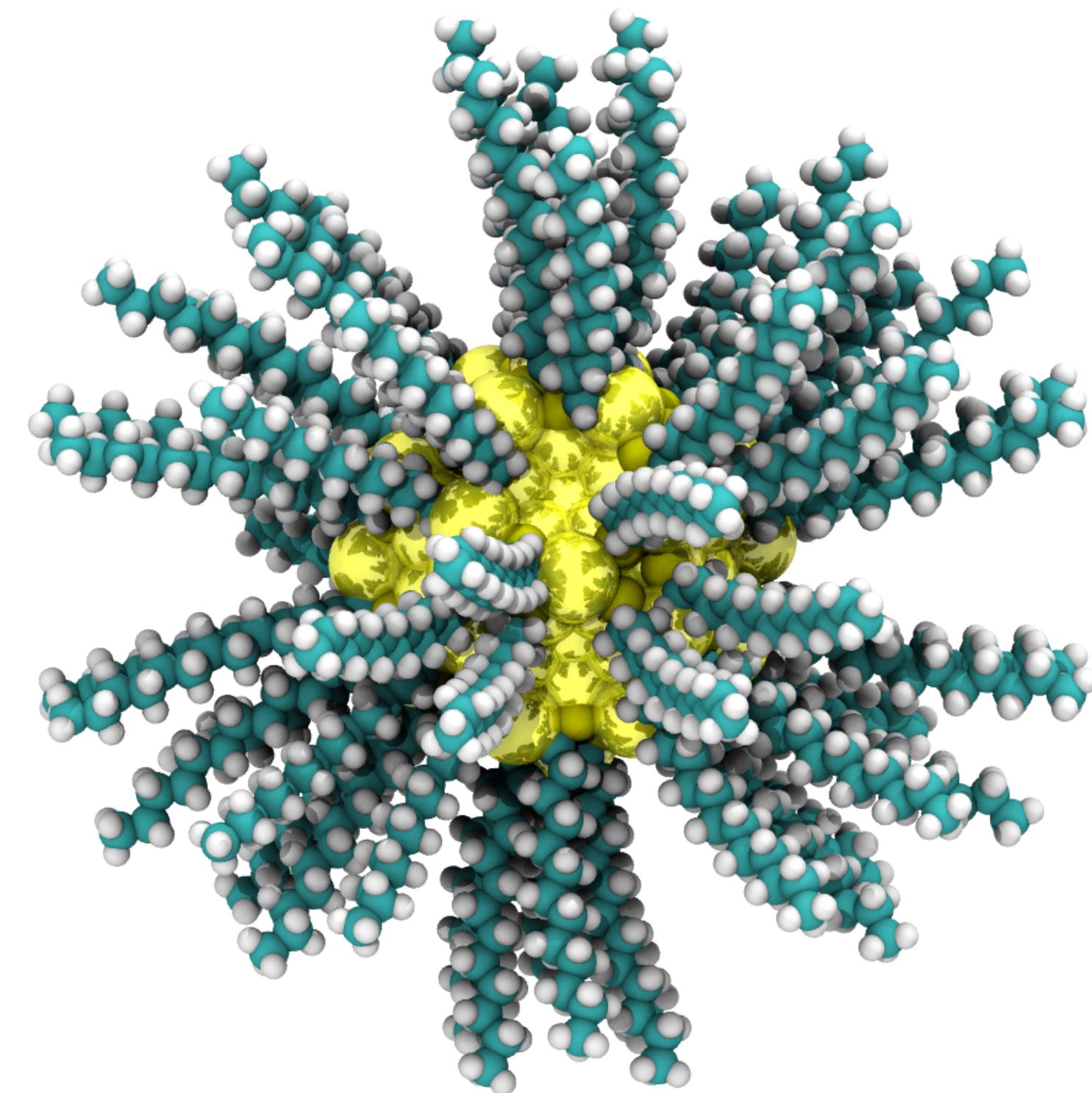


Exploring the Bionanotechnology Interface

CCIB Seminar

Jahmal Ennis 9/12/23



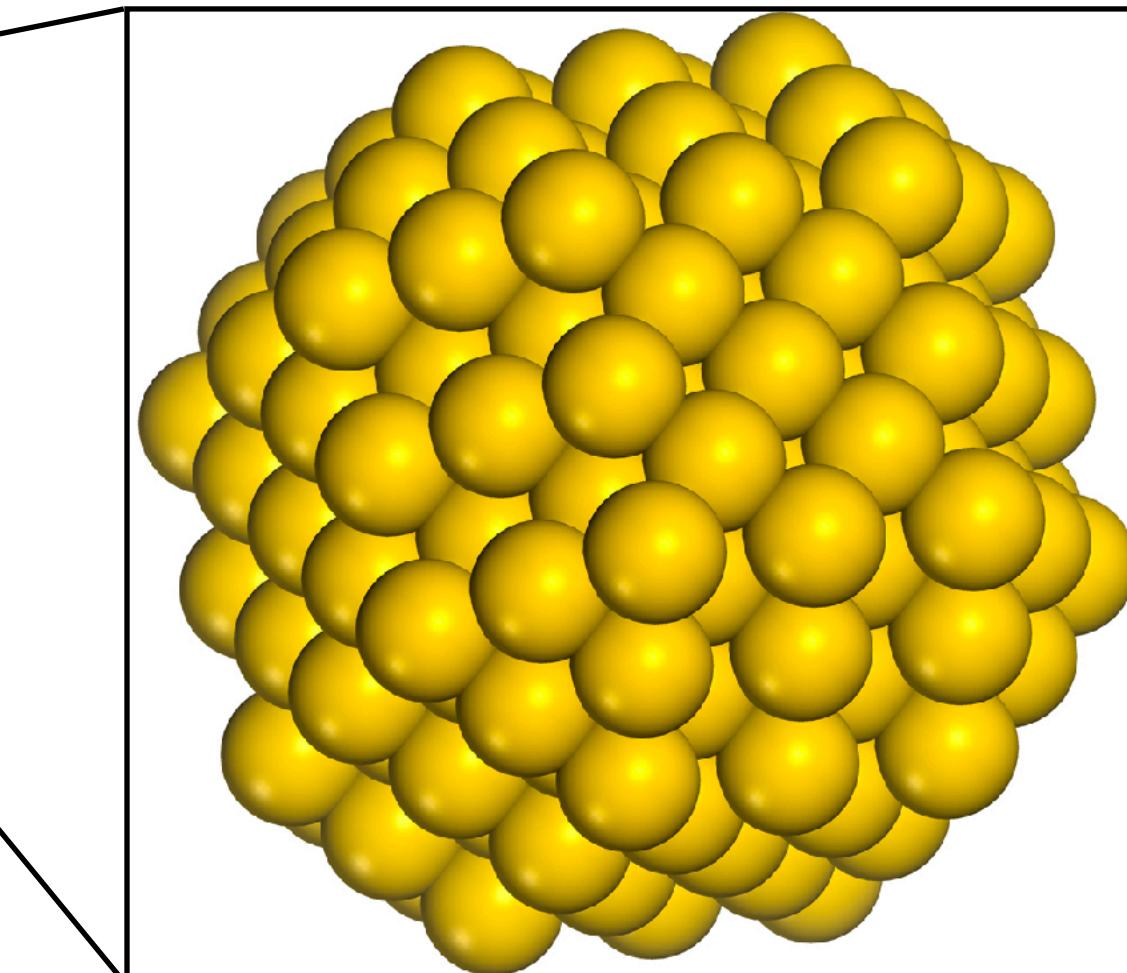
Outline

- Background/Motivation
- Results
 - Core parameter effects on the membrane
 - Ligands cause lipid disordering
 - Aggregation is dependent on both core parameters and ligand length
- Summary
- Future Directions

Why are metals of interest, particularly gold?

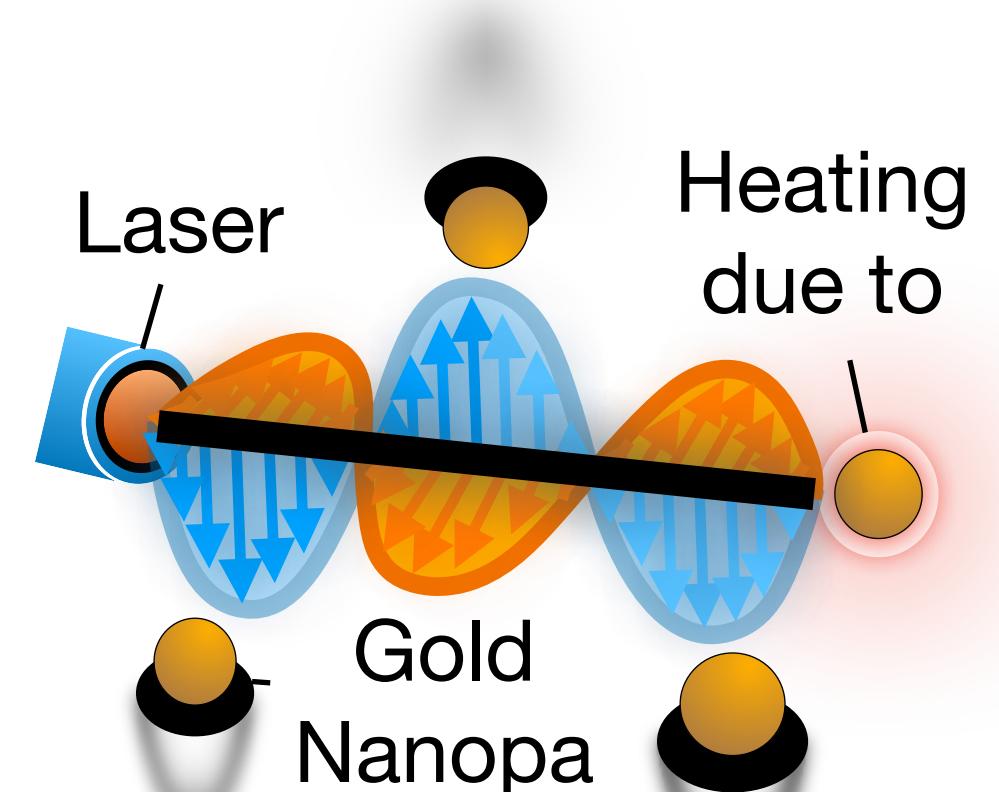
Bulk Gold

- Non-reactive
- Very stable
- No light sensitivity



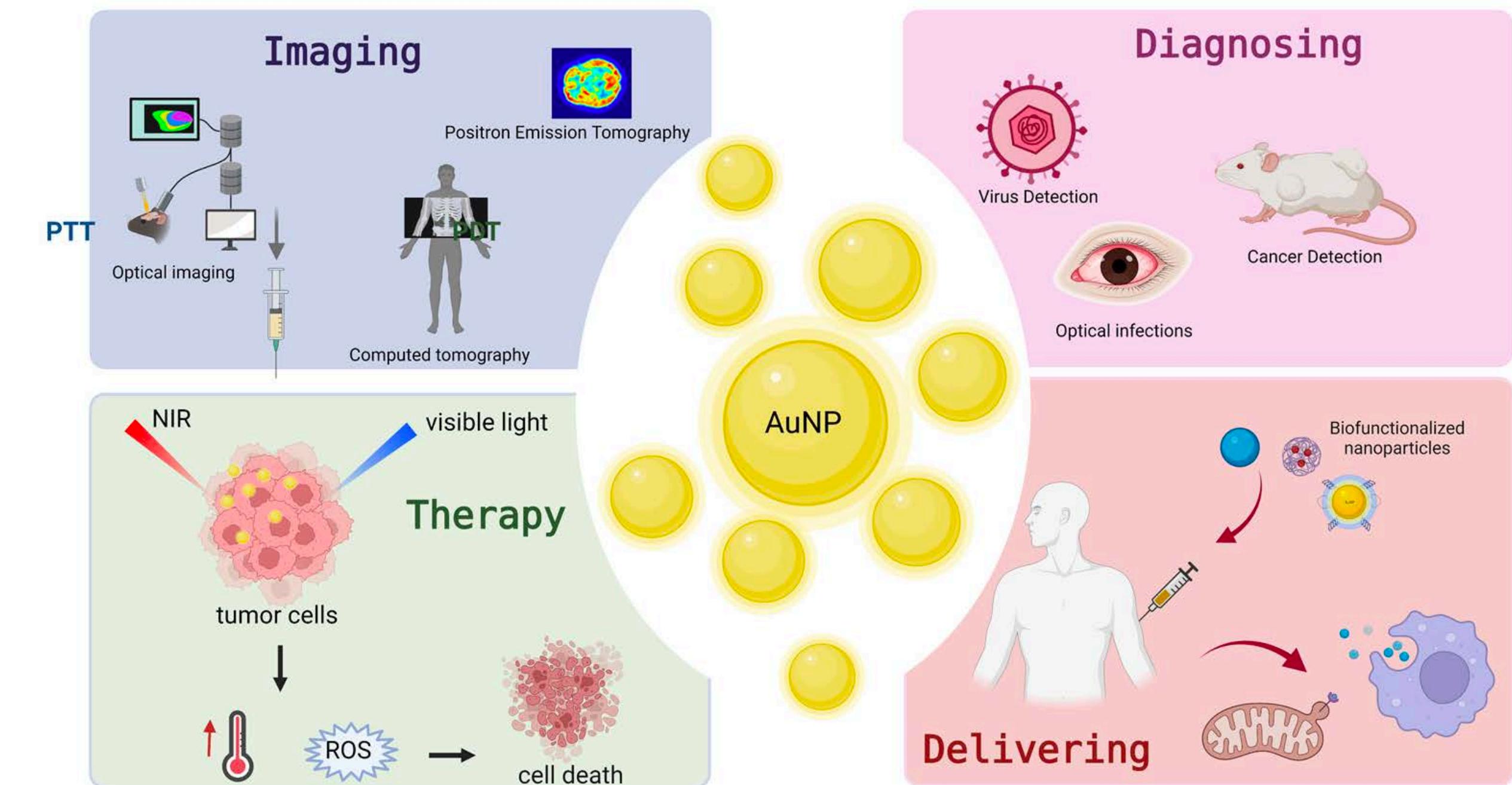
Nano Scale
Gold

- Reactive
- Light sensitivity

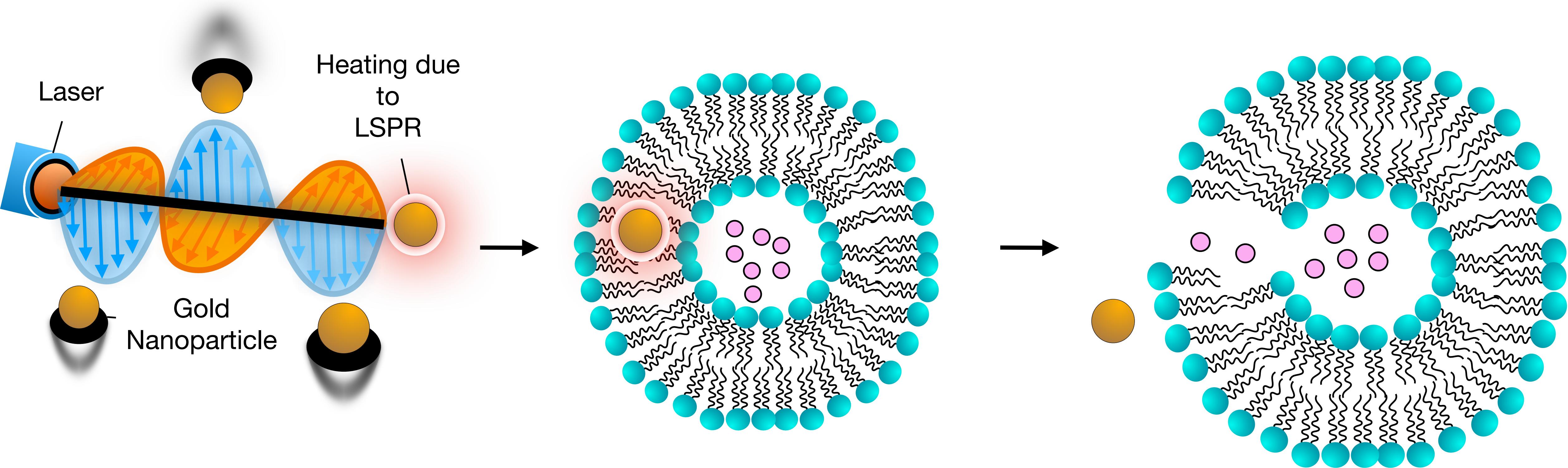


Nanoparticles: A versatile tool that needs to be better understood

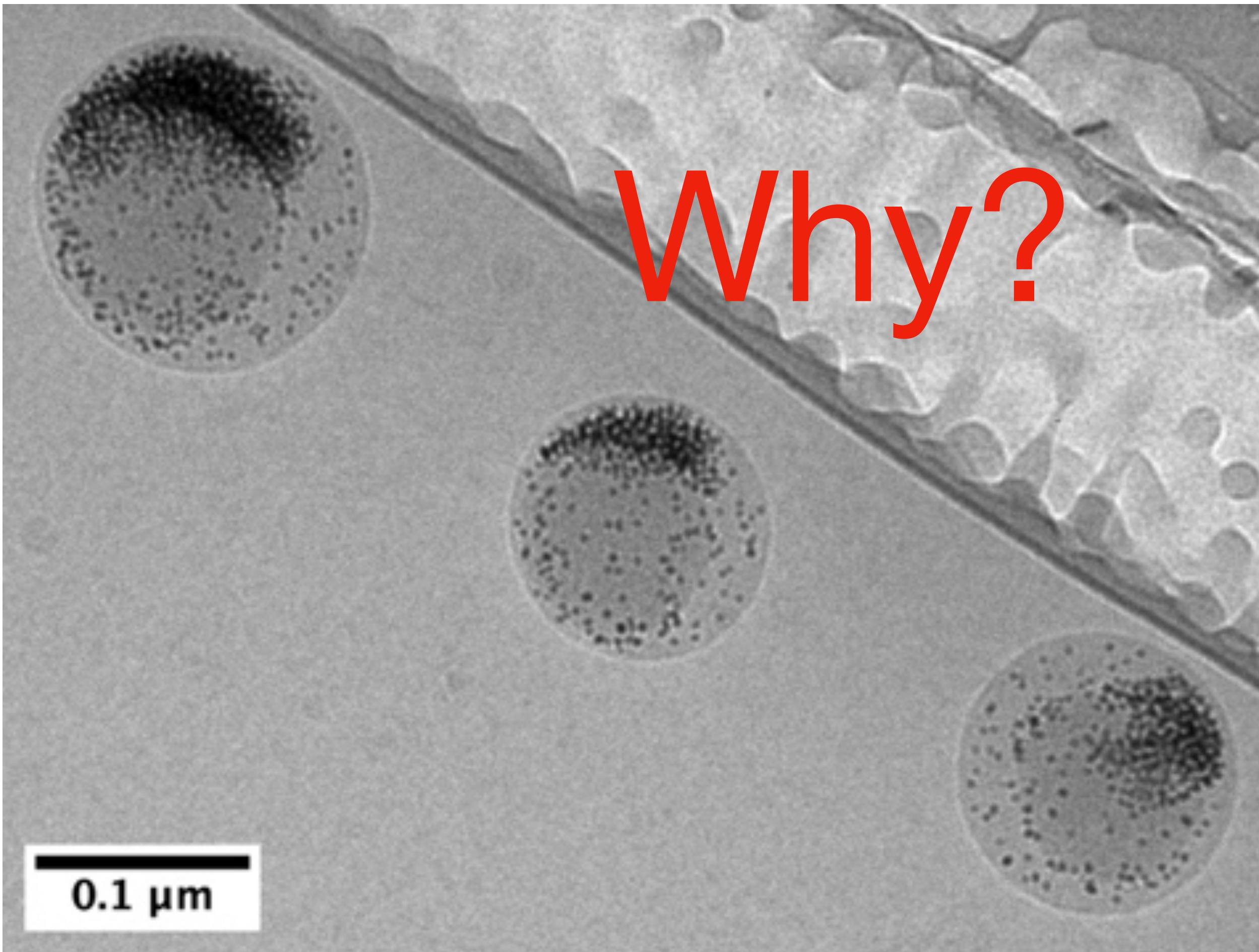
- Photodynamic Imaging
- Diagnostic Tool
- Targeted Drug Delivery Systems



Nanoparticles: A versatile tool that needs to be better understood

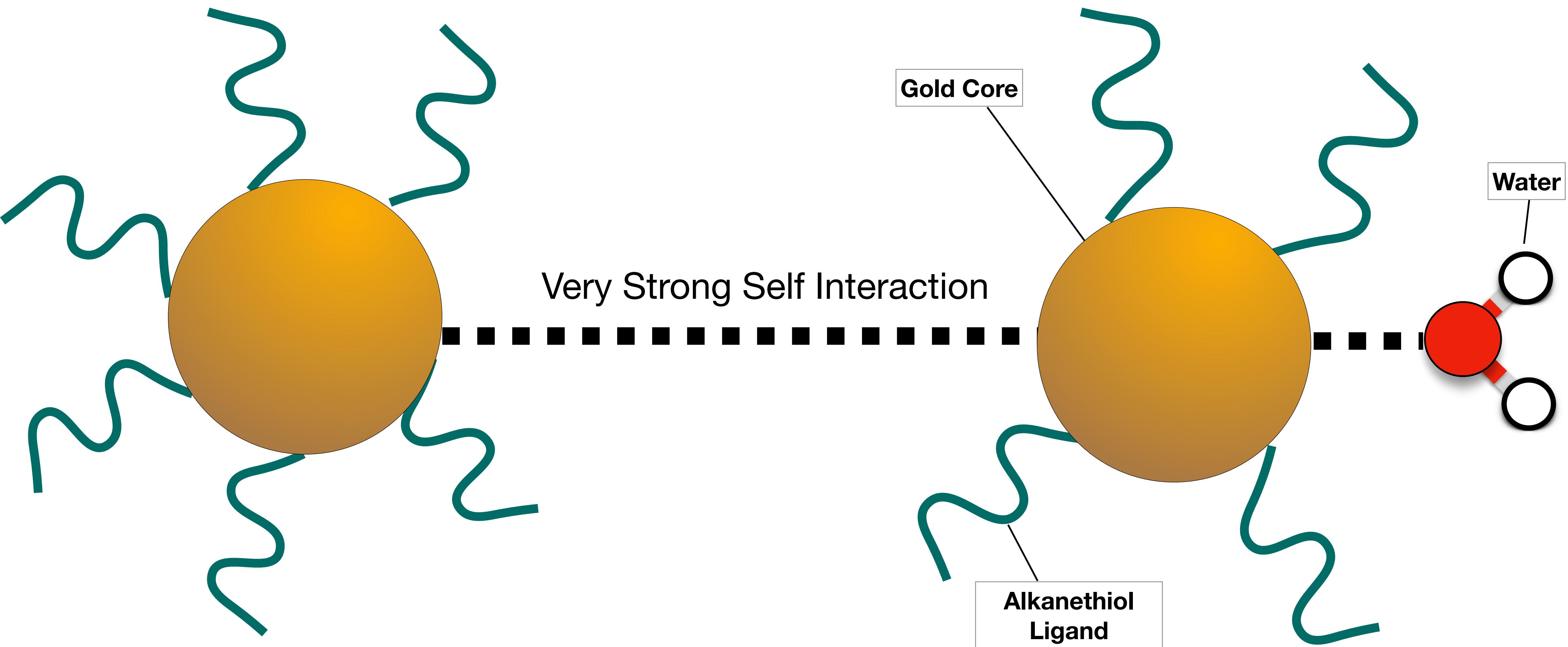


Experimental work shows nanoparticles aggregate in membrane

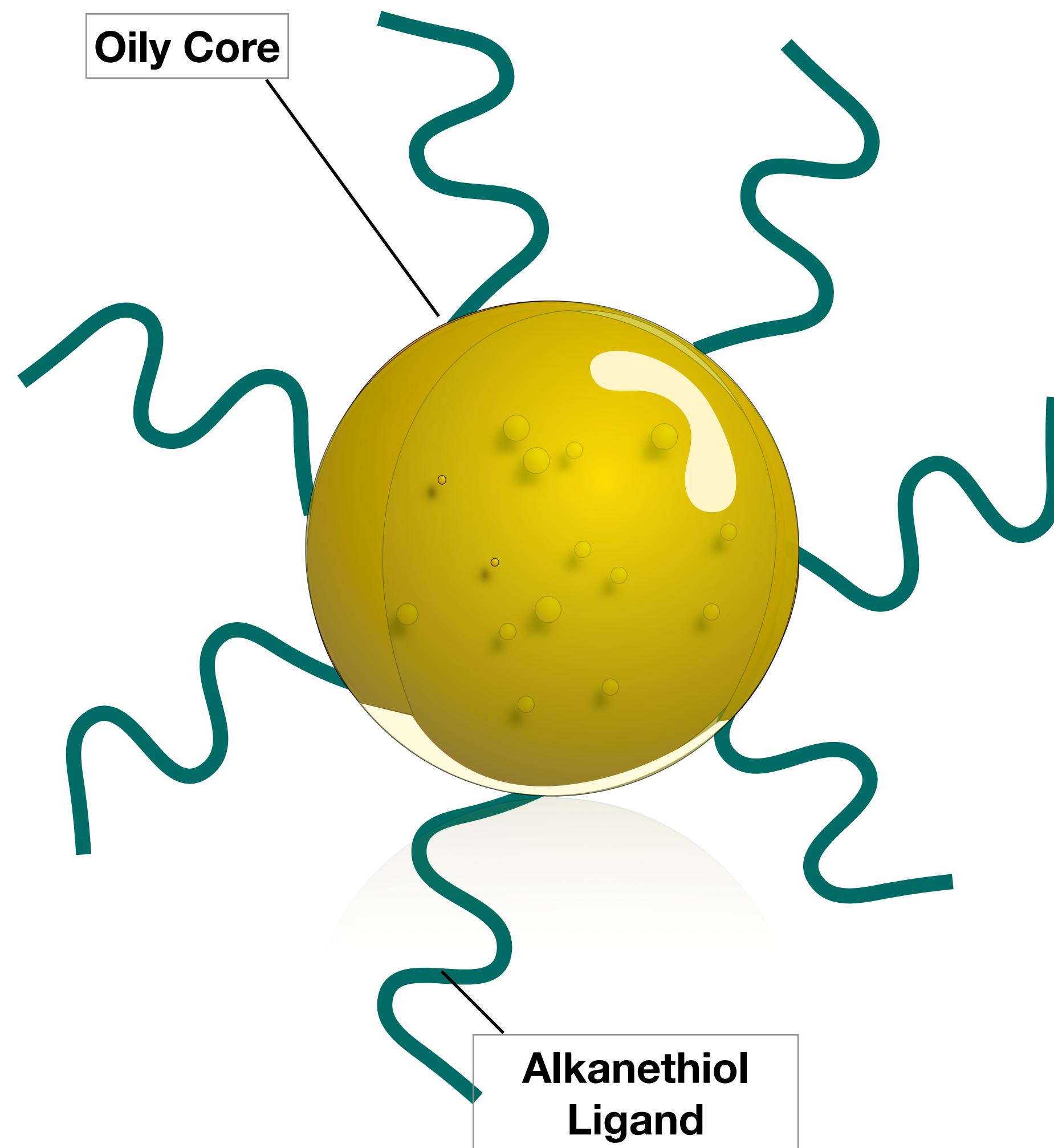


Large movie was here

Ideal gold core model

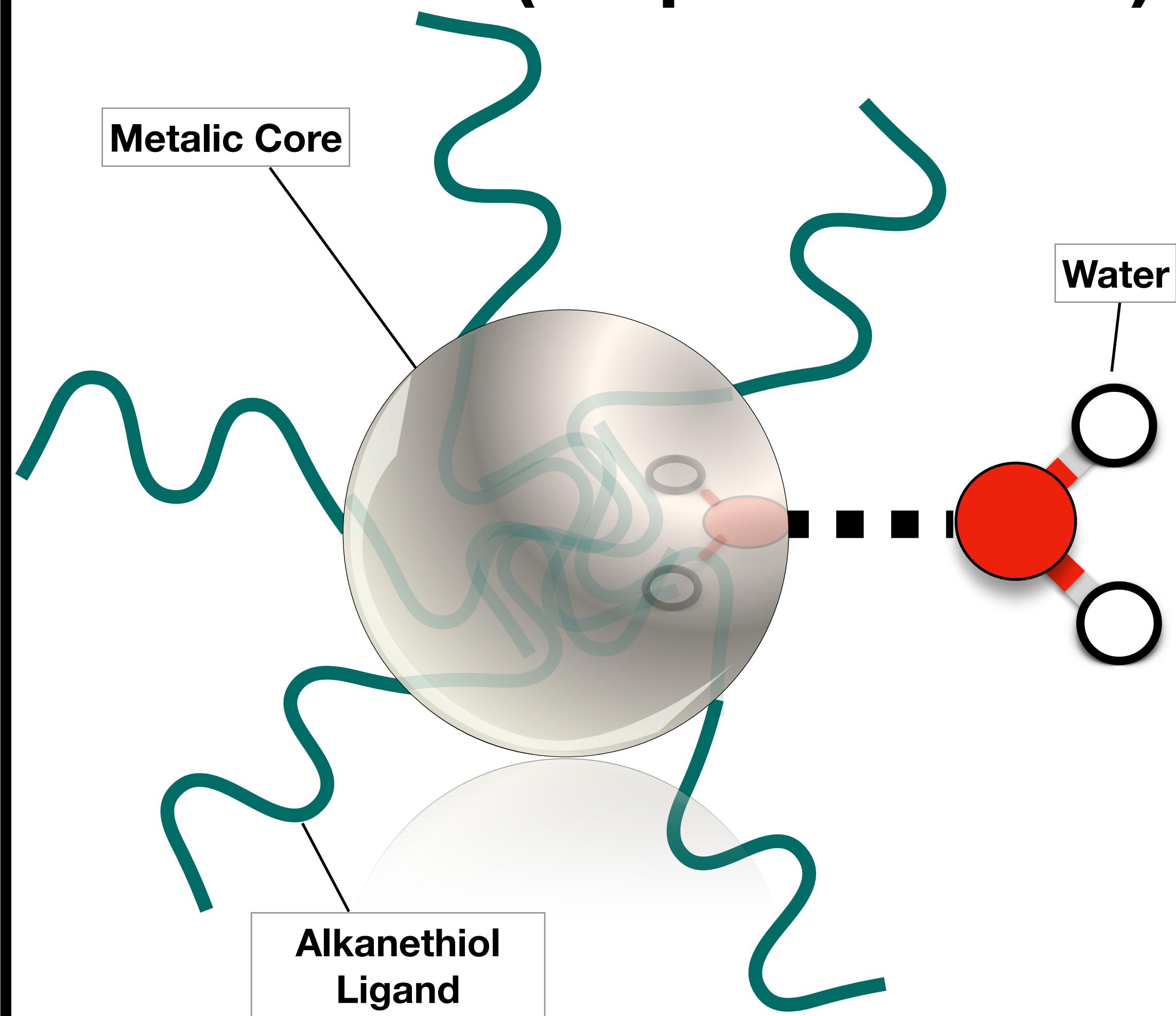


Oily Model (Current Model)



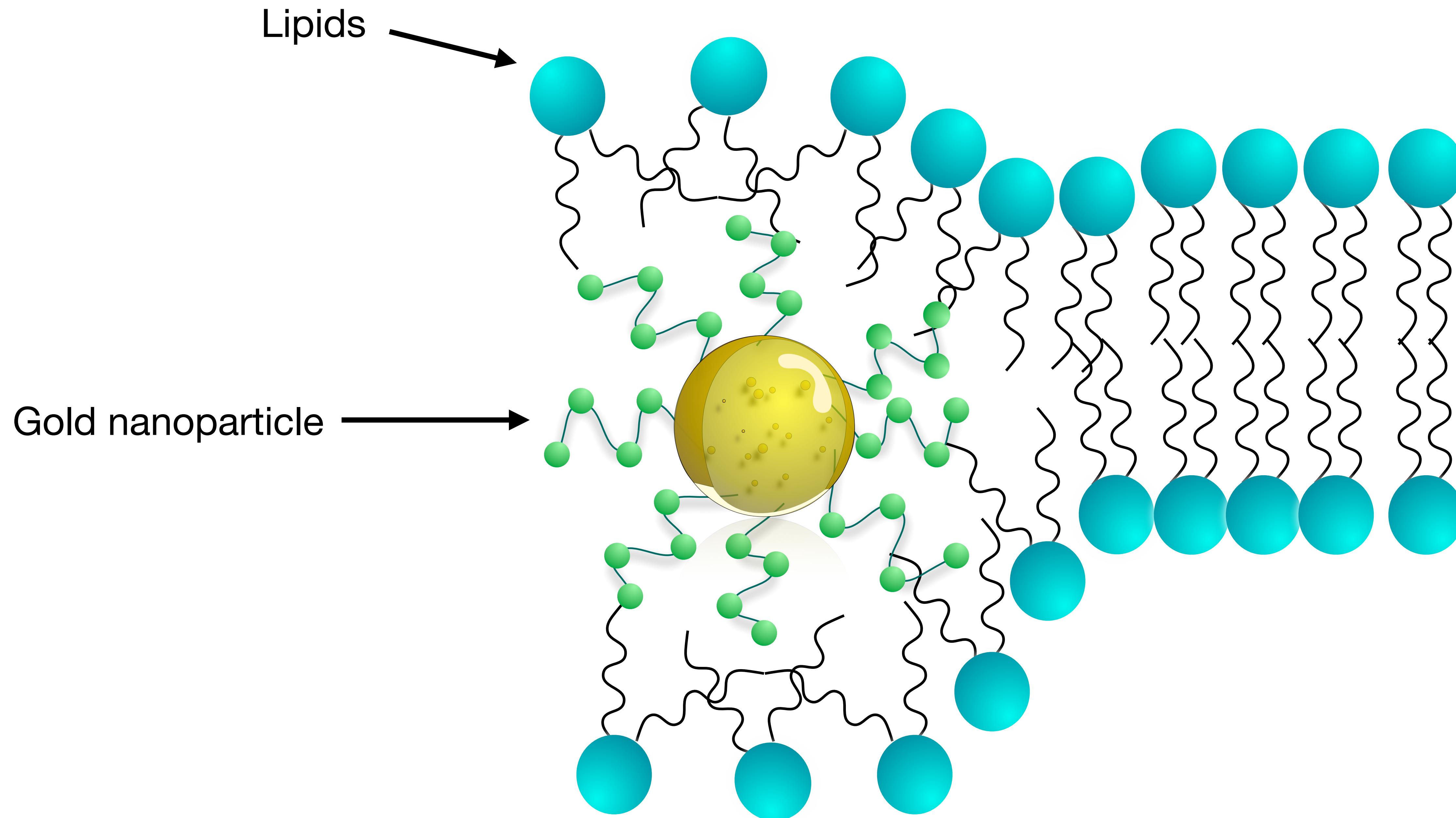
- No hydrogen bonding
- No self Interactions

Polar Model (Proposed Model)



- Hydrogen bonding
- Self Interactions

The interface between gold and lipid



Research Question:

- What is the mechanism of ligand coated gold nanoparticle aggregation in lipid membranes?

How does ligand length affect nanoparticle aggregation?

How is aggregation dependent on gold core model?

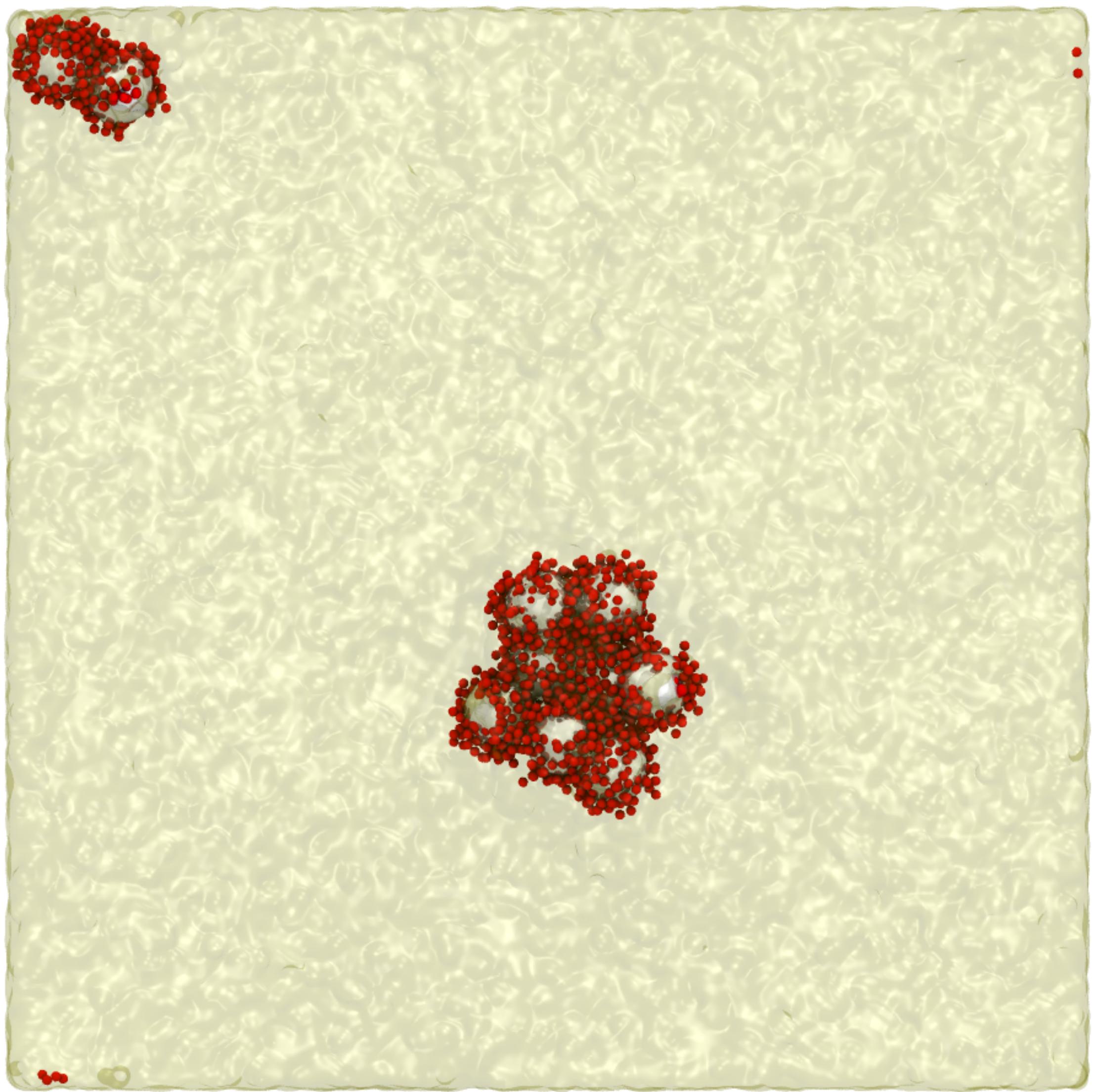
Can we model complex nanoparticle aggregation behavior observed experimentally by tuning these?

Outline

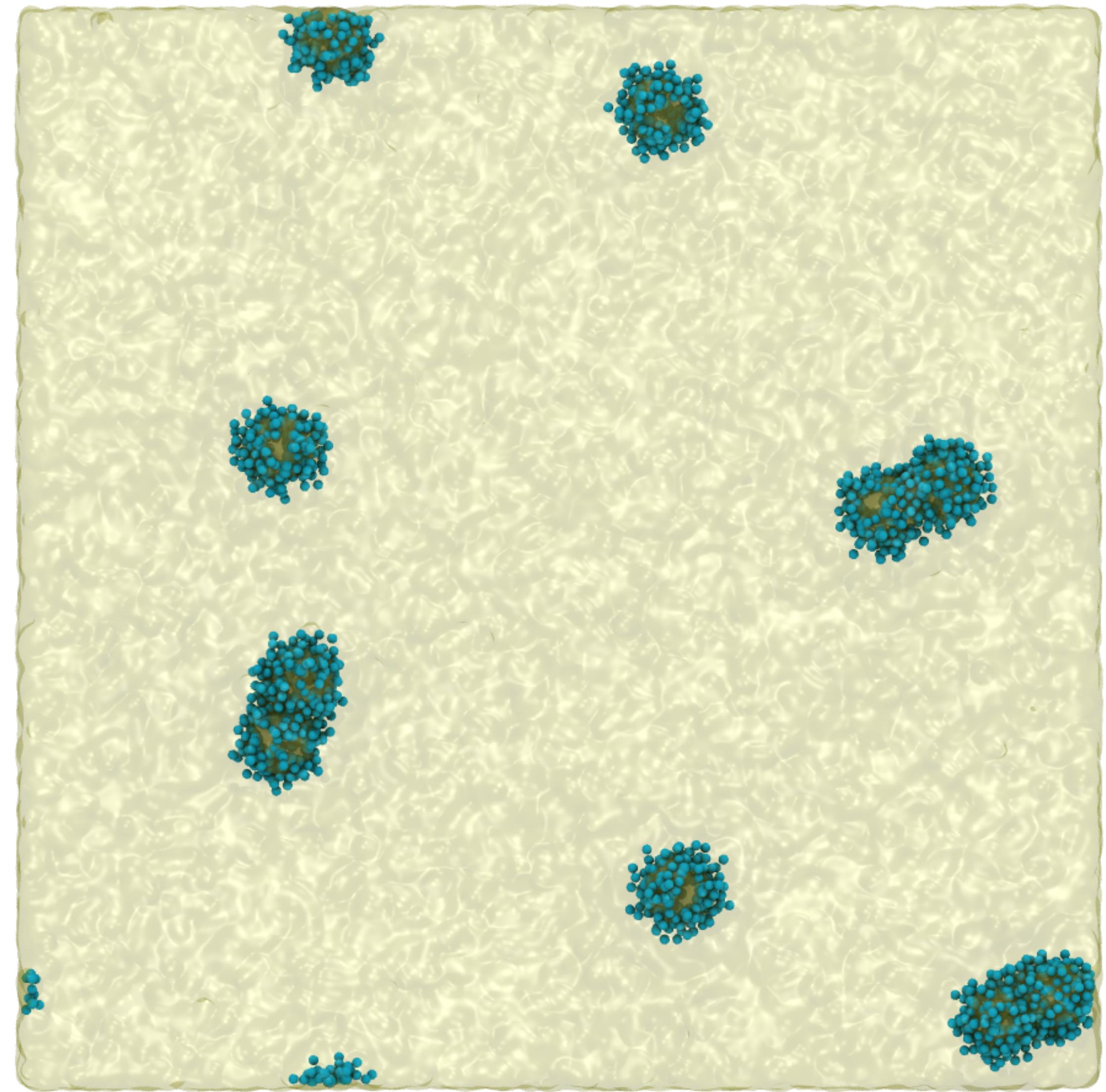
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How does the new model compare to the old model?

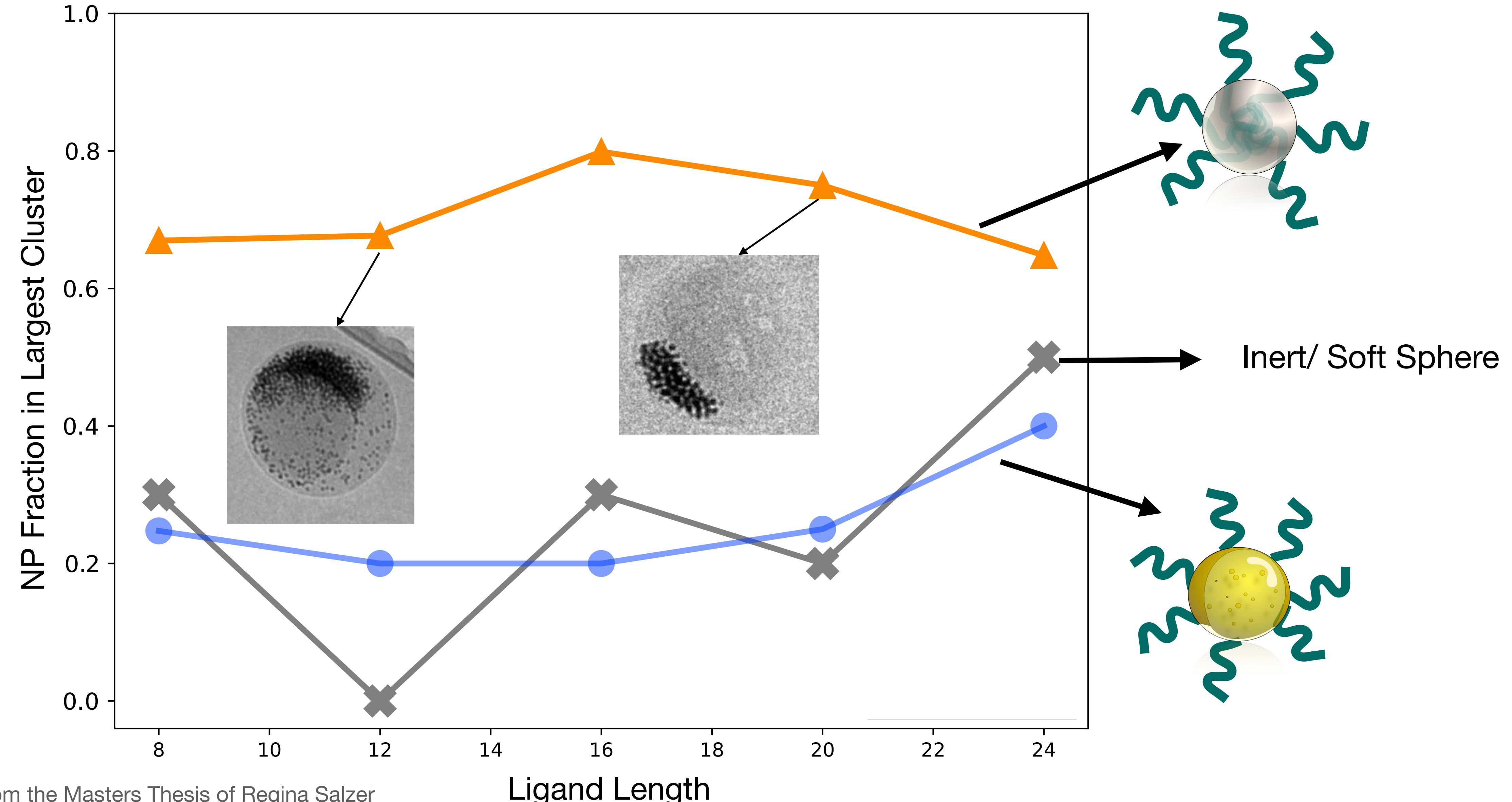
Polar Core Model



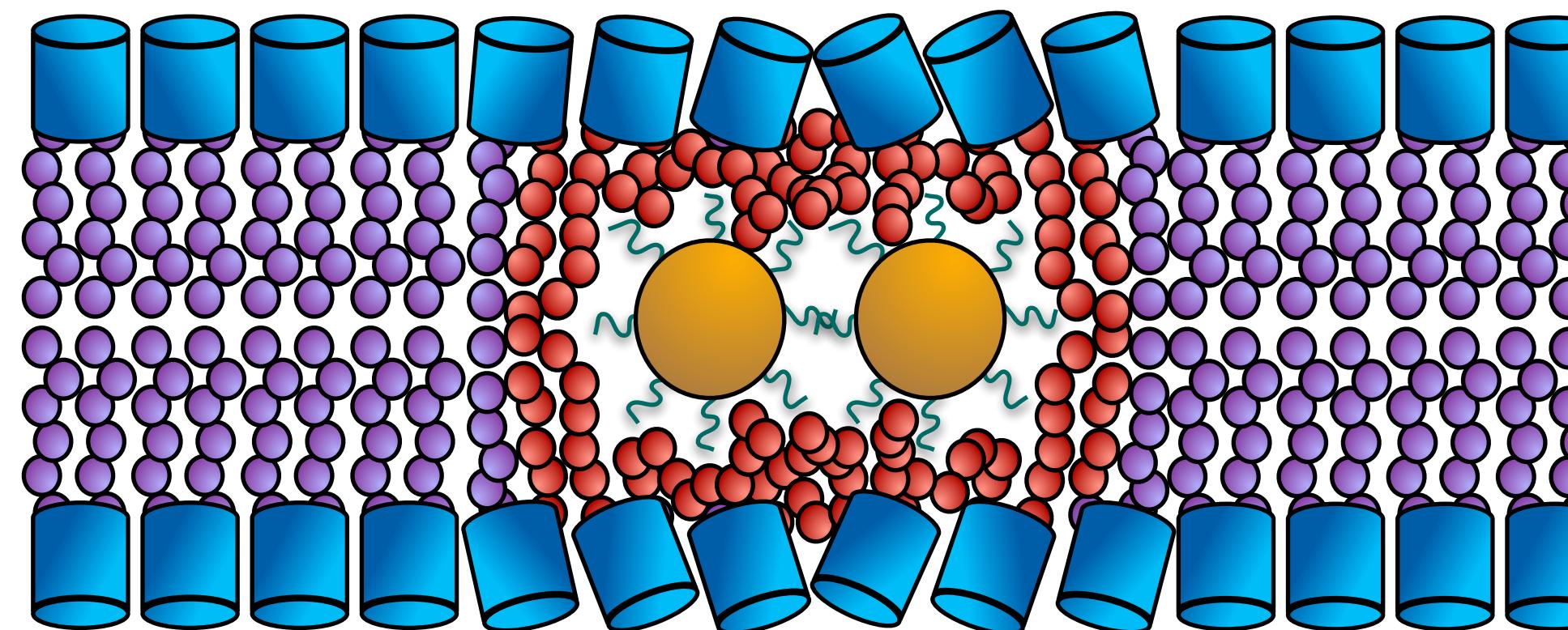
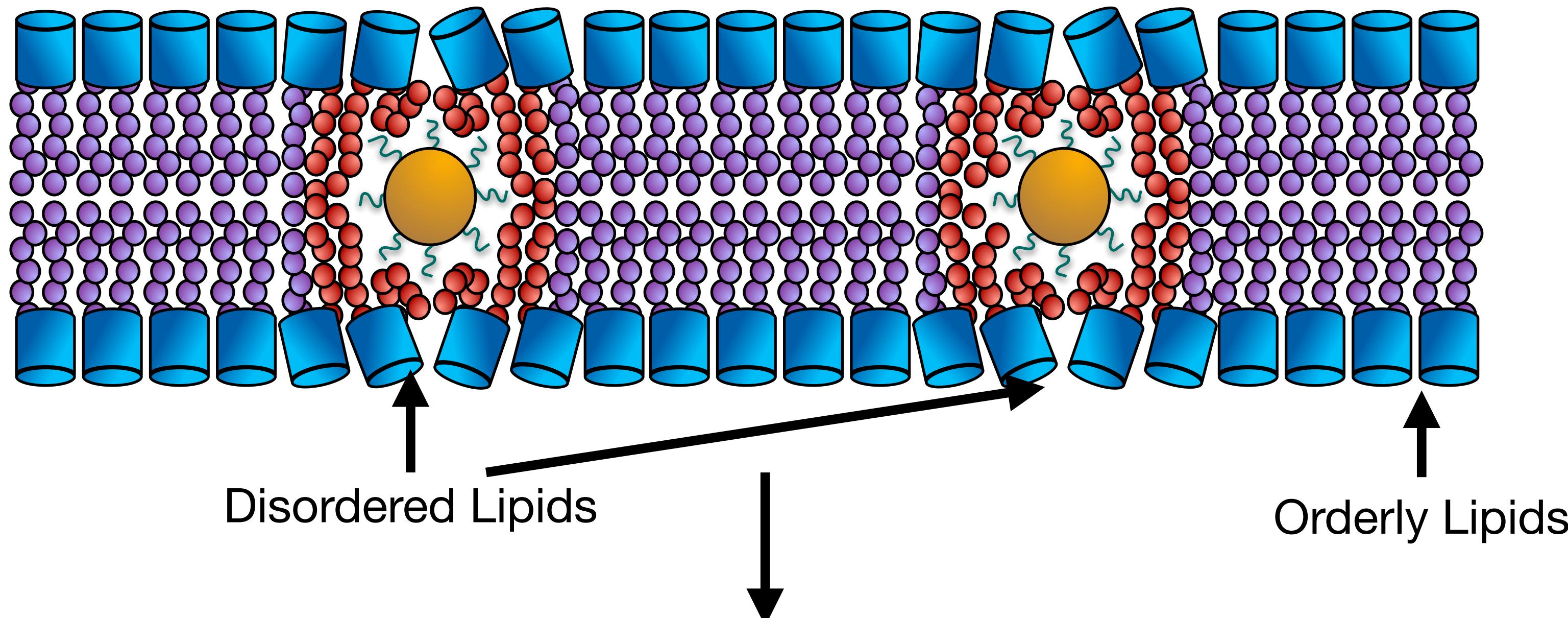
Oily Core Model



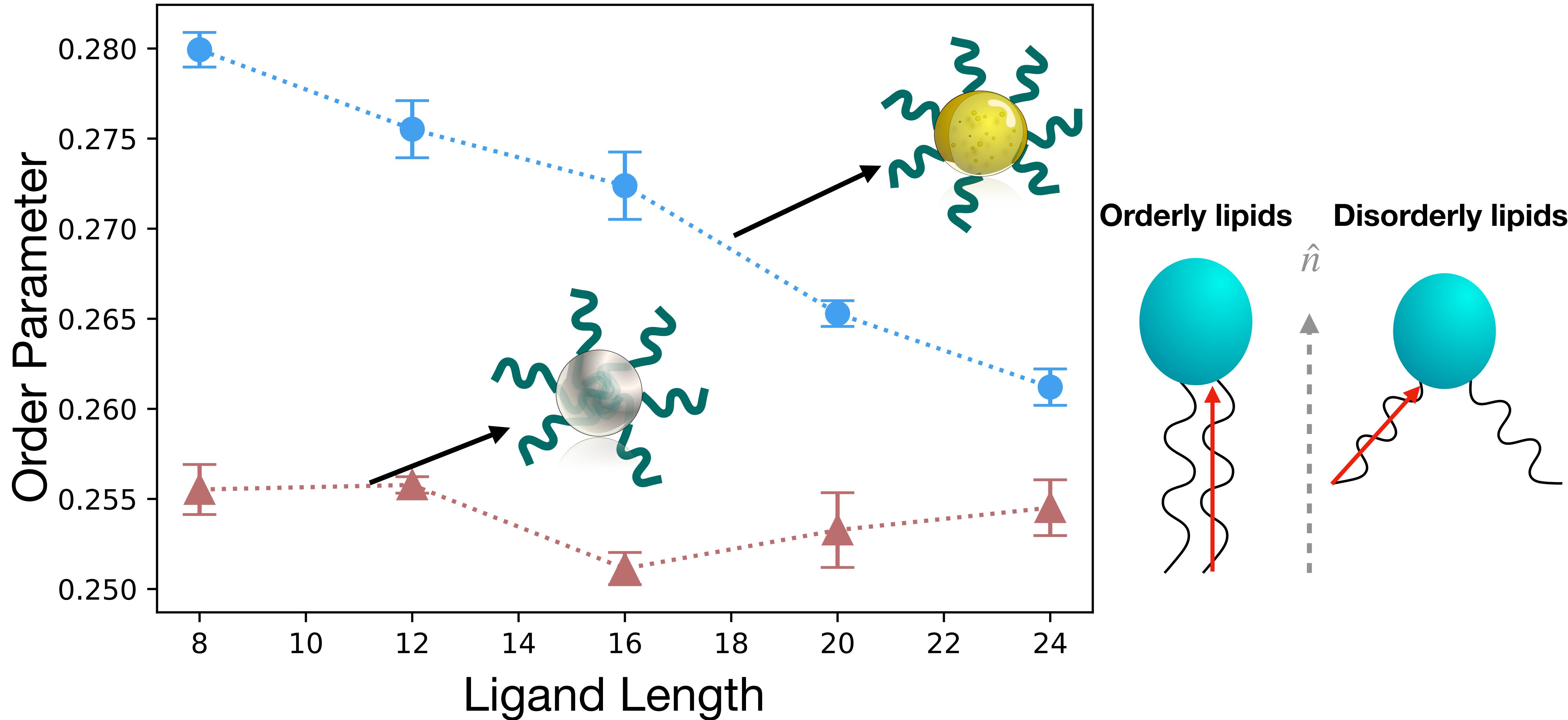
Aggregation behavior is sensitive to ligand length and core parameter



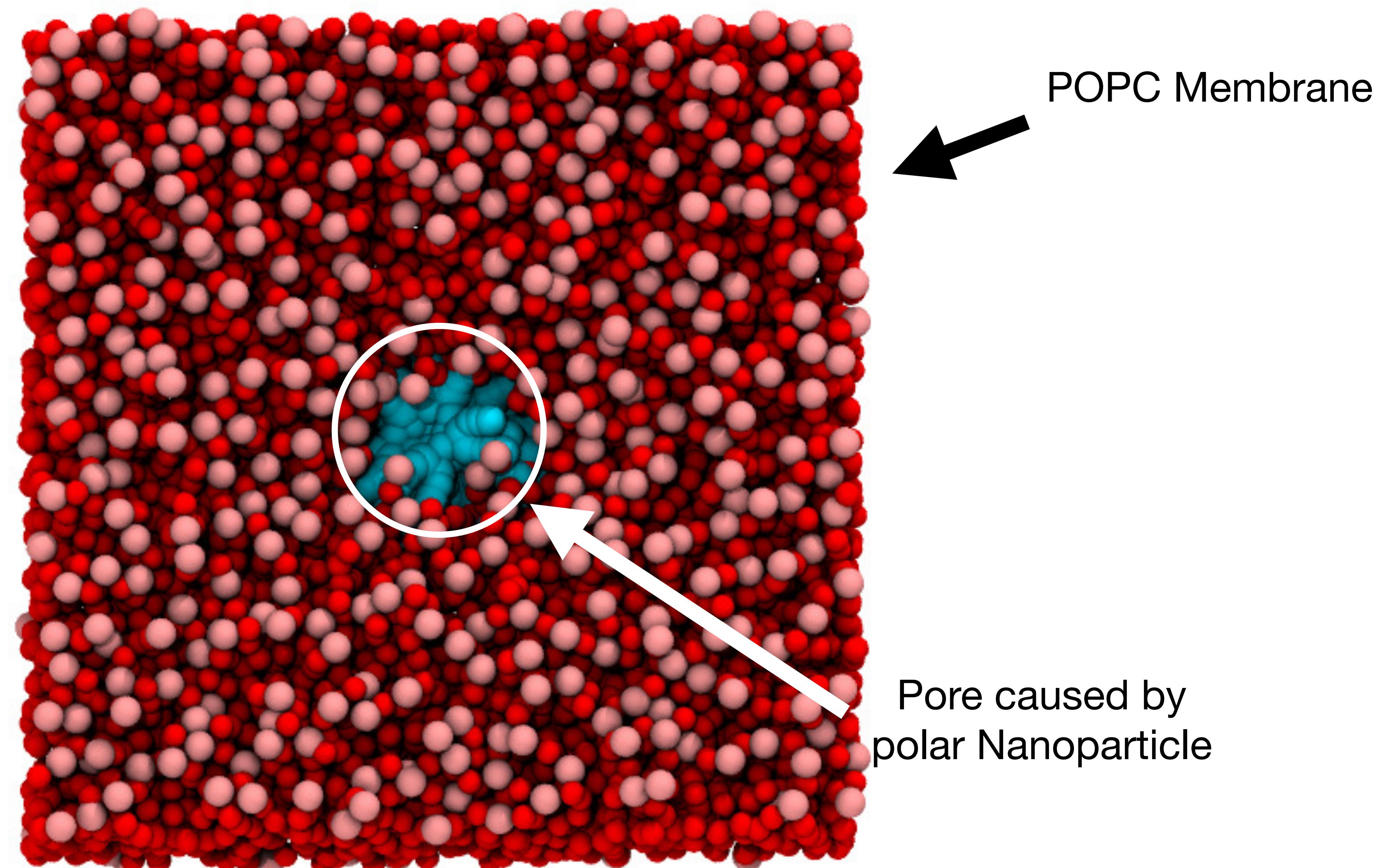
Can lipid disorder drive gold nanoparticle aggregation?



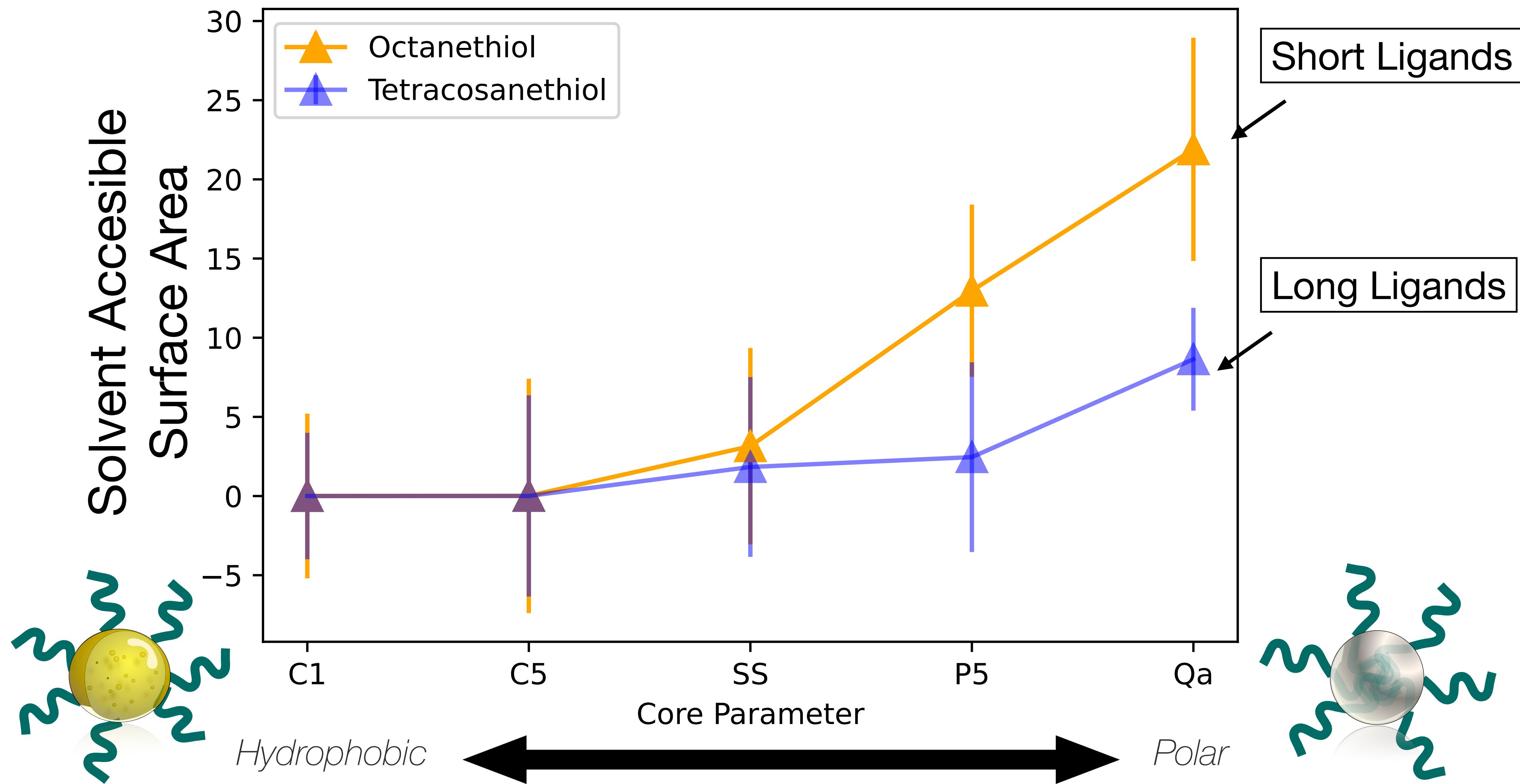
Do ligands drive gold nanoparticle aggregation?



Increasing nanoparticle polarity leads to exposure of hydrocarbon chains to water



Core polarity increases surface accessibility of nanoparticles embedded in the membrane



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Summary

- Mechanisms driving aggregation
 - Longer ligands disrupt lipid packing, contributing to aggregation regardless of core model
 - Polar cores with short ligands can porate the membrane and have strong direct interactions with other polar cores, further driving aggregation
- The polar core model matches preliminary experimental data better than the conventional hydrophobic core model
- The model is one step towards the integration of metals into coarse-grained biological force fields.

Outline

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Future Directions

- Development of a metal bead that can interface in both solution and membrane environments
- Further comparison of aggregation results to experimental results
- Gaining mechanistic insight into aggregation of gold nanoparticles in various membranes

Acknowledgements



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- Dr. Grace Brannigan
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- Connor Pitman
- Regina Salzer

Questions?