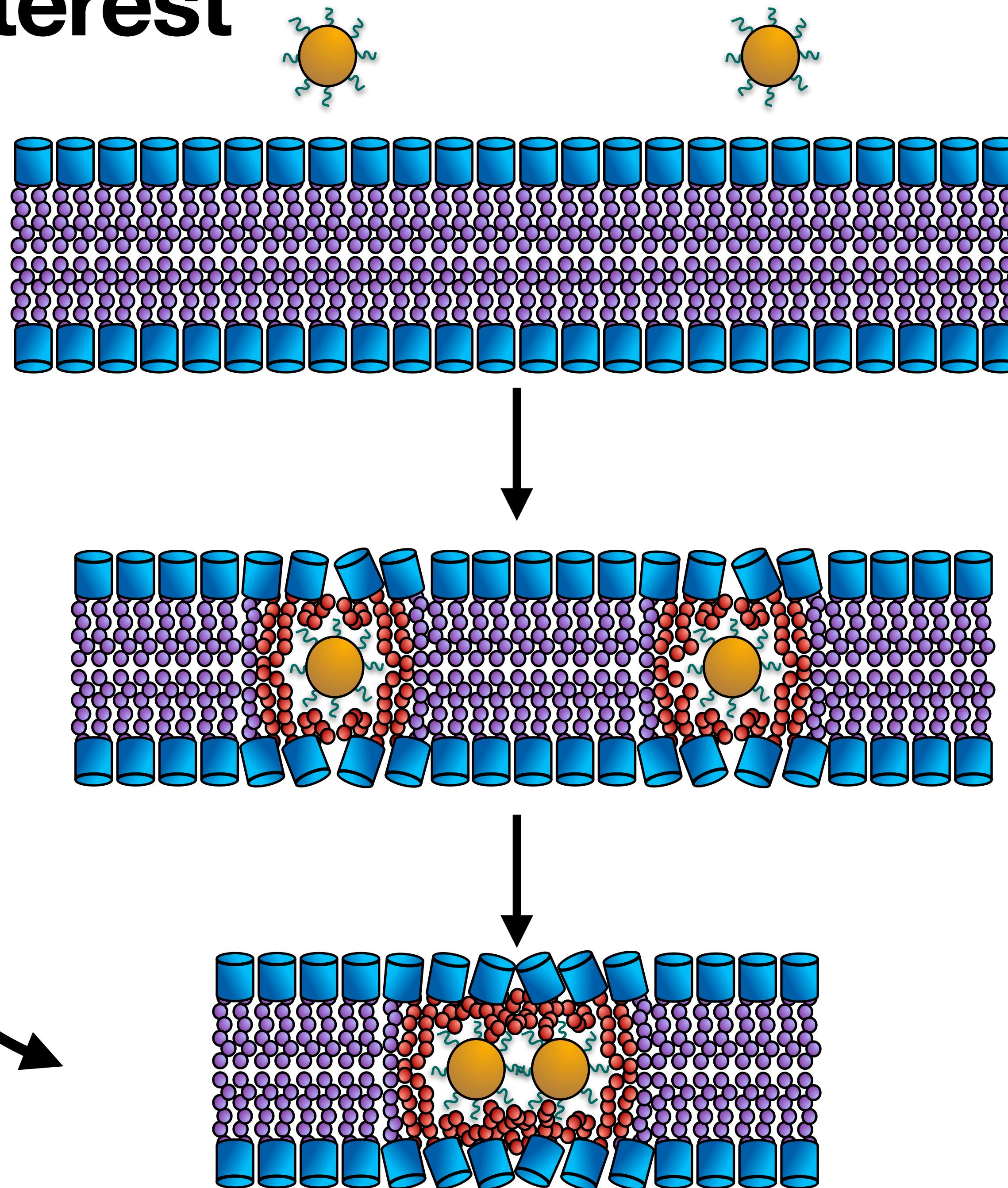
# Agenda

- Background & Motivation
- Microscopic Lipid Deformation
- Membrane Bending Deformations
- Summary

# Background

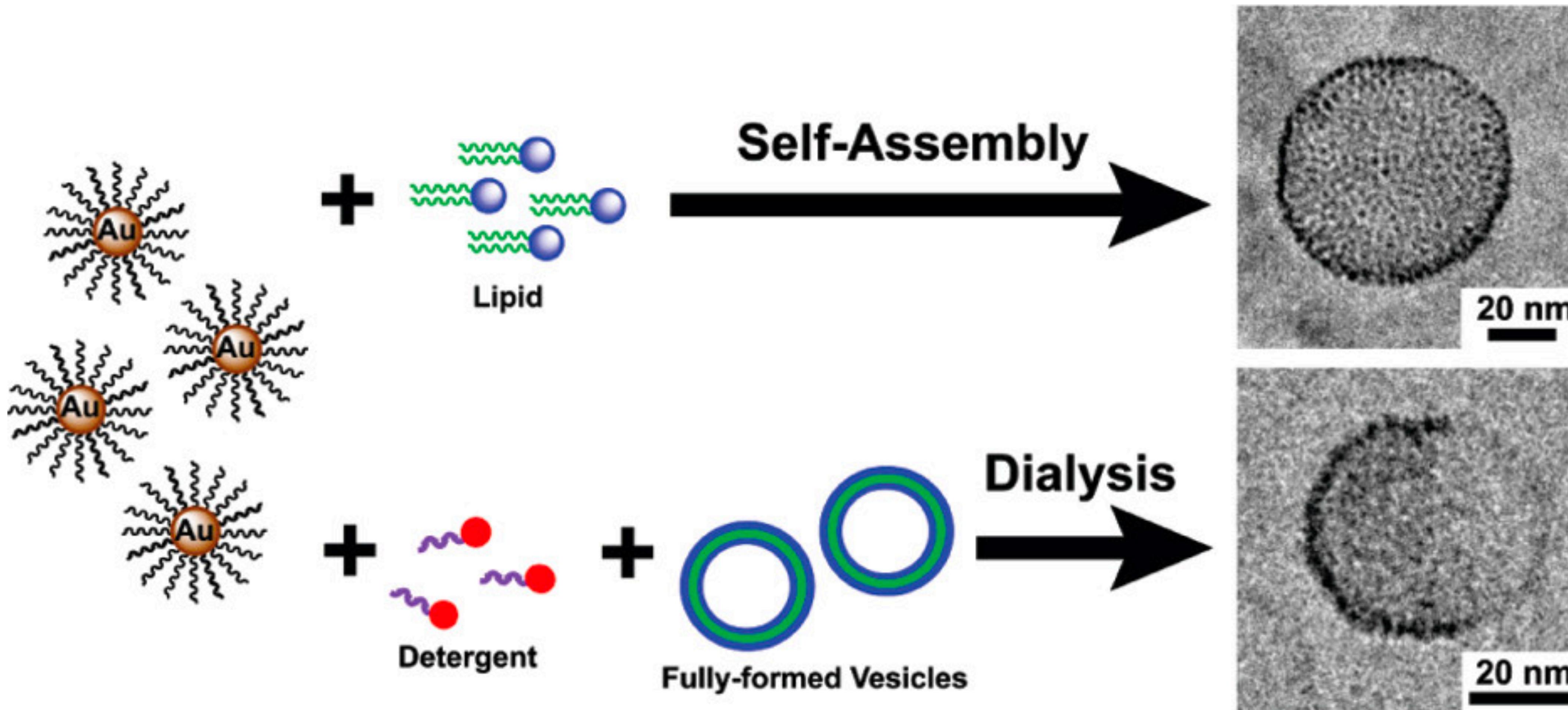
# System of Interest

How do we  
go from the  
separated  
state to the  
condensed  
state?



# Hydrophobic Gold Nanoparticle Self-Assembly with Phosphatidylcholine Lipid: Membrane-Loaded and Janus Vesicles

Michael R. Rasch<sup>†</sup>, Emma Rossinyol<sup>‡</sup>, Jose L. Hueso<sup>†</sup>, Brian W. Goodfellow<sup>†</sup>, Jordi Arbiol<sup>§</sup>, and Brian A. Korgel<sup>\*†</sup>

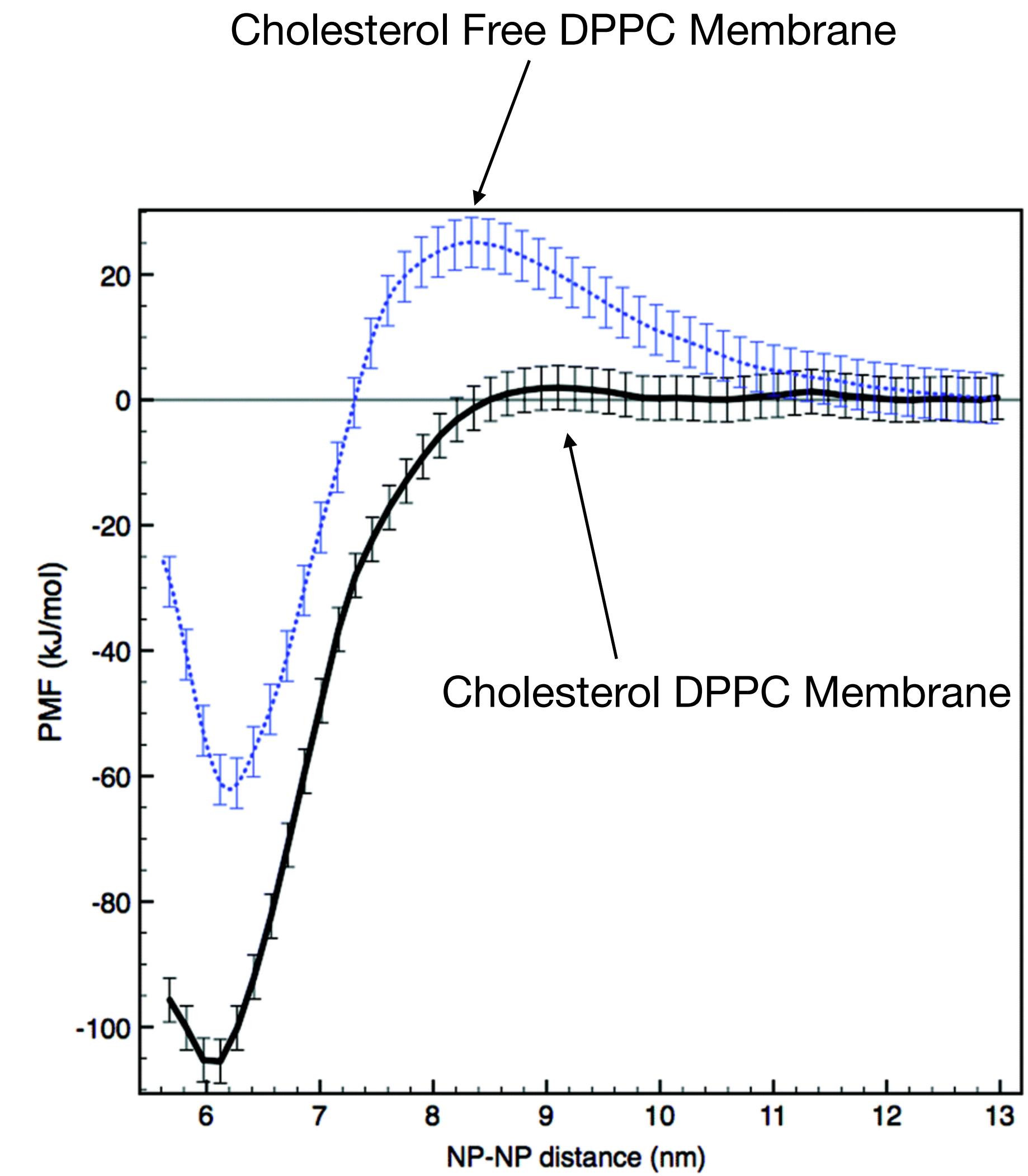
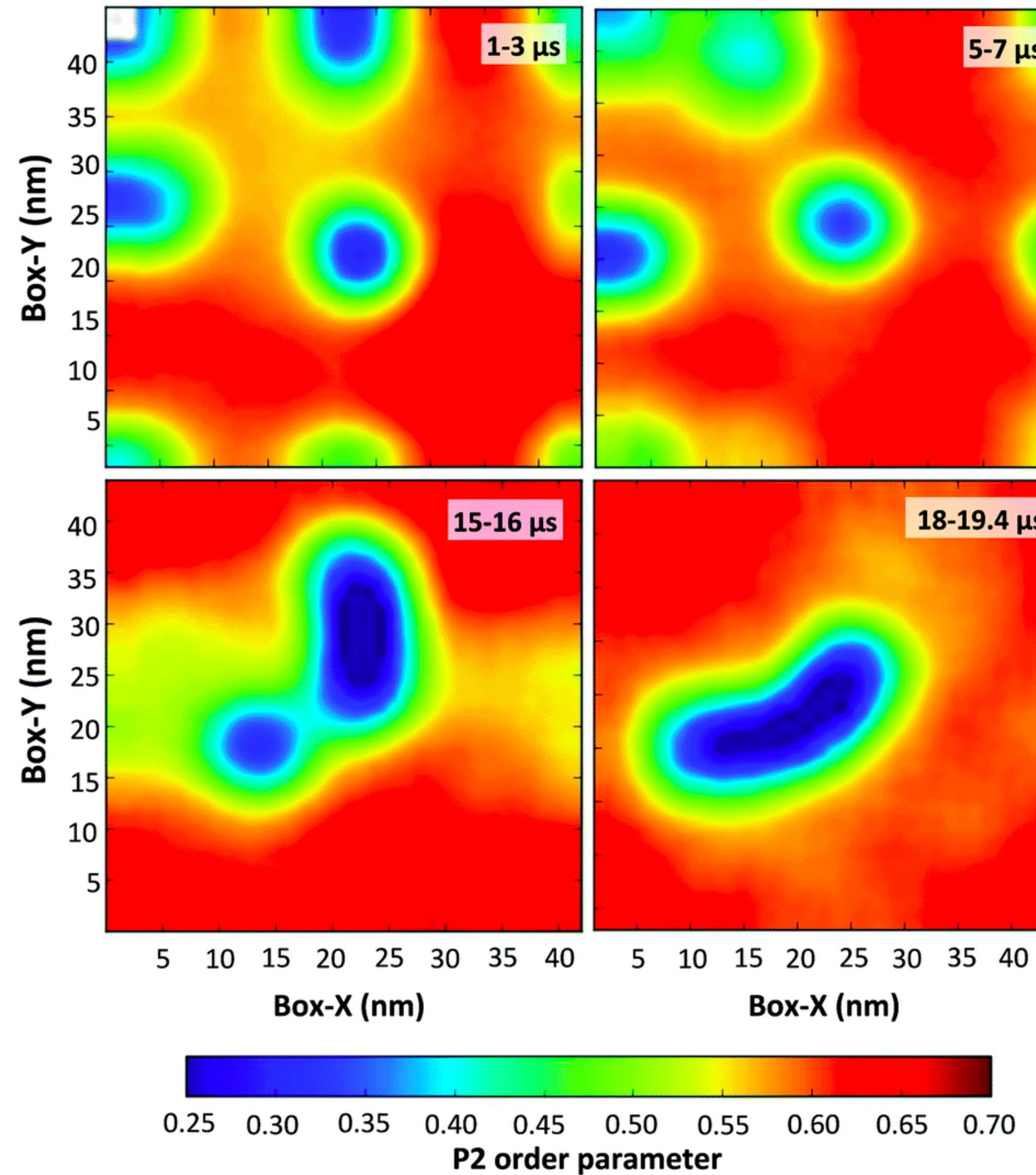


# Self-assembly of anionic, ligand-coated nanoparticles in lipid membranes<sup>†</sup>



Check for updates

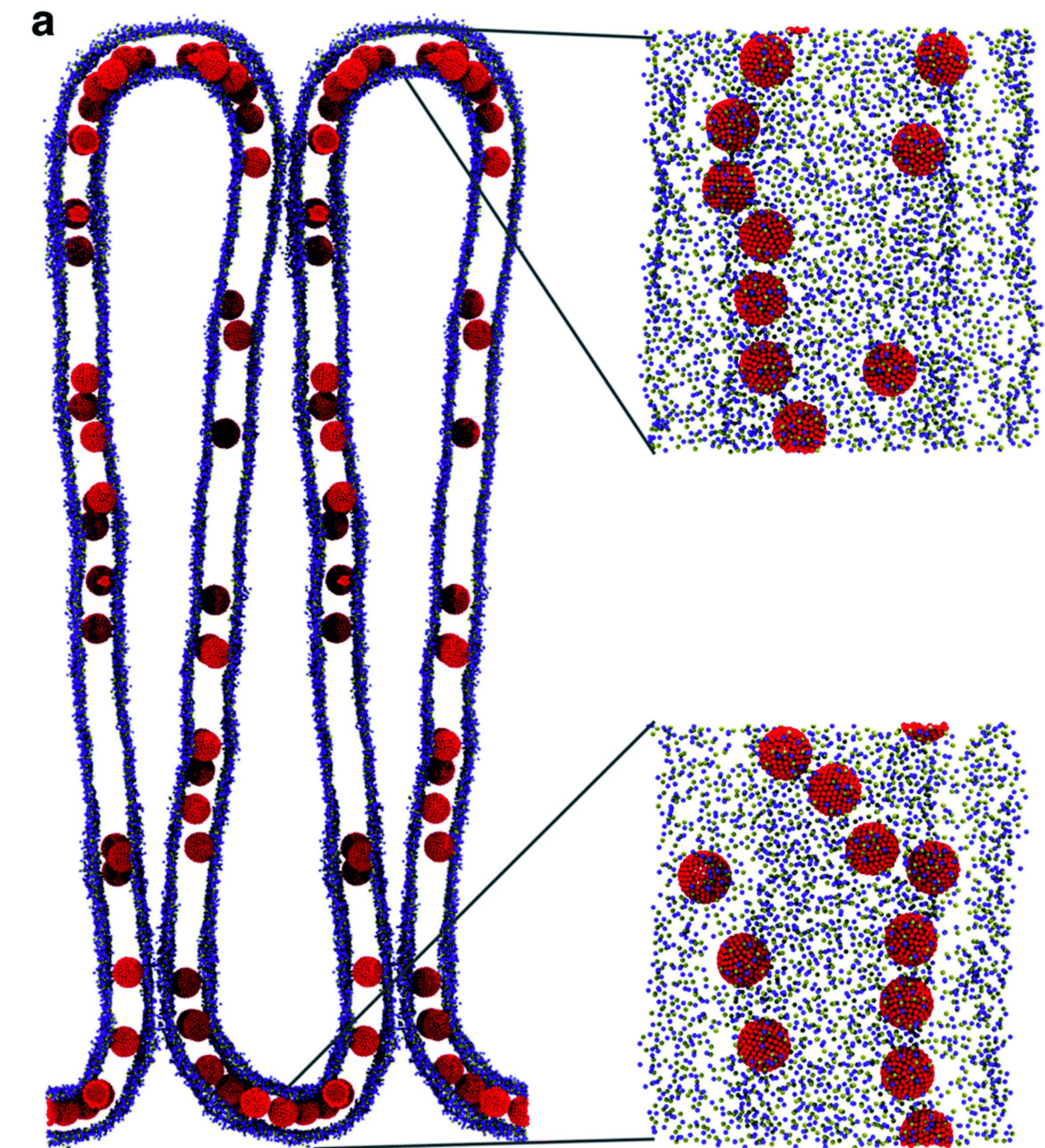
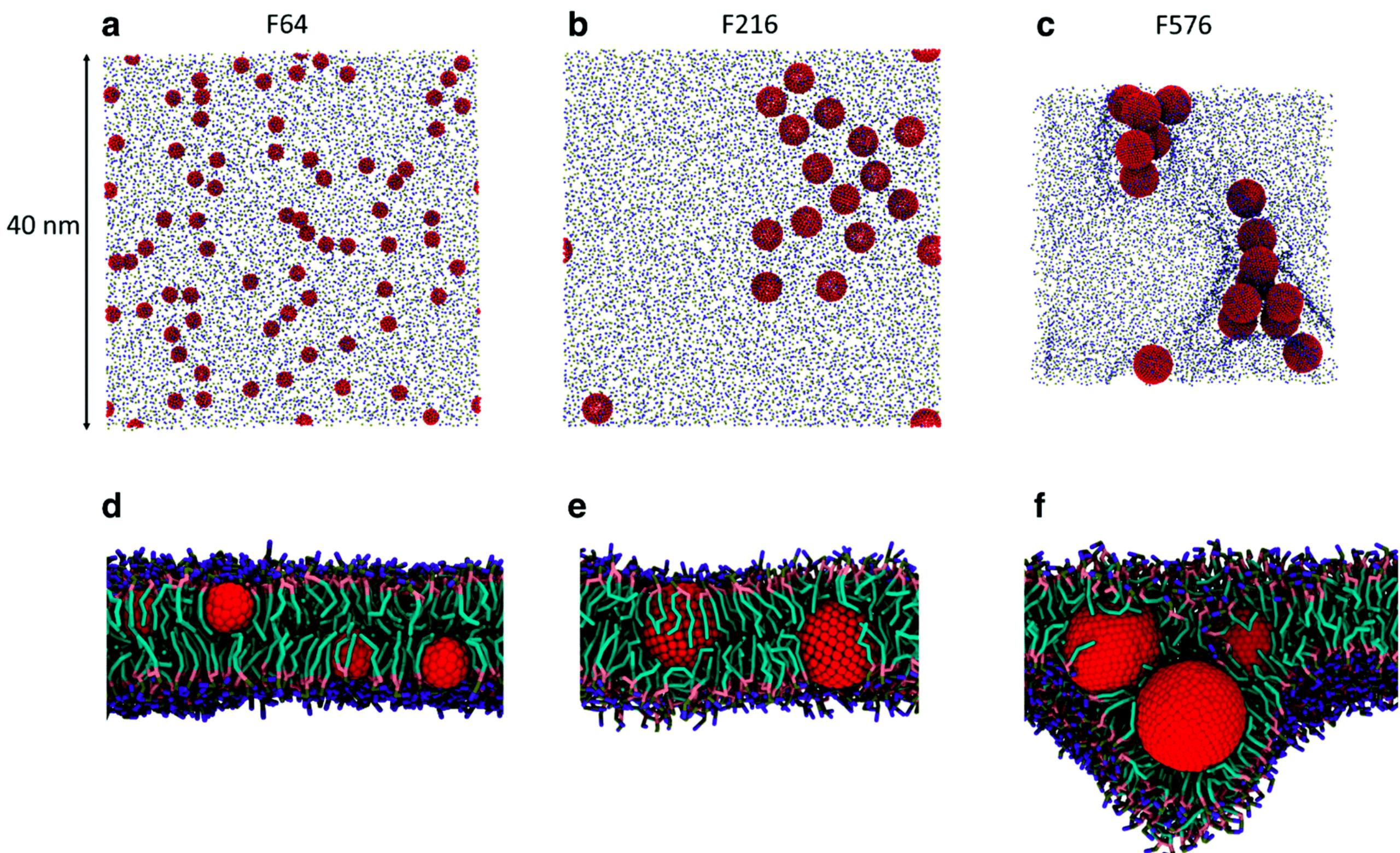
Panagiotis Angelopoulos,<sup>‡ a</sup> Lev Sarkisov,<sup>b</sup> Zoe Cournia<sup>c</sup> and Paraskevi Gkeka <sup>§ \*c</sup>



# Size-dependent aggregation of hydrophobic nanoparticles in lipid membranes

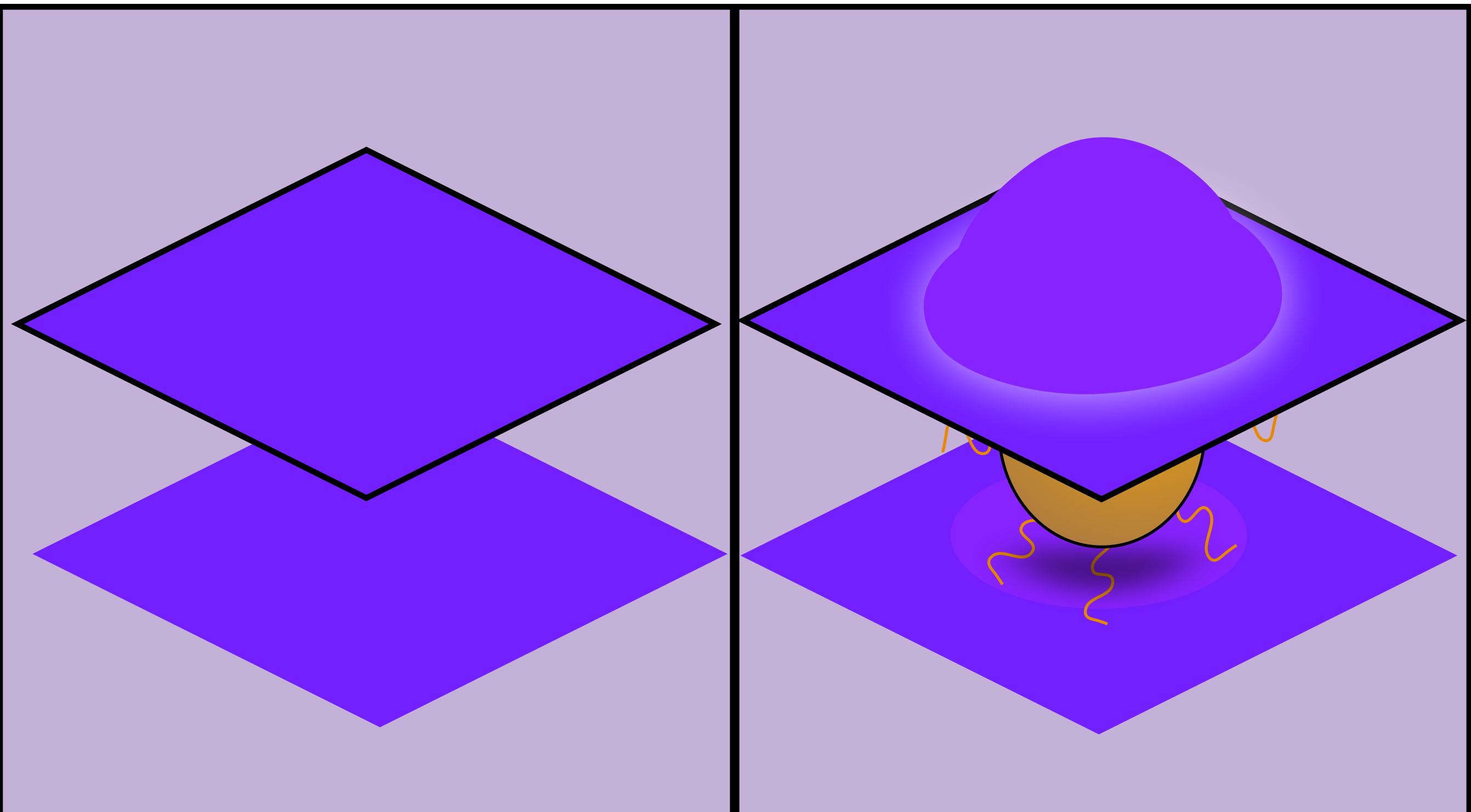
Enrico Lavagna,<sup>a</sup> Jonathan Barnoud,<sup>† b</sup> Giulia Rossi  \*<sup>a</sup> and Luca Monticelli  \*<sup>c</sup>

 Author affiliations



# Nanoparticle Deformations In Lipid Bilayer

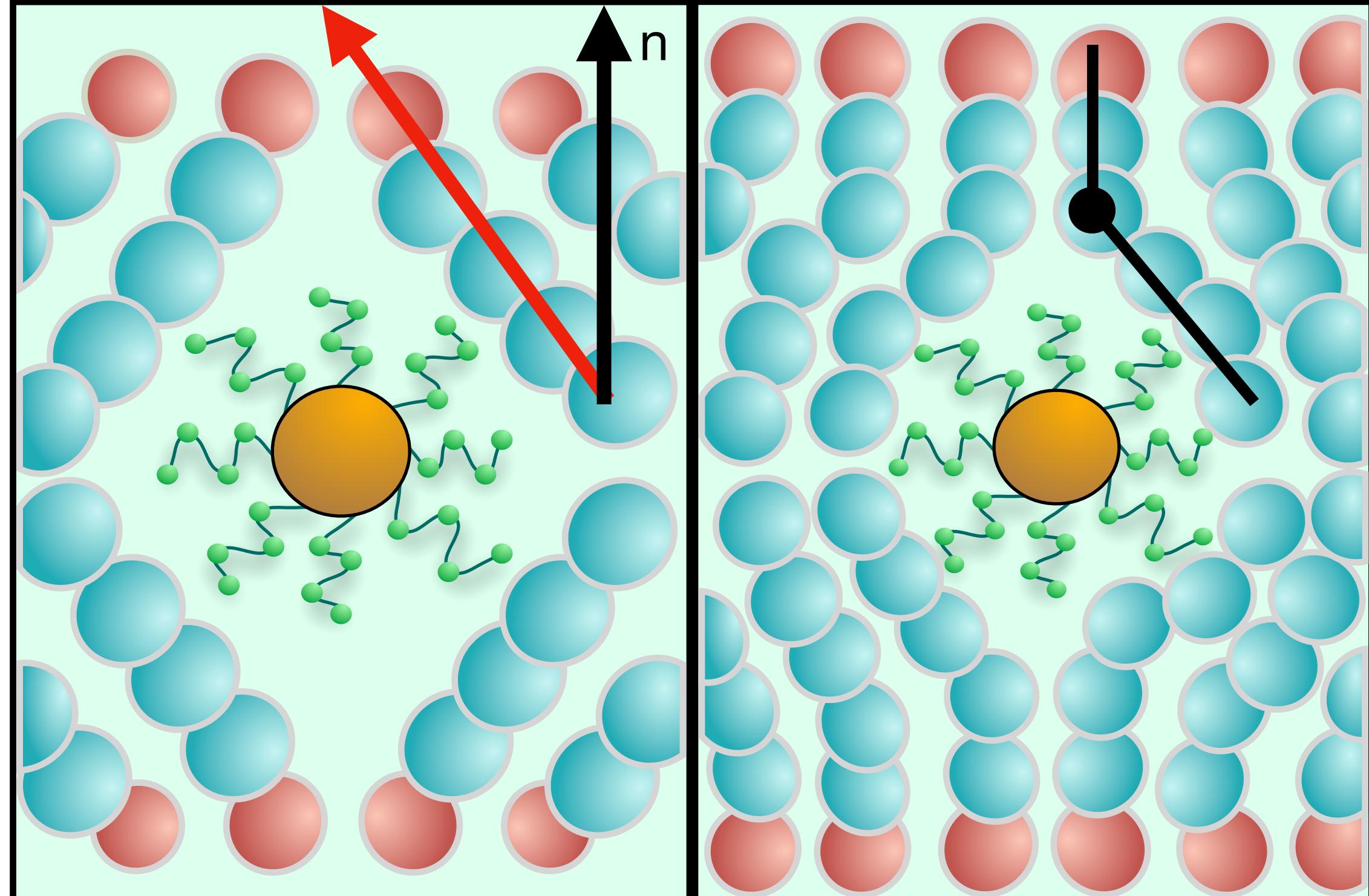
Membrane Deformation



Flat Lipid Membrane

Deformed Lipid Membrane

Lipid Deformation



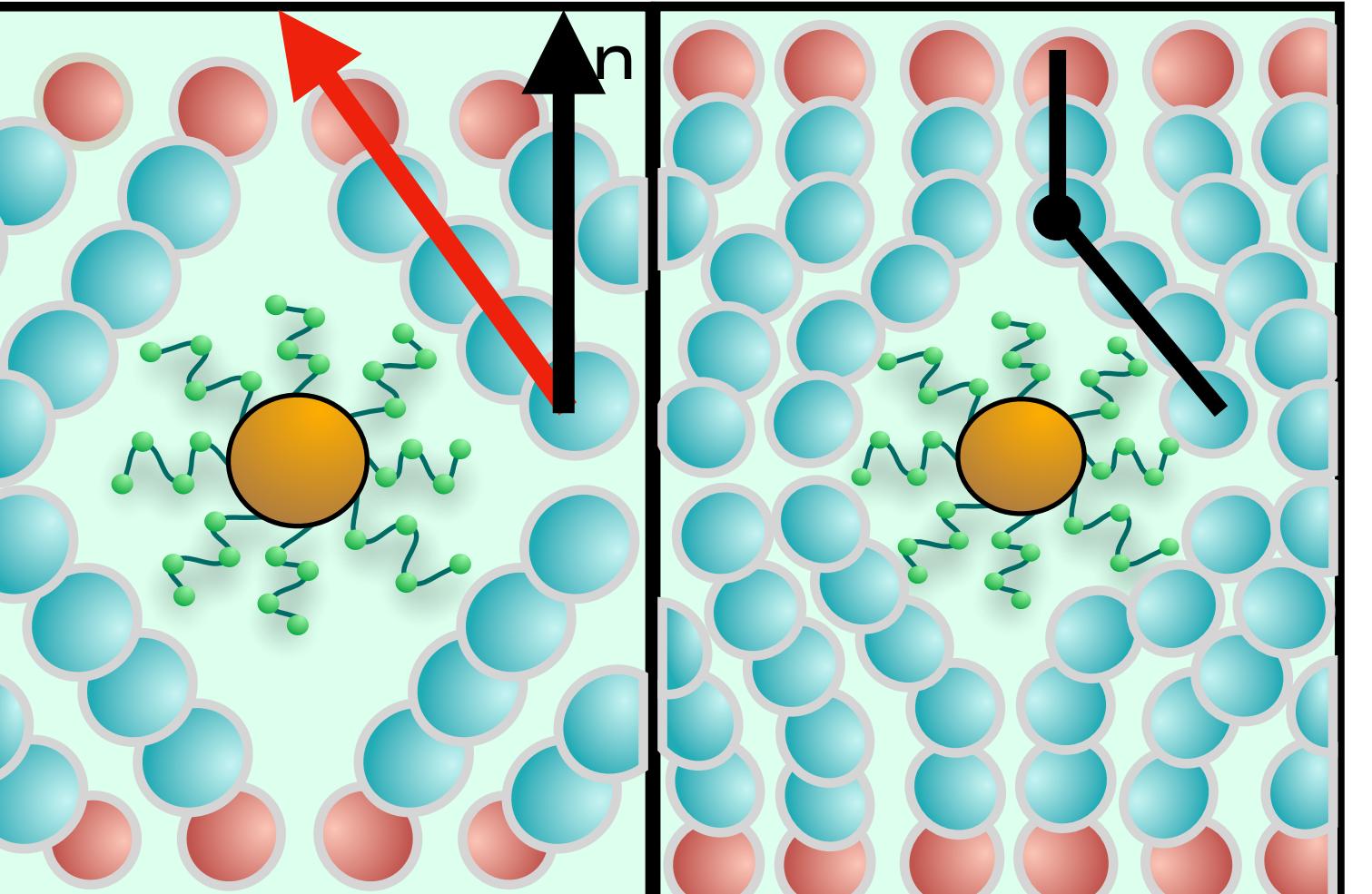
Lipid Tilt

Acyl Chain Bending

**Main Question: What is the primary mechanism of ligand coated nanoparticle aggregation?**

# Microscopic Lipid Deformation

Lipid Deformation

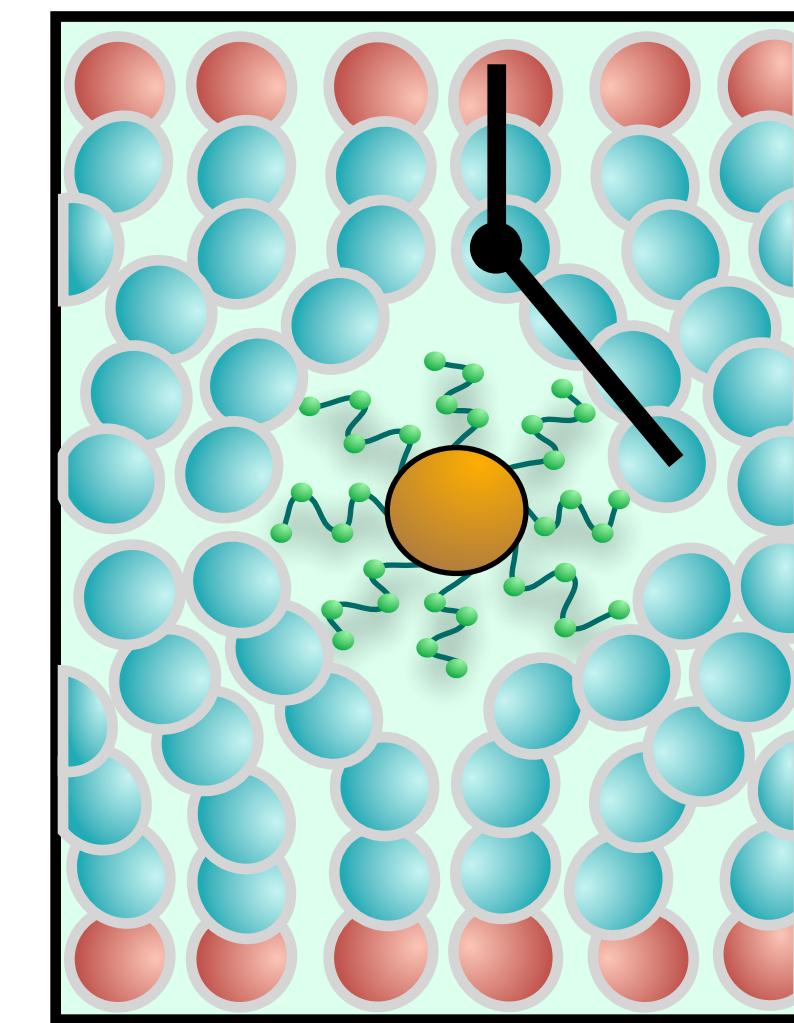
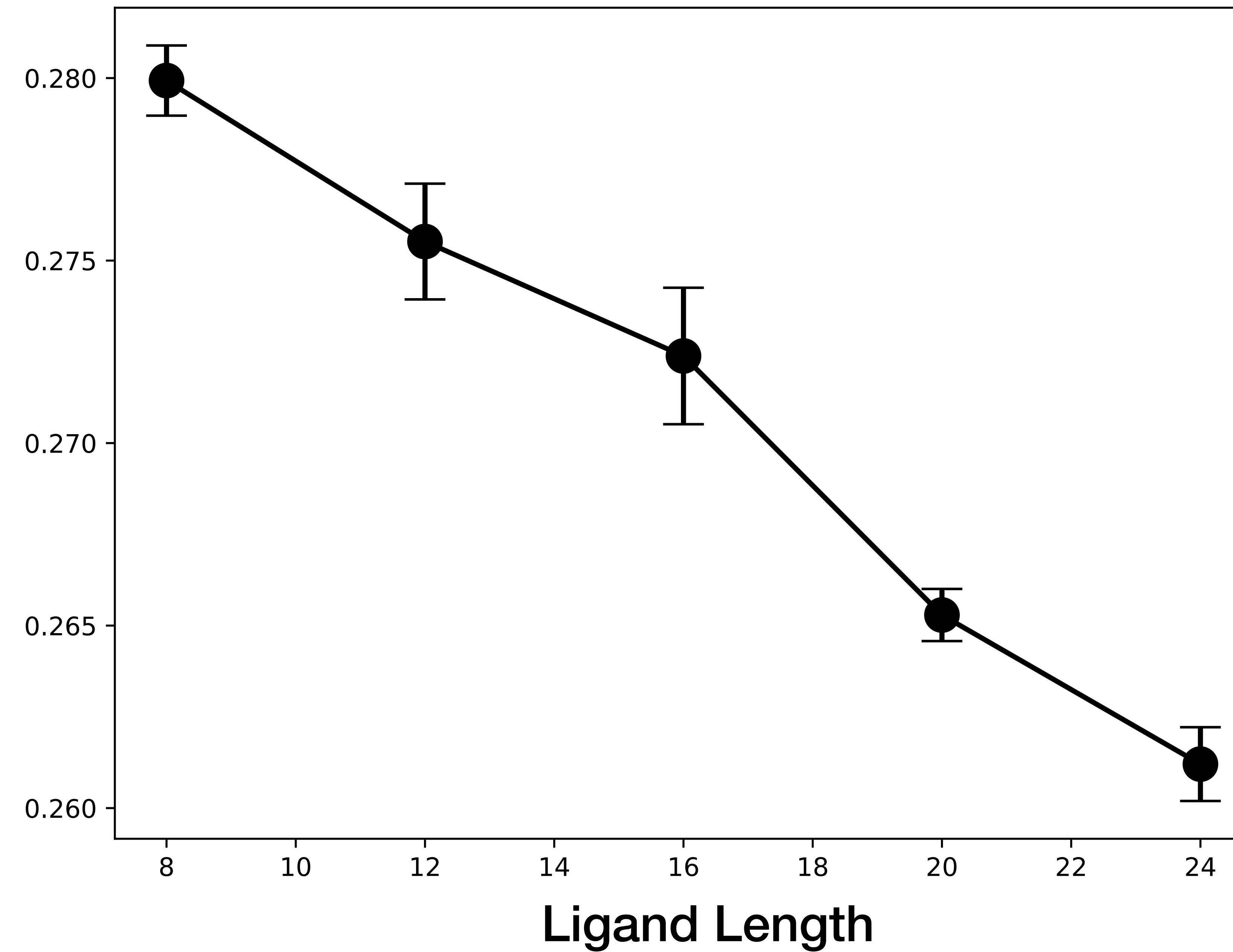


Lipid Tilt

Acyl Chain Bending

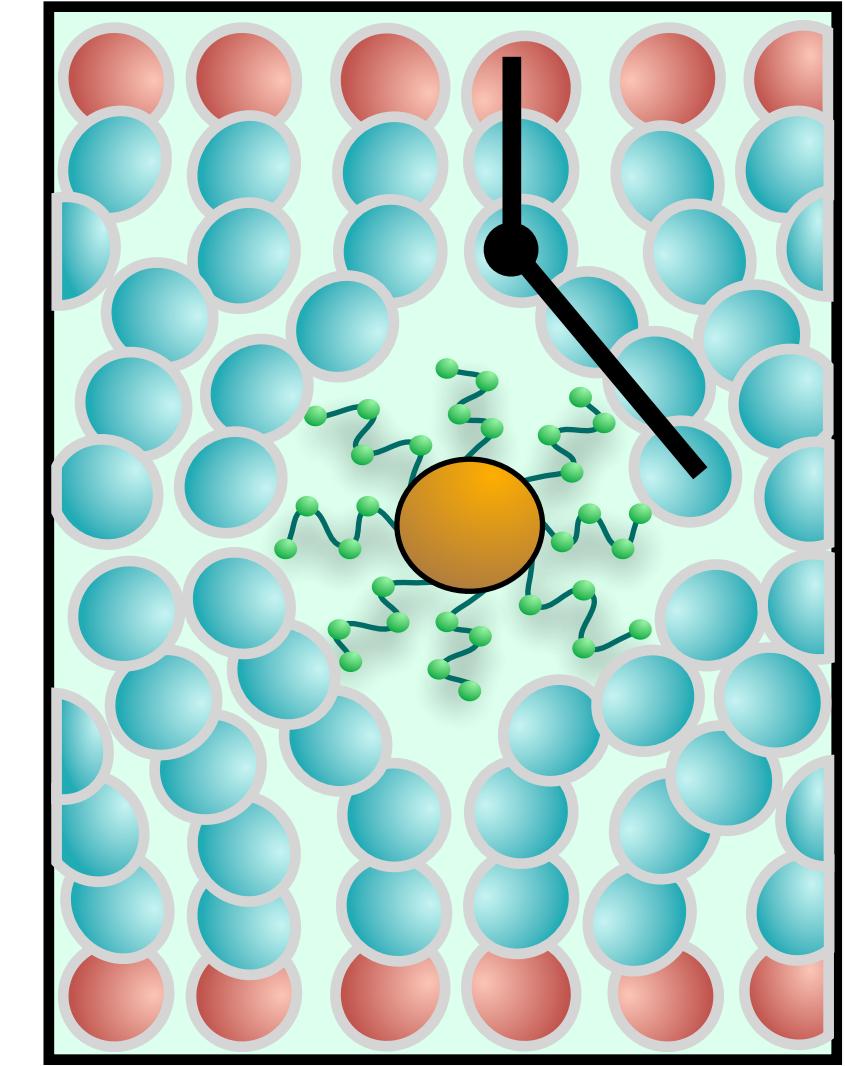
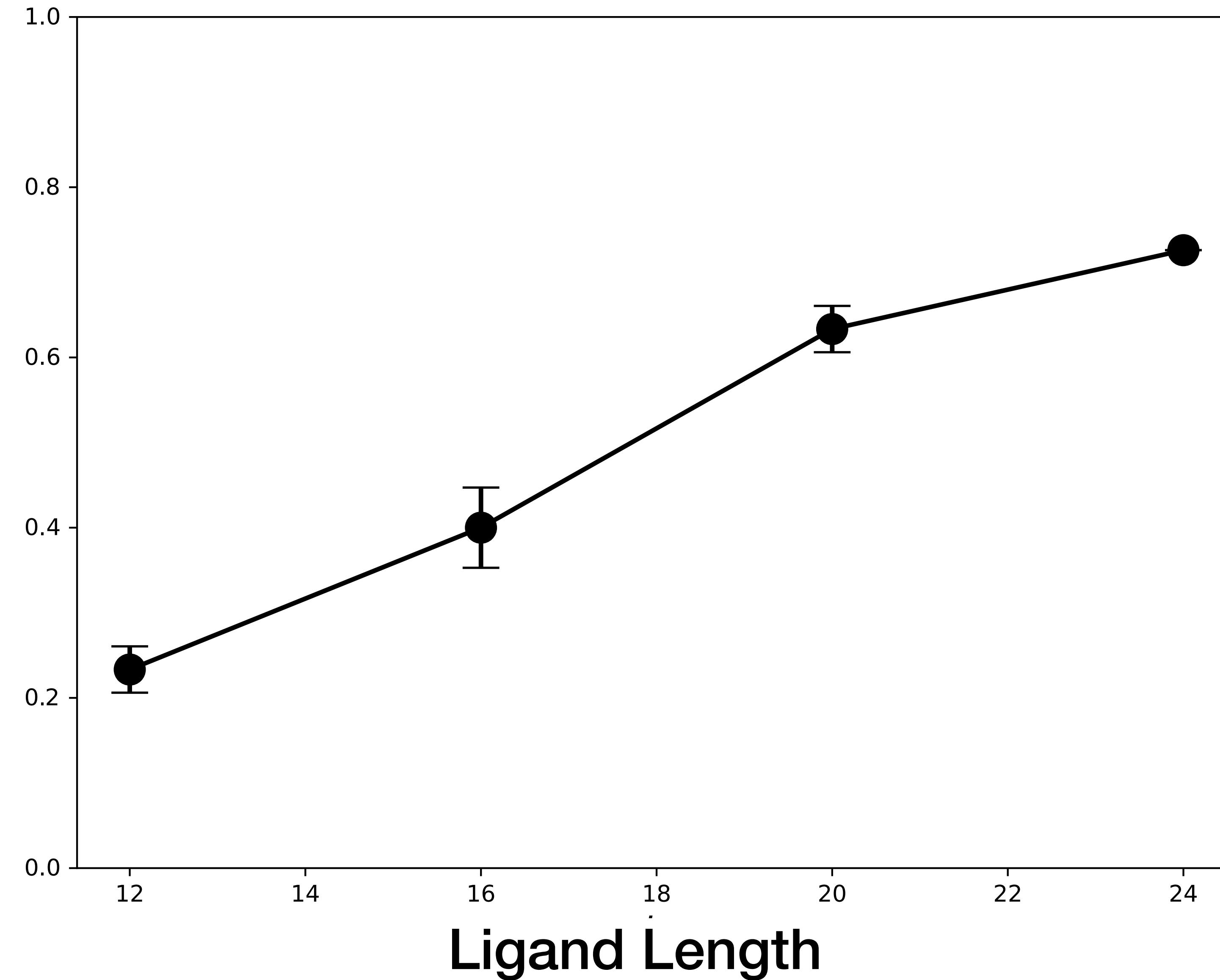
# Does hydrophobic nanoparticle ligand length disrupt lipid acyl chain order?

Acyl Chain  
Order  
Parameter



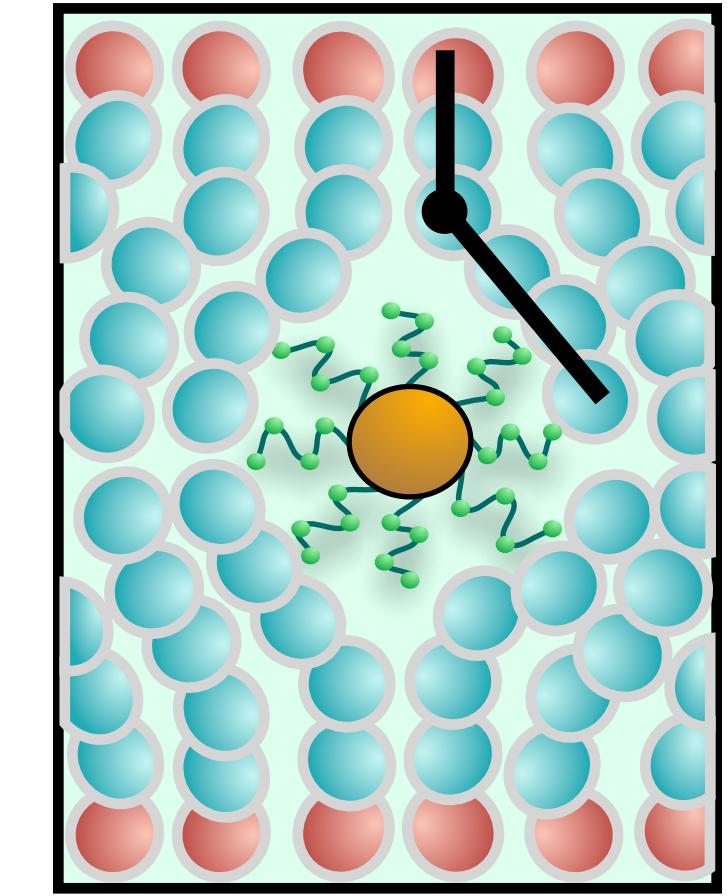
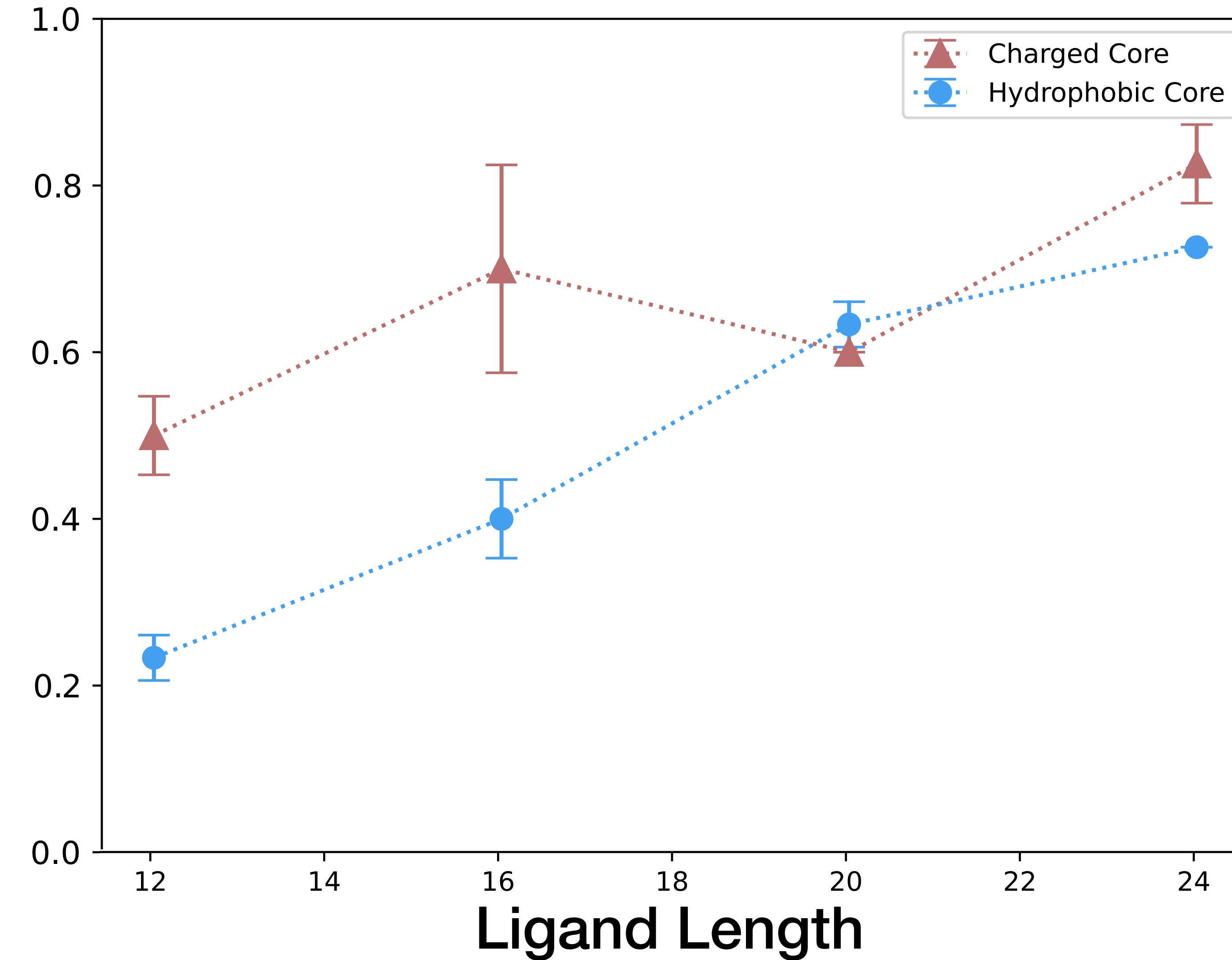
# Does increasing ligand length, increase hydrophobic nanoparticle aggregation?

Fraction of  
NP's in  
Largest  
Aggregate



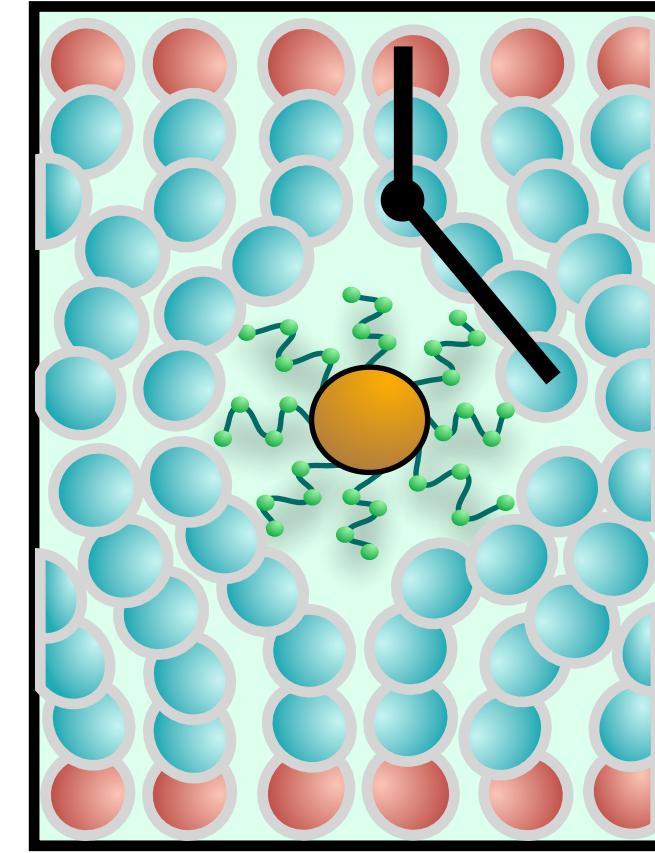
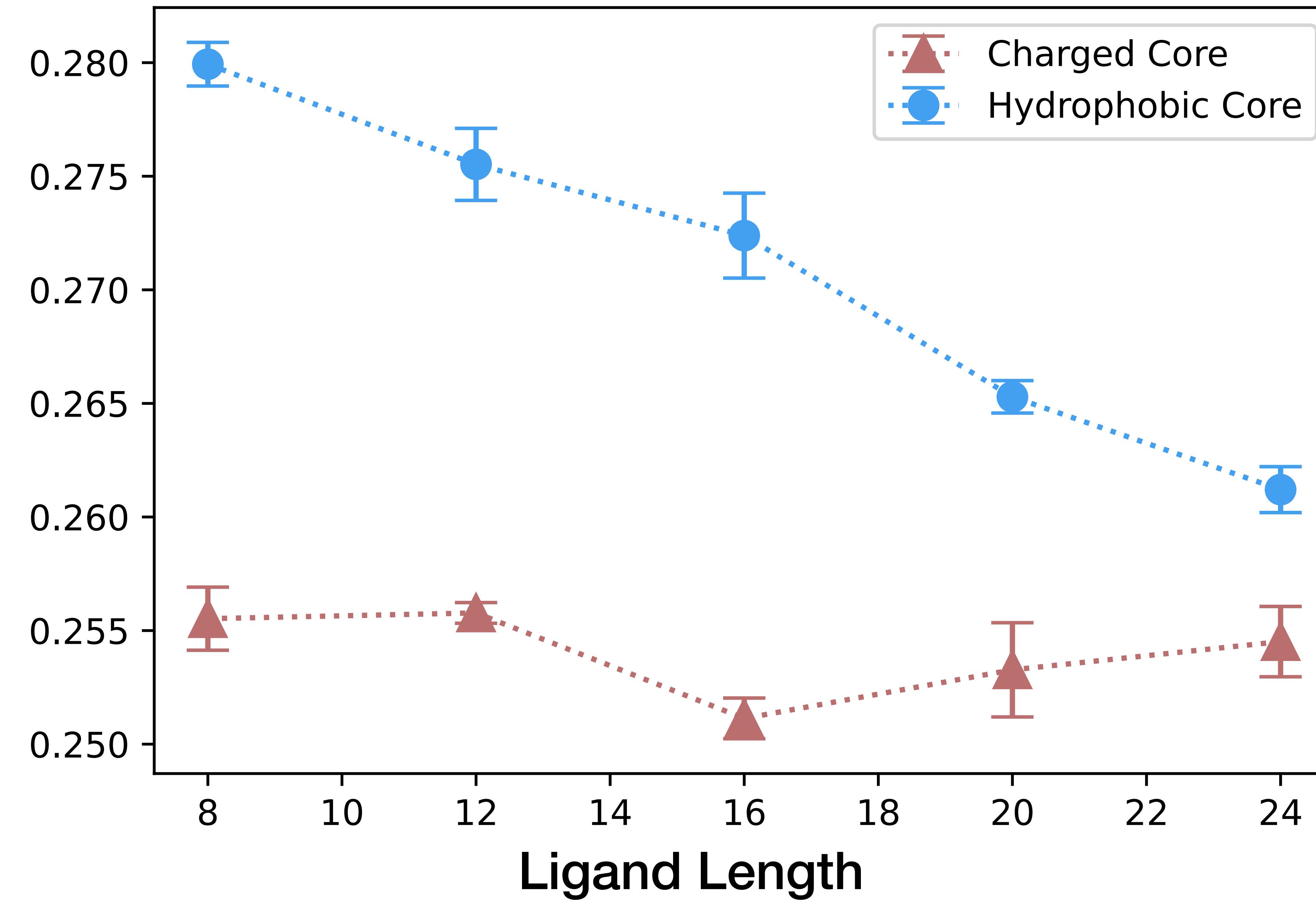
# Does increasing lipid disorder increase charged nanoparticle aggregation?

Fraction of  
NP's in  
Largest  
Aggregate



# Does charged nanoparticle ligand length disrupt lipid acyl chain order?

Acyl Chain  
Order  
Parameter

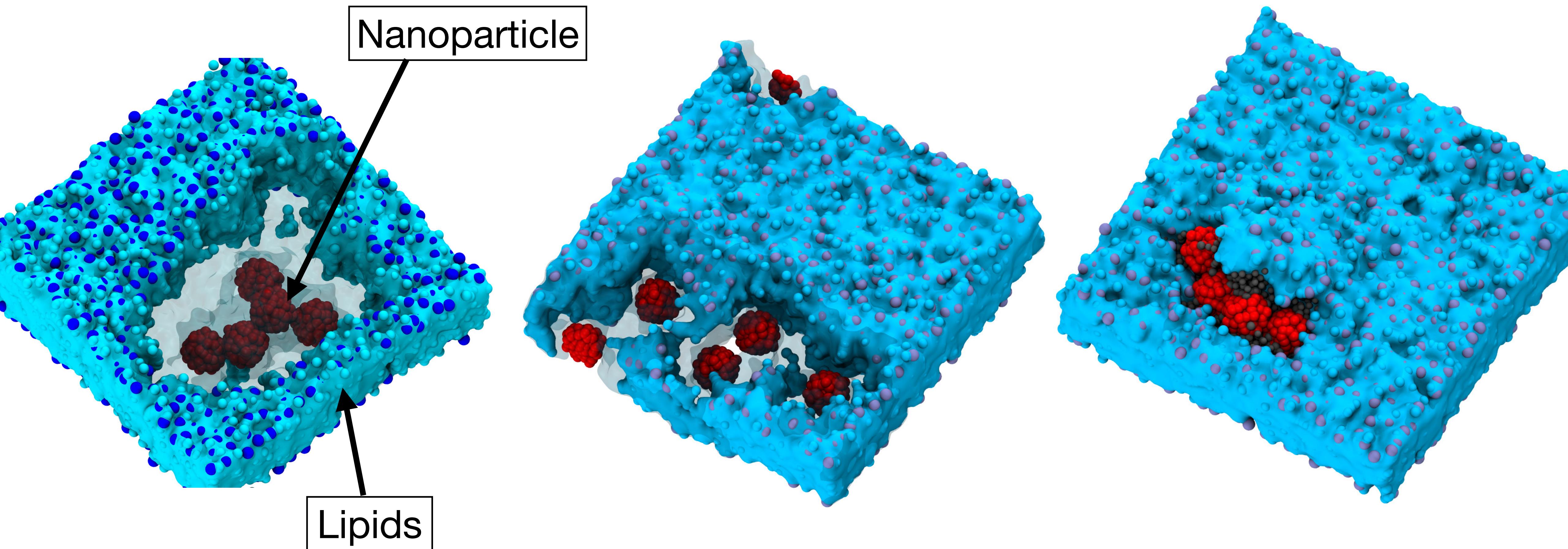


# How does nanoparticle surface charge affect aggregation?

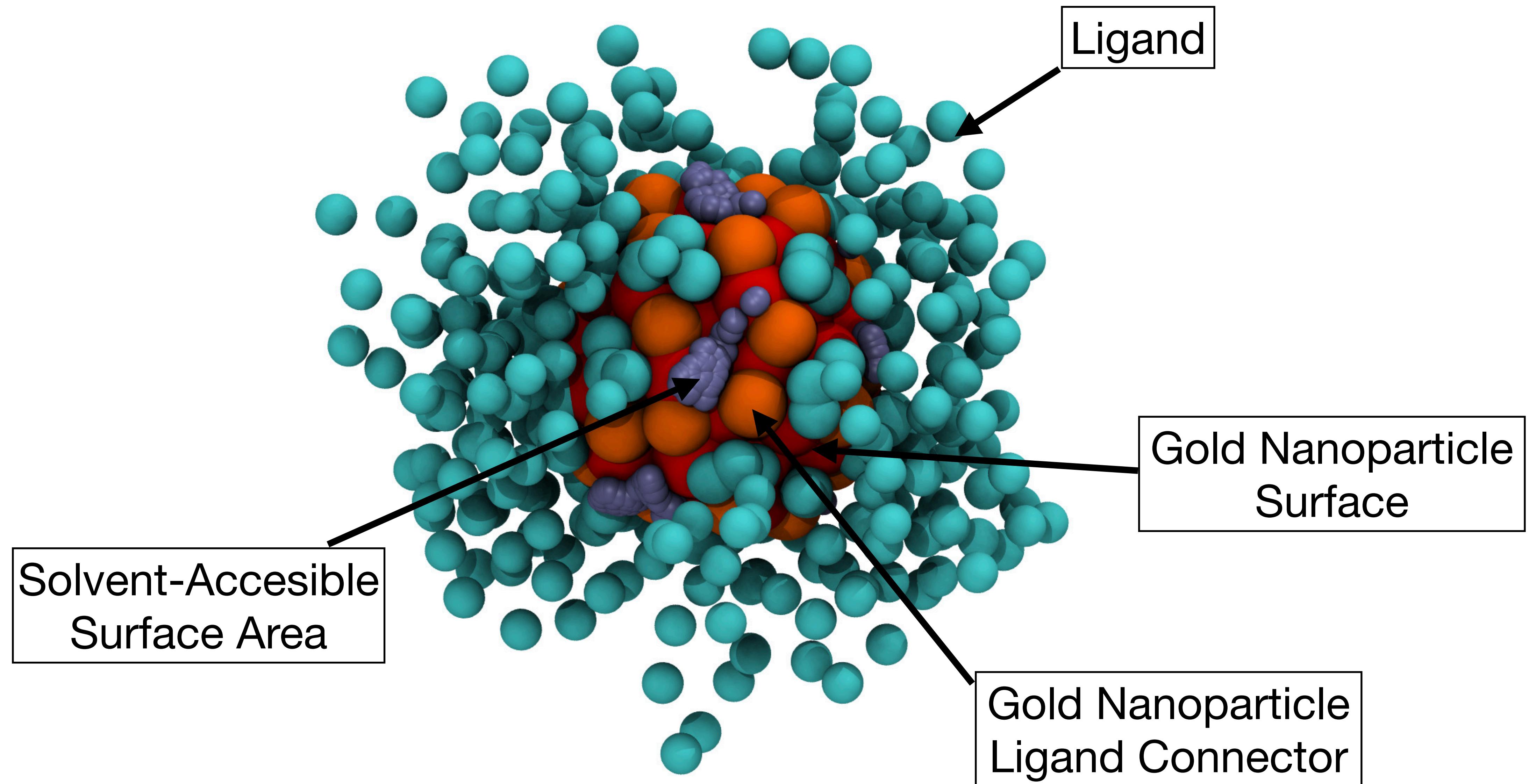
70% Ligand Coverage

60% Ligand Coverage

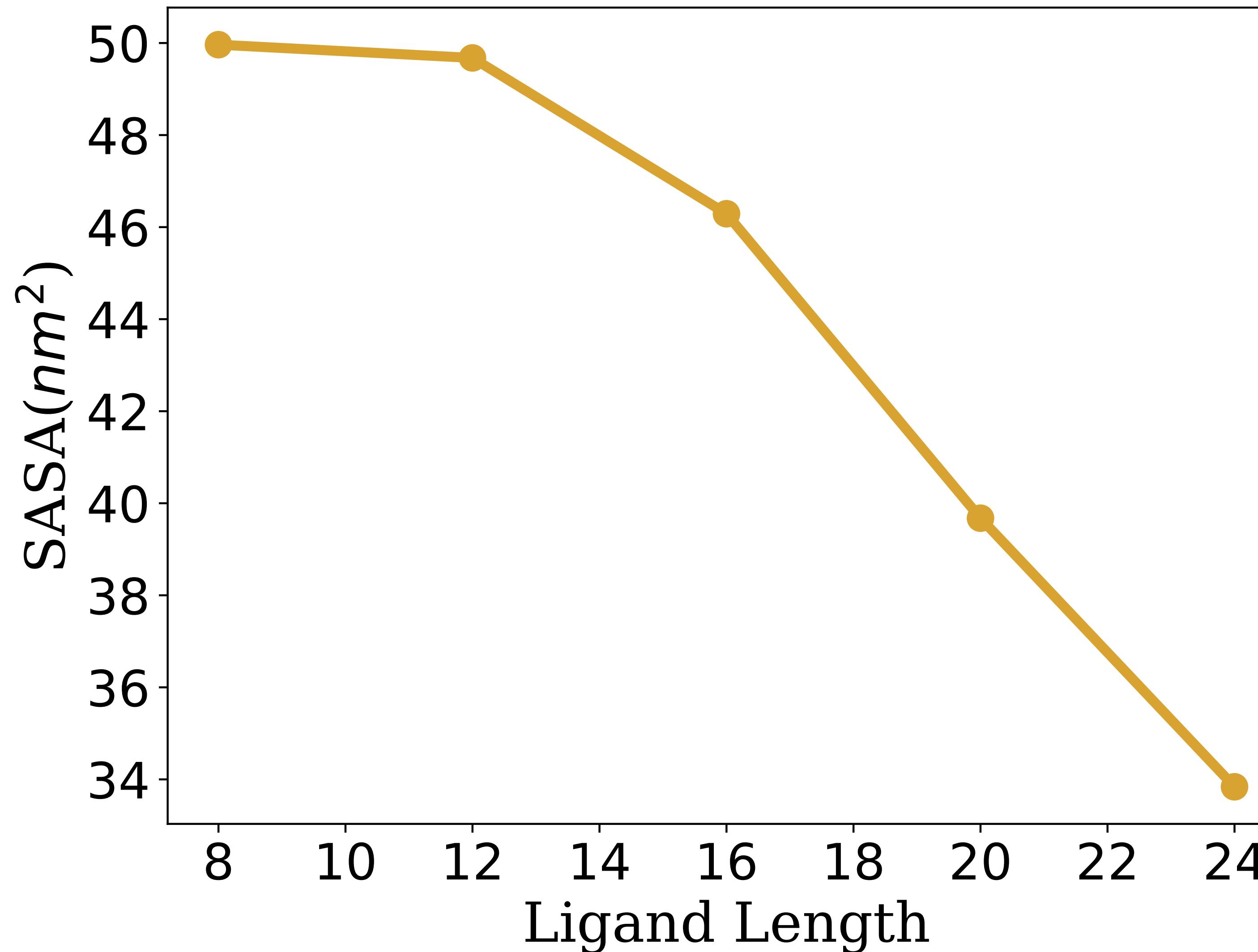
40% Ligand Coverage



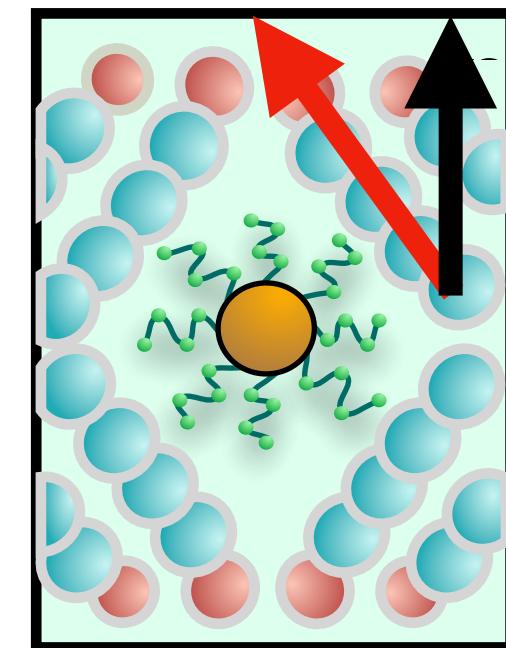
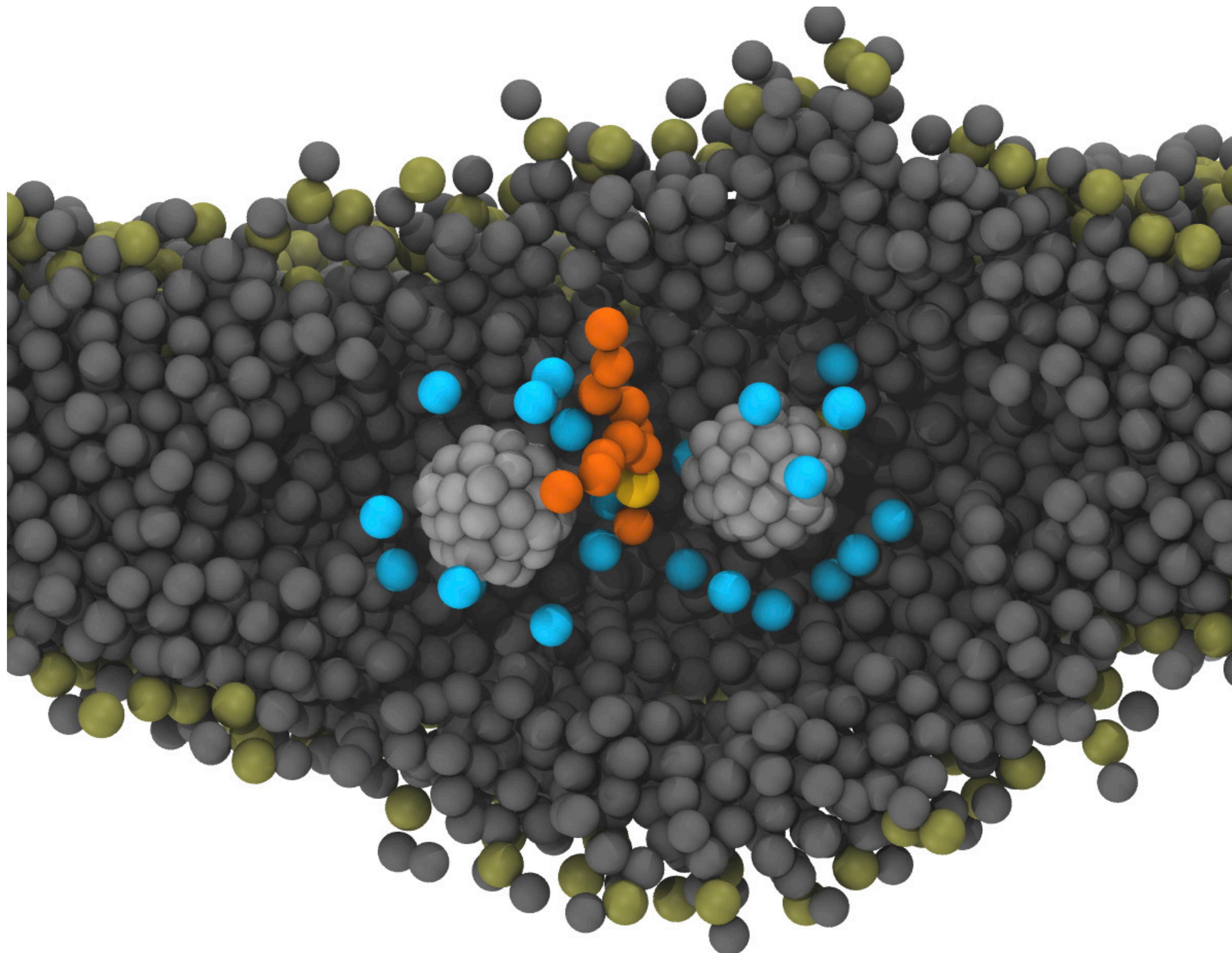
# Small charged nanoparticles have exposed surface regions



# Does increasing ligand length decrease nanoparticle surface exposure?

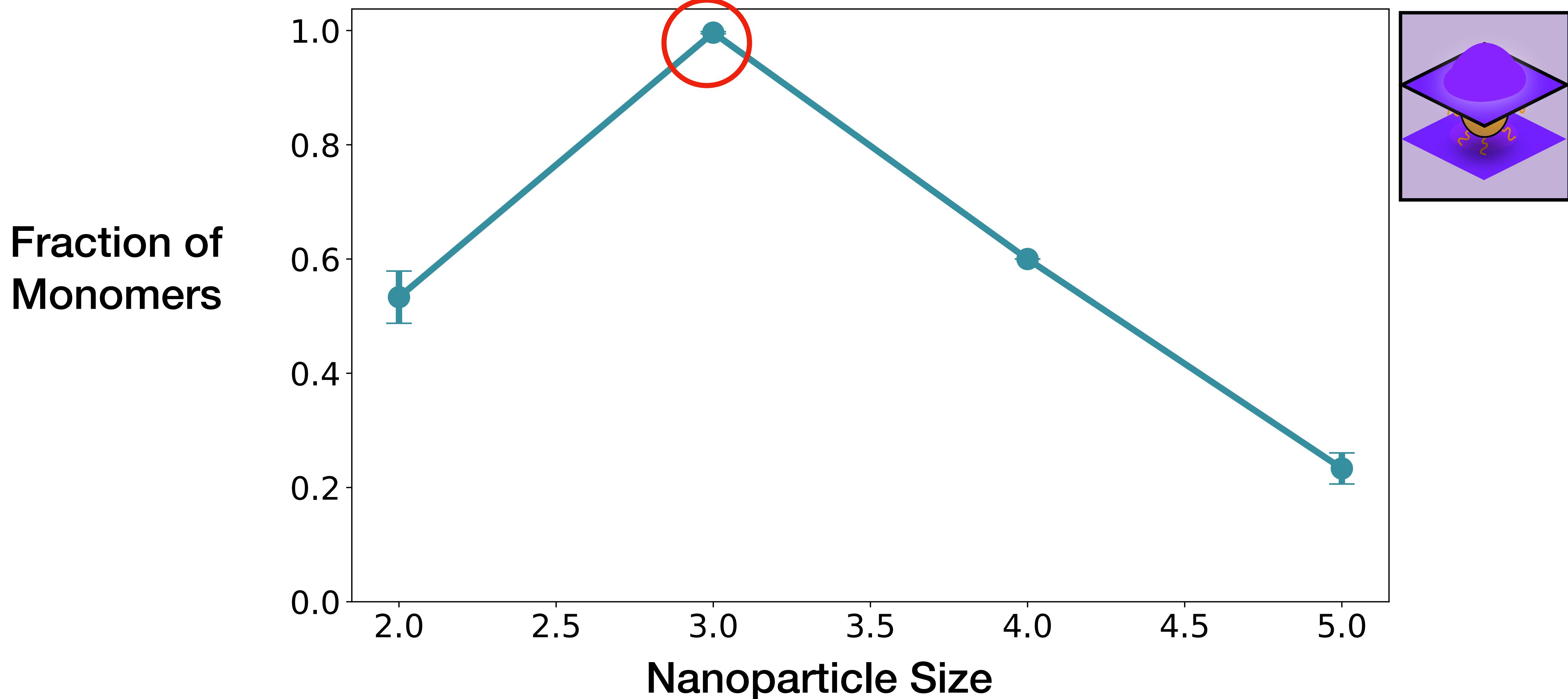


# Are the lipids around charged nanoparticles tilted?

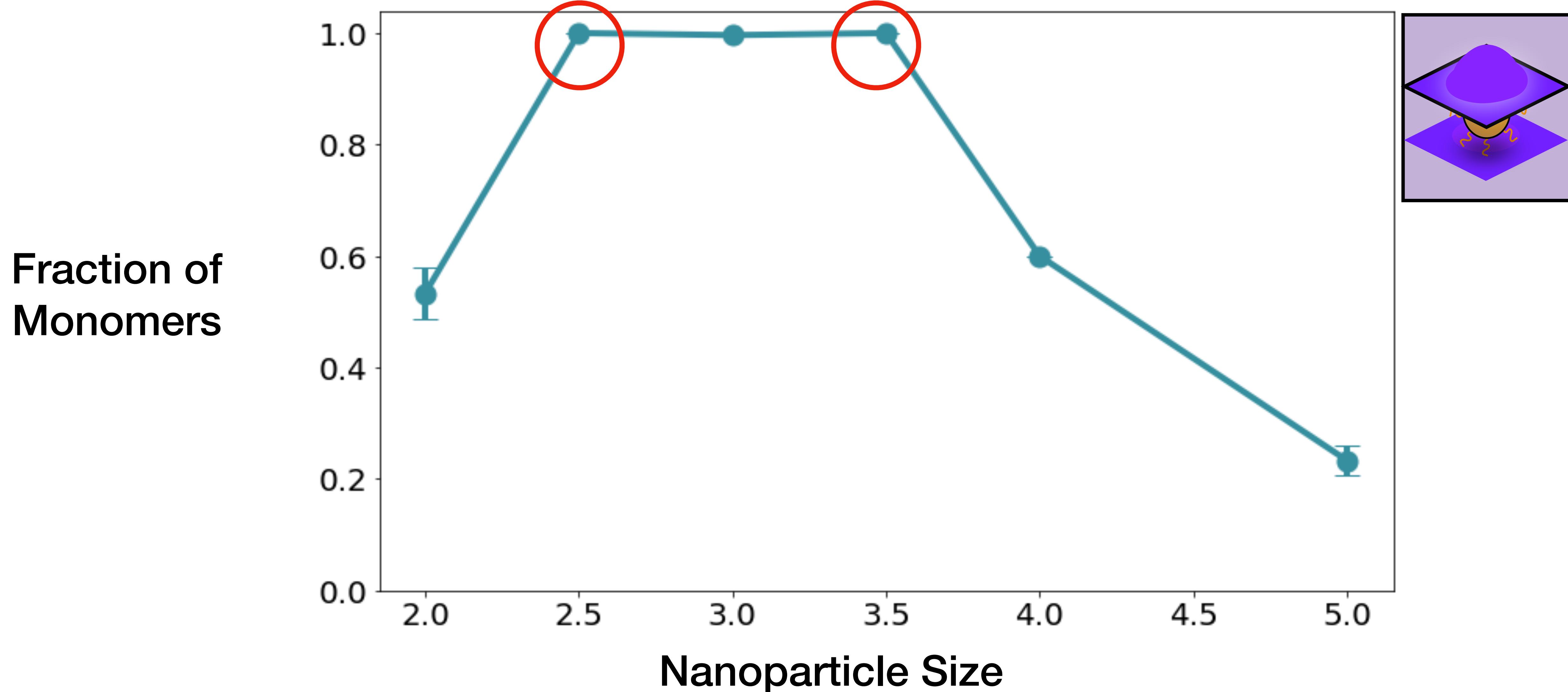


# **Membrane Deformations**

# Does nanoparticle aggregation increase with nanoparticle size?

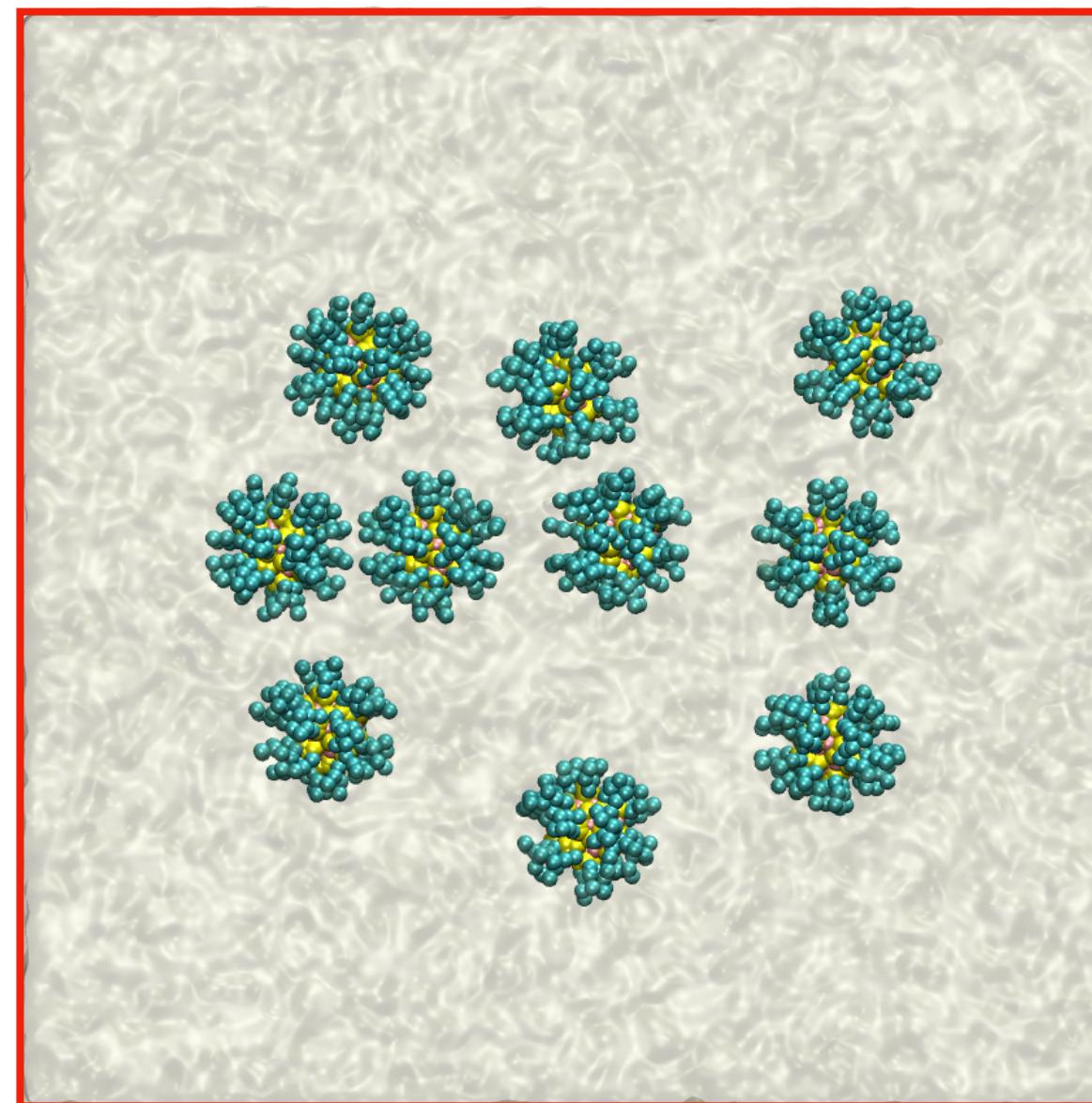


# Does nanoparticle aggregation increase with nanoparticle size?

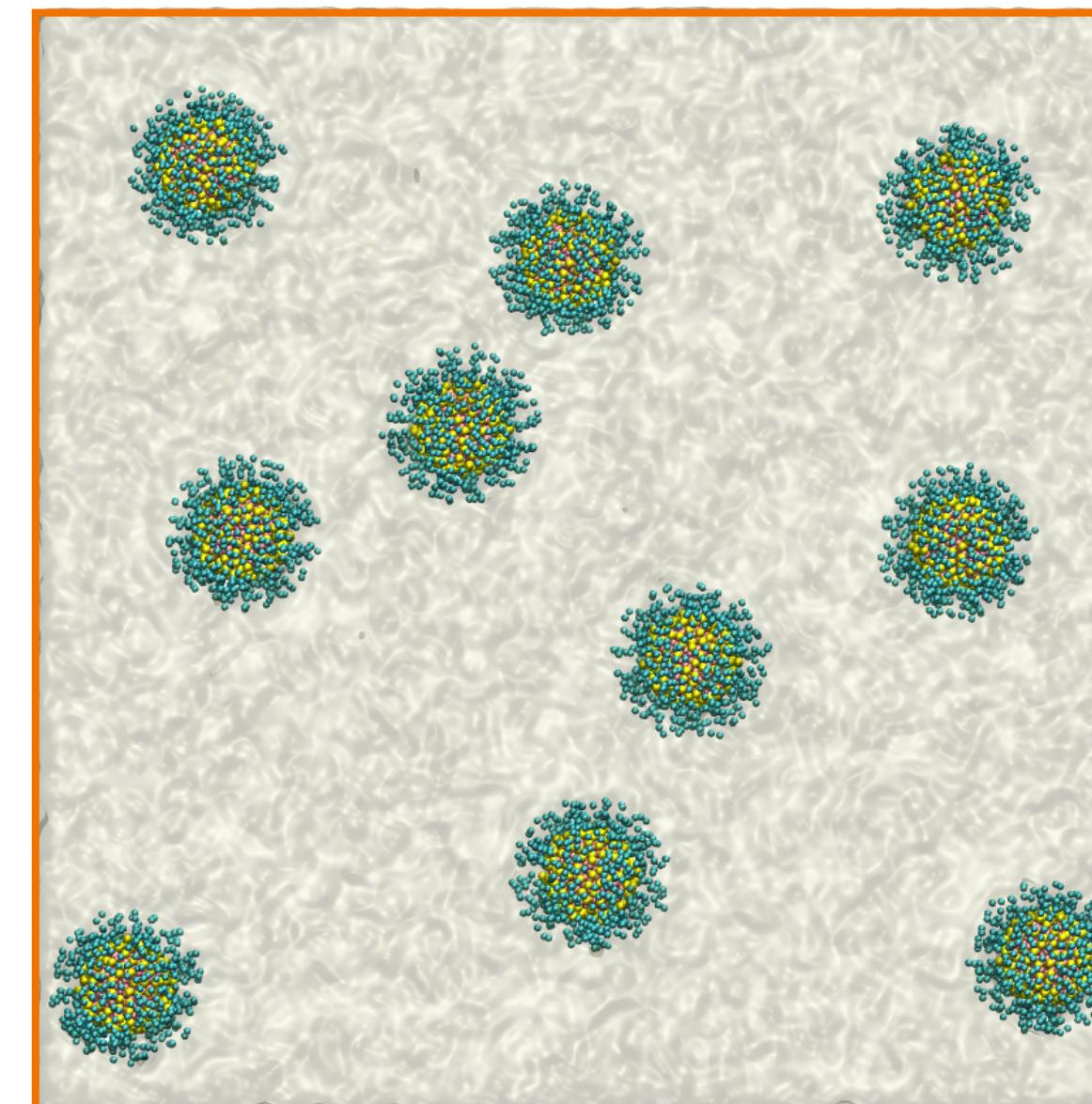


# Starting Configurations of Nanoparticles at Varying Sizes

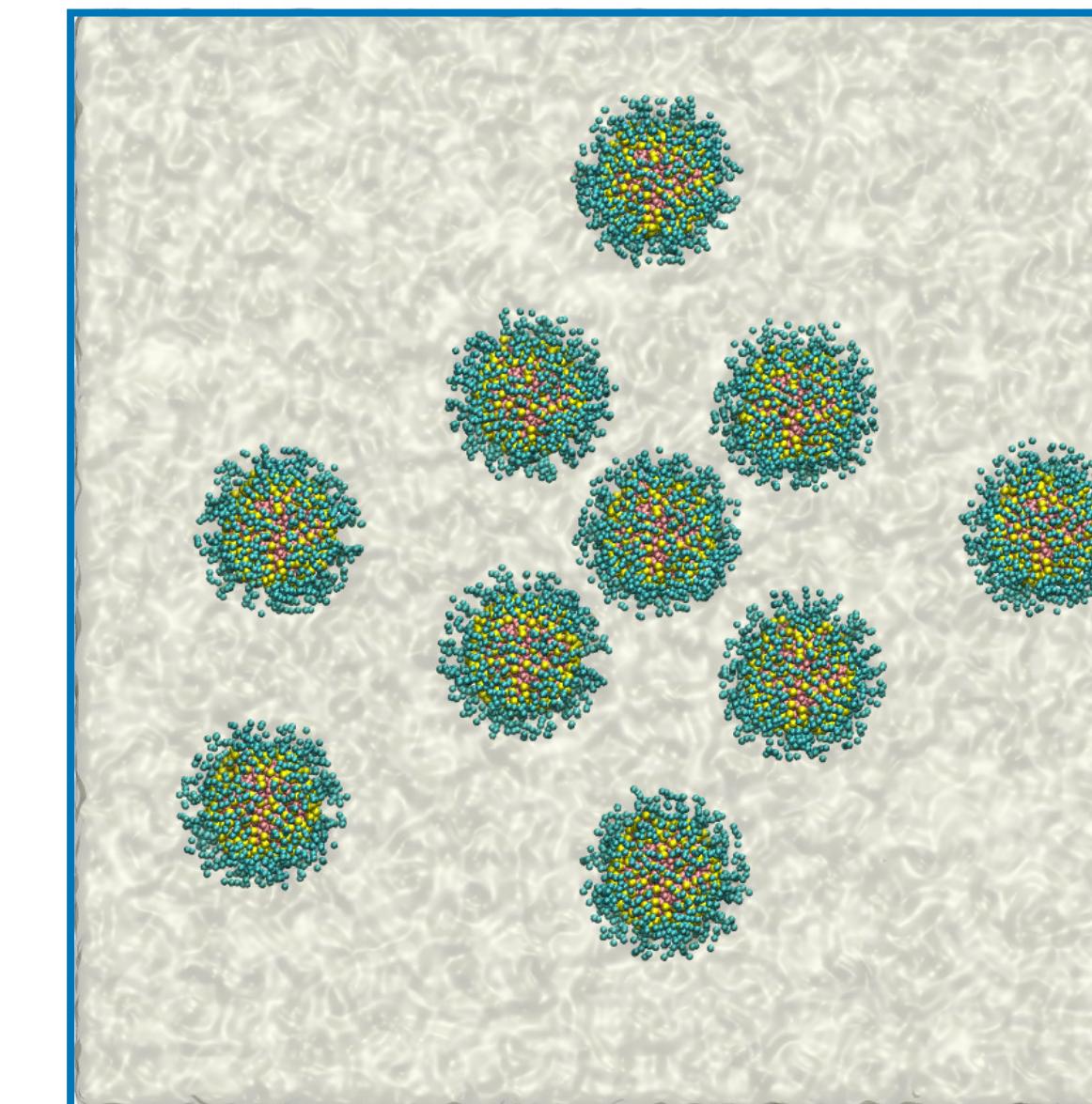
2nm Nanoparticles



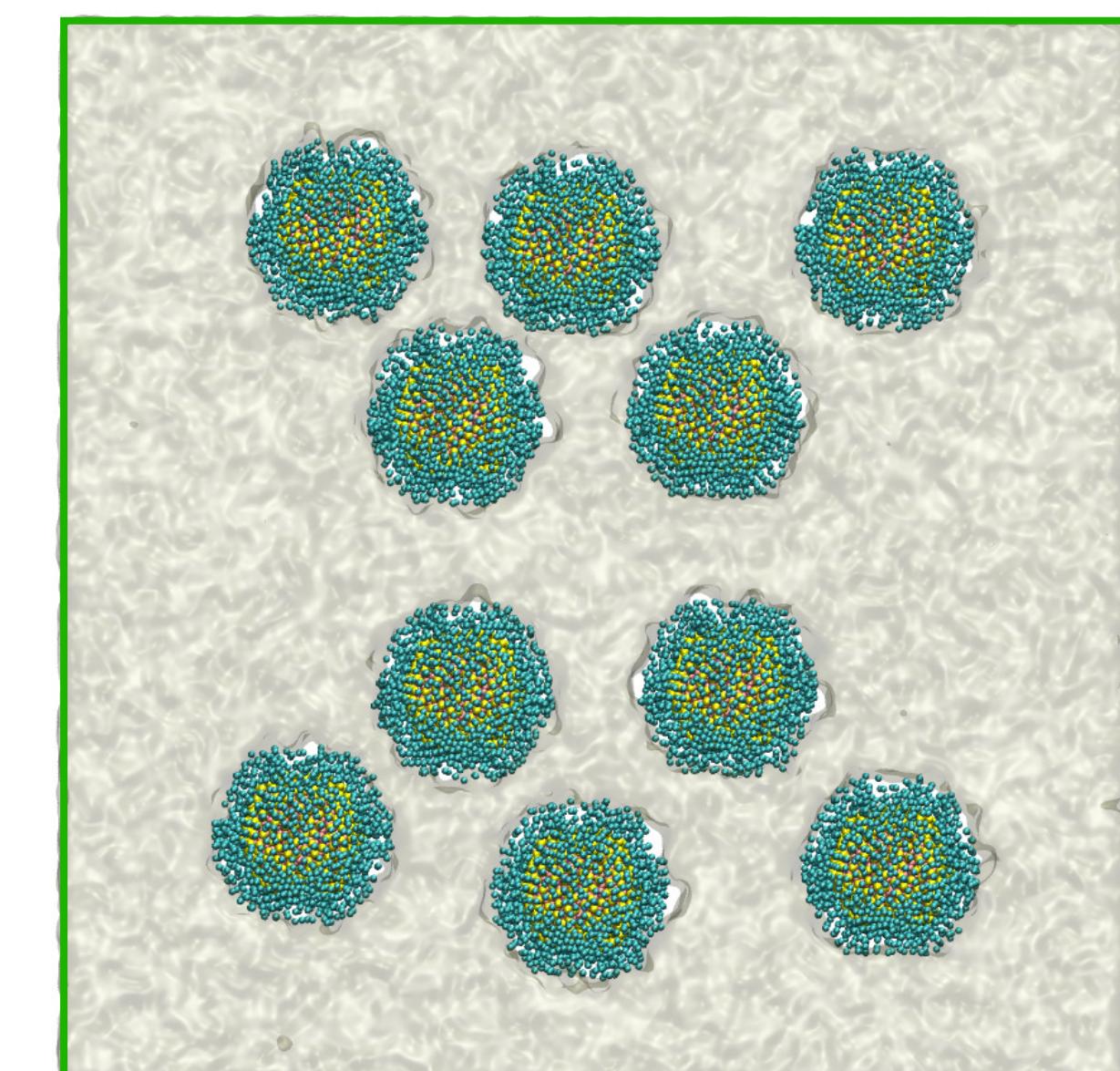
3nm Nanoparticles



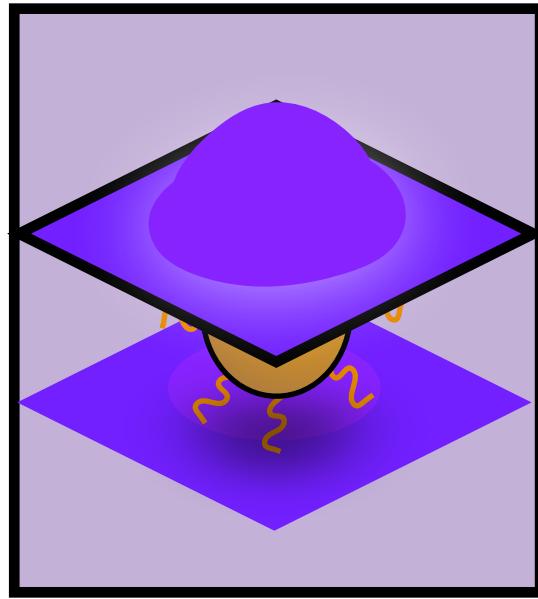
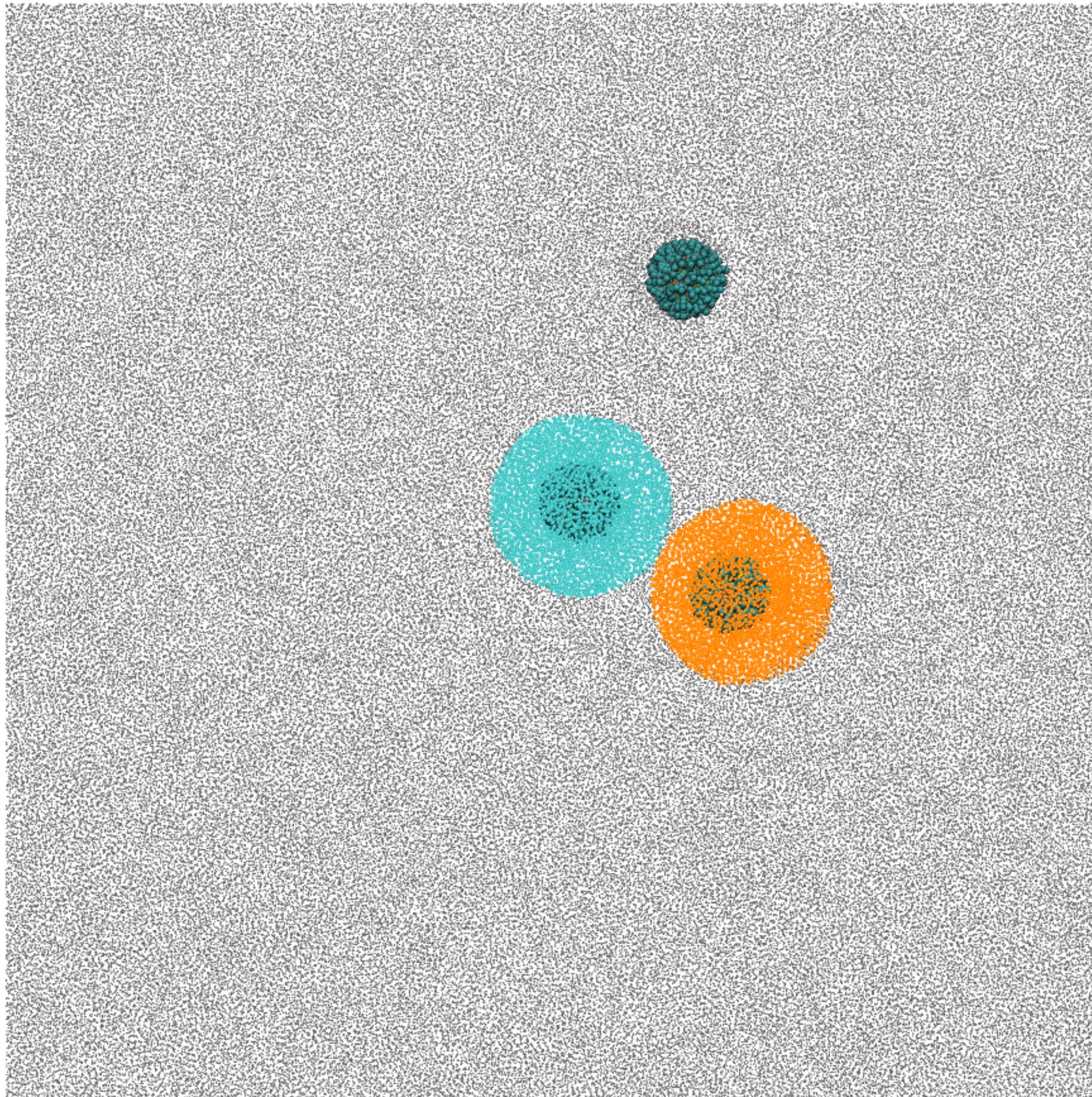
4nm Nanoparticles



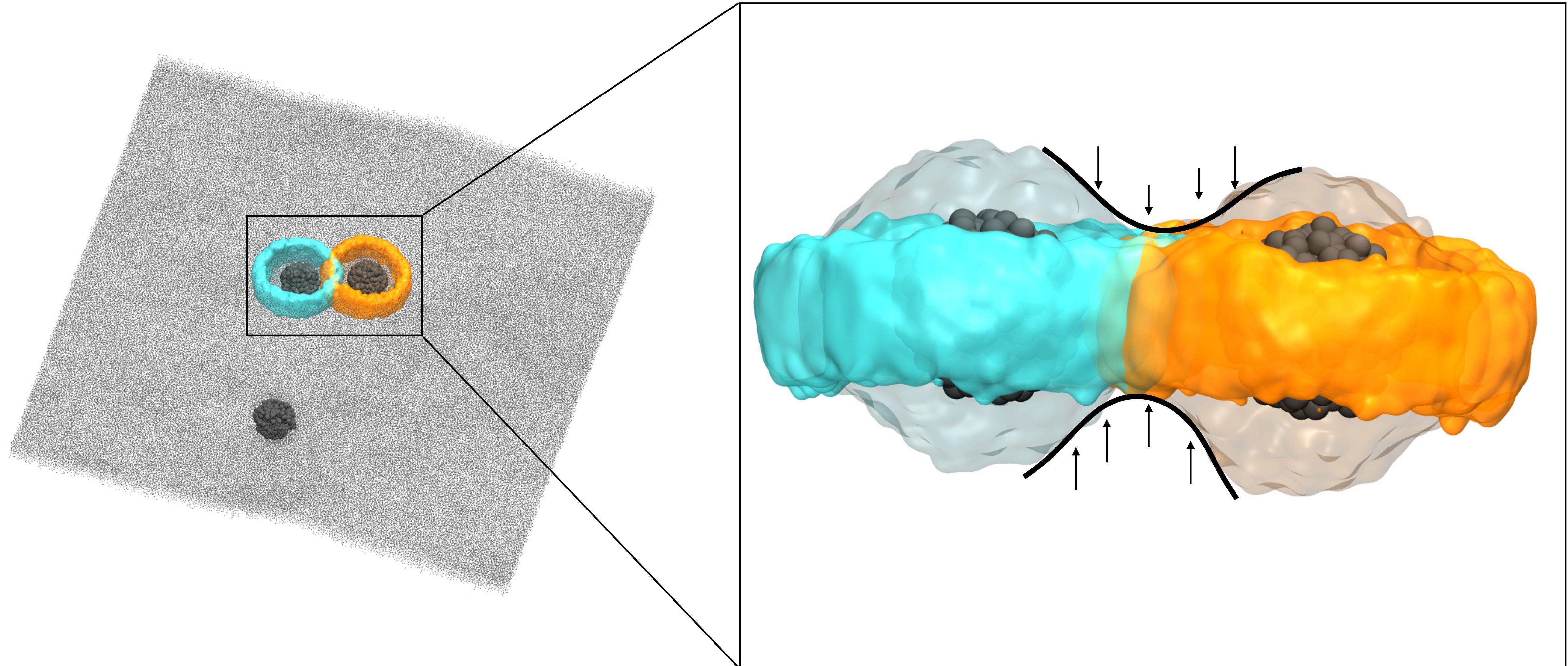
5nm Nanoparticles



# 3nm Nanoparticles in Large POPC Membrane



# Negative Curvature may Increase Equilibration Time



# Summary

- Nanoparticle ligand length disrupts lipid order in the membrane leading to more aggregation
- Charged nanoparticles disrupt packing more than their hydrophobic counterparts
- Equilibration of large nanoparticle systems may be slowed by unfavorable membrane bending