Center For Hierarchical Materials (CHEM)

Planning Meeting

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August 3-4, 2020

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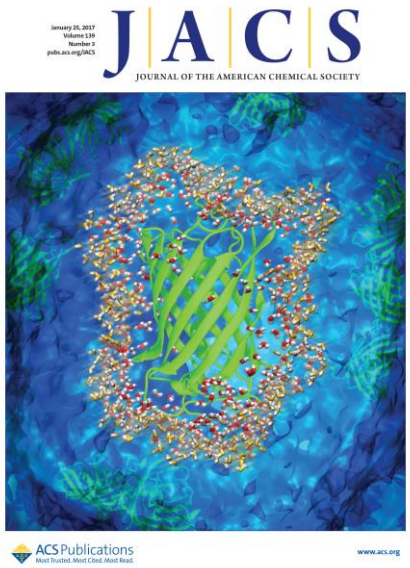
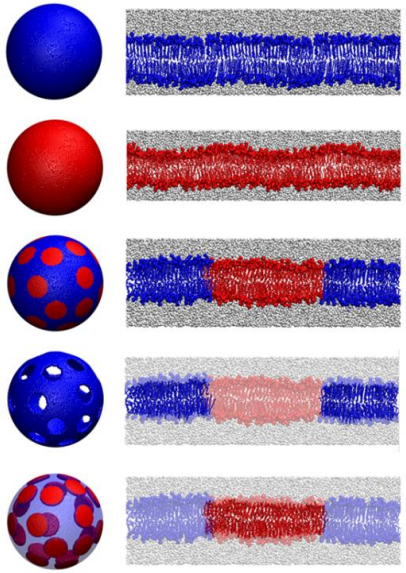
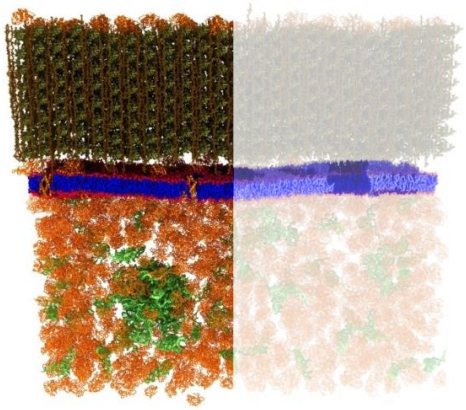
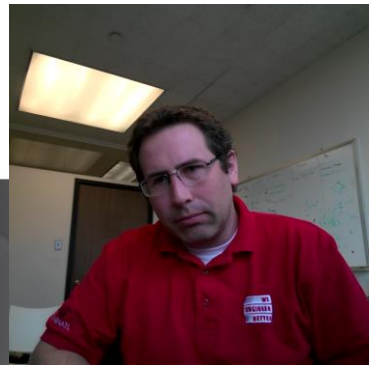
Introduction









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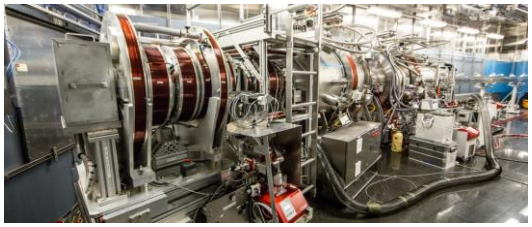
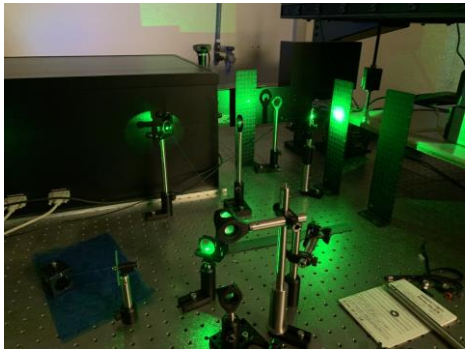
Tools



Inelastic Scattering / Dynamics
Direct / Backscattering / Neutron Spin Echo

Elastic Scattering / Structure
SANS/SAXS



Inelastic Light Scattering

Fluorescence / FRET / Polarization

GPU Accelerat
Small S

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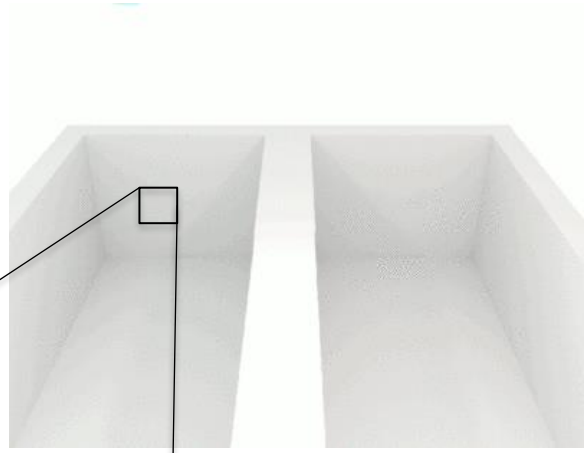
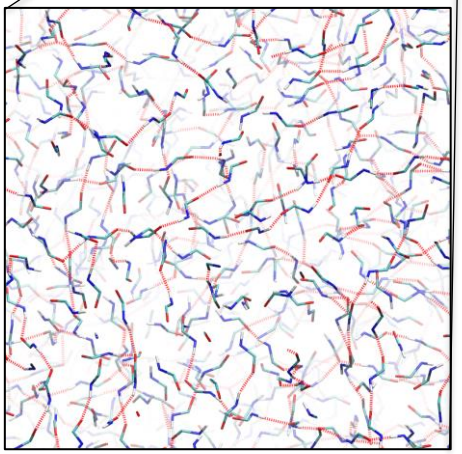
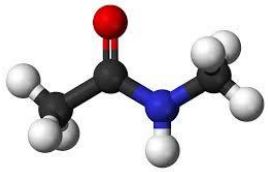
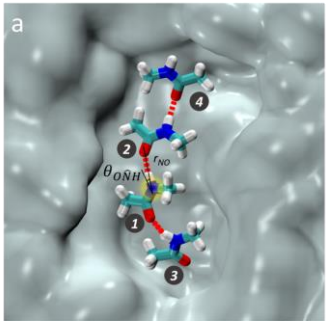
Small to Big

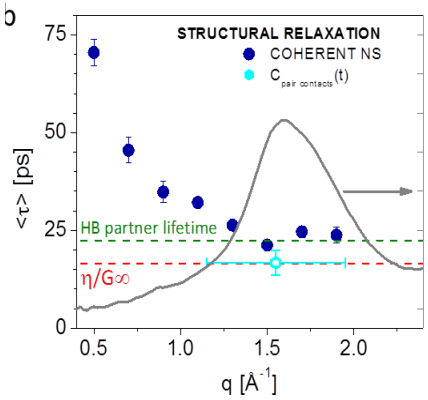


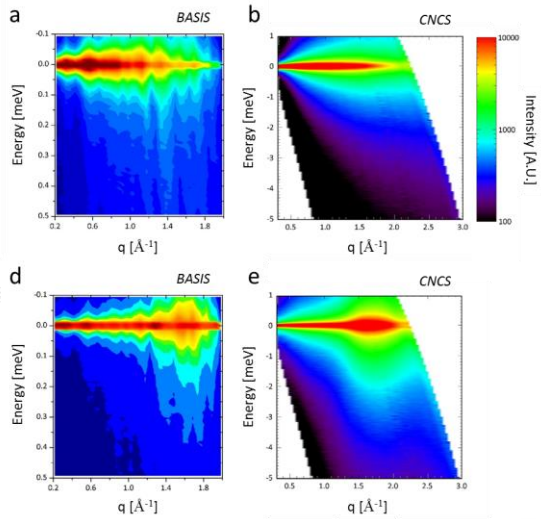




N-methylacetamide







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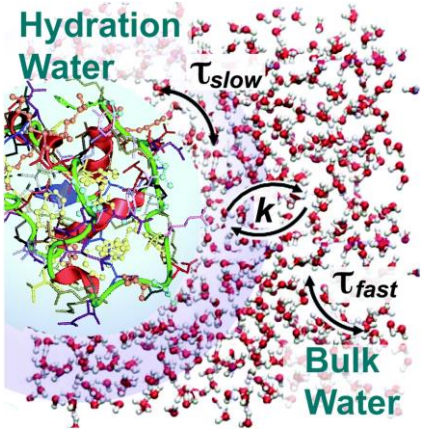
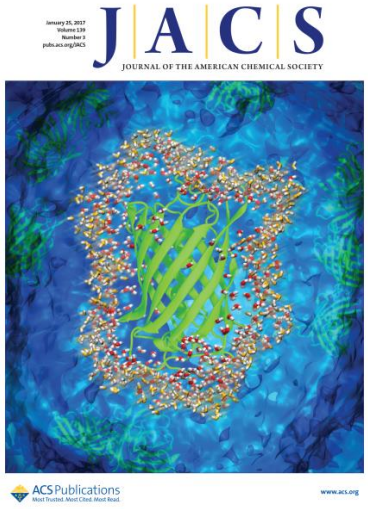
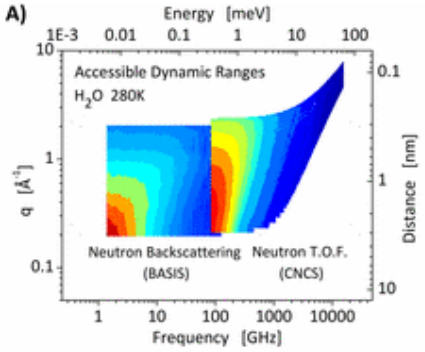
Small to Big

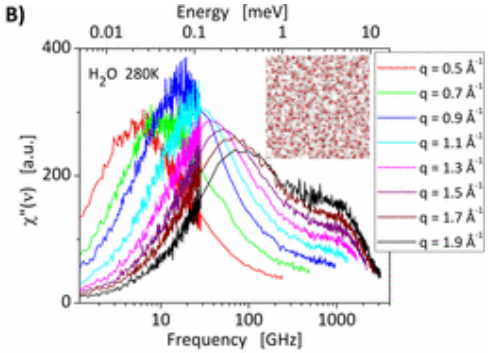


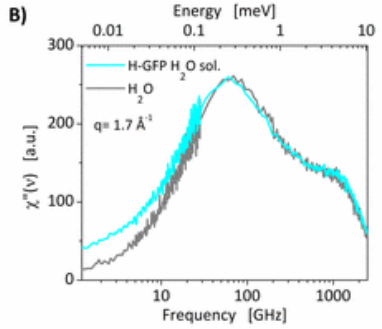
Comez et al Soft Matter 2016

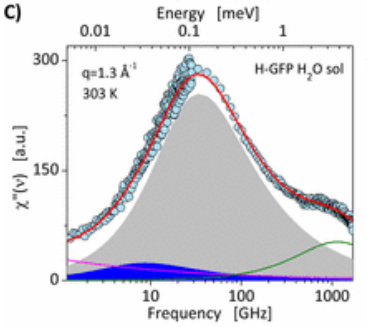


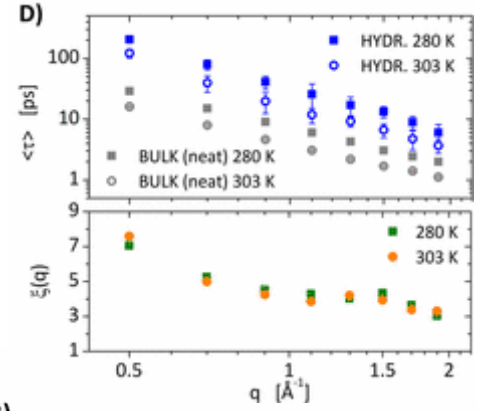
Perticaroli et al. JACS 2017.

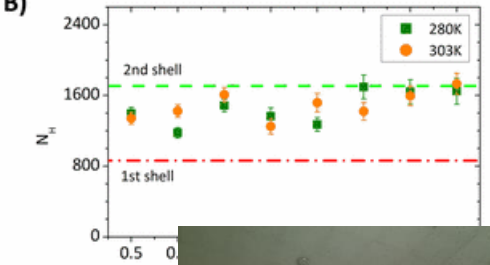












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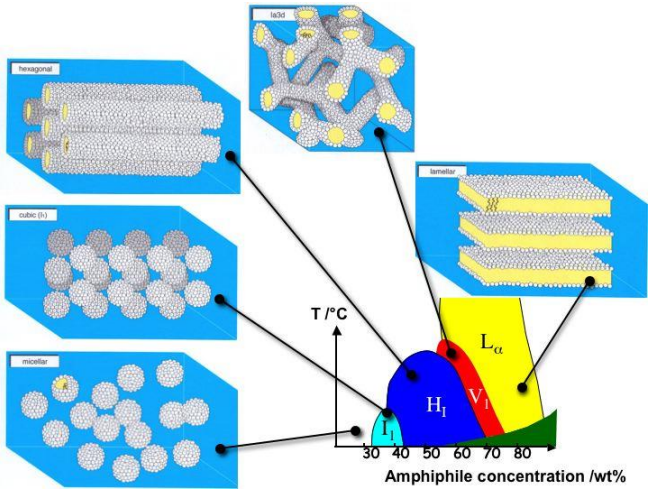
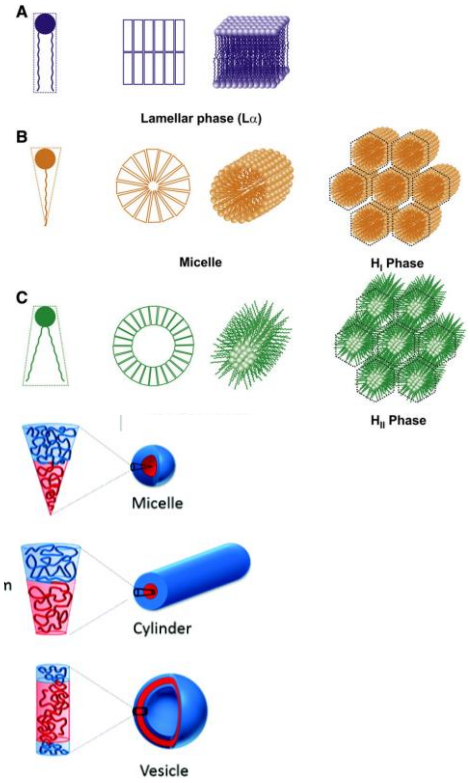
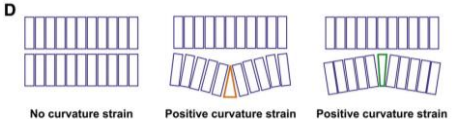
Phase Separation within Lyotropic Liquid Crystal Materials

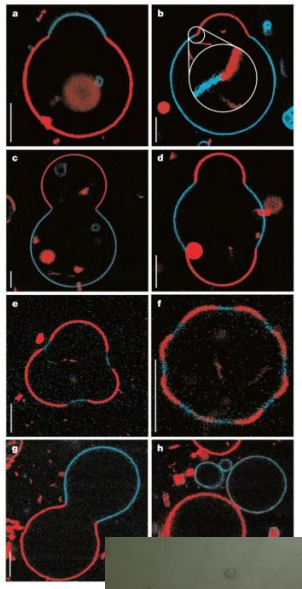
Lyotropic Liquid Crystal Phases

Solvent dispersed liquid crystals with 1D or quasi 1D order



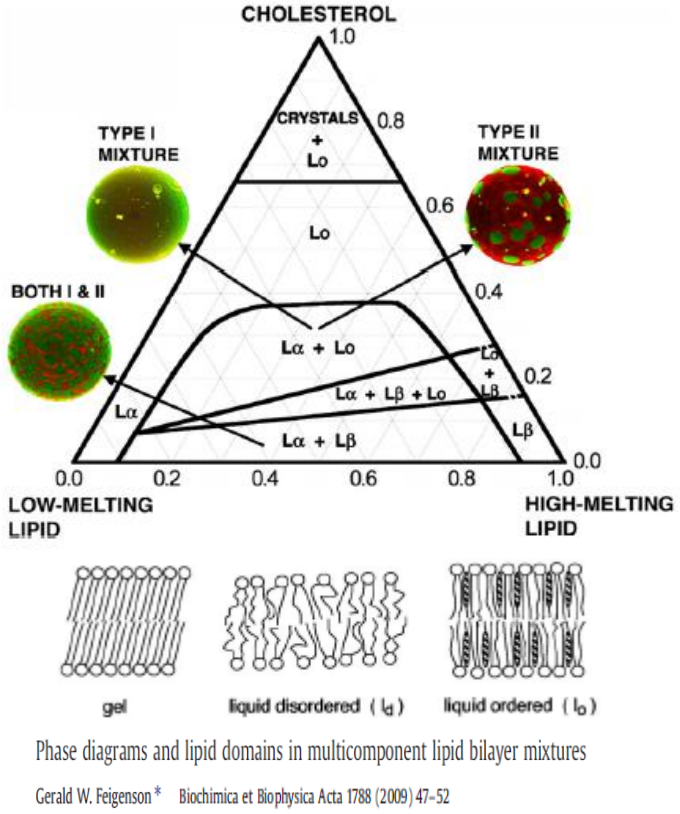






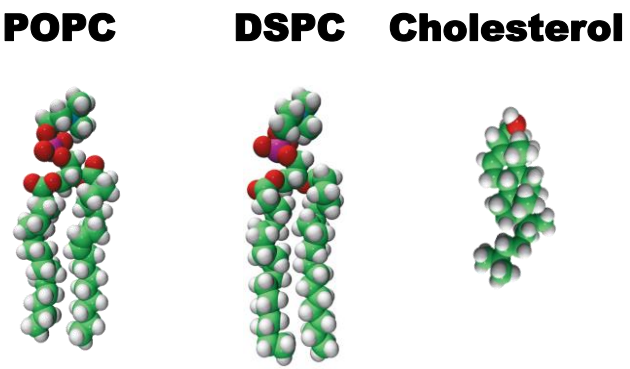
Baumga
Webb N

Phase behavior in mammalian model membrane mimics

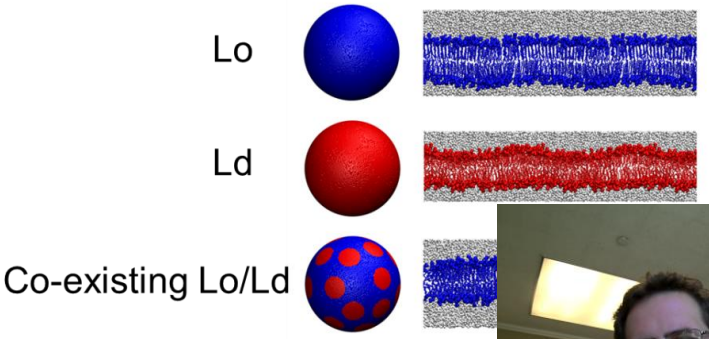


Phase diagrams and lipid domains in multicomponent lipid bilayer mixtures

Gerald W. Feigenson* Biochimica et Biophysica Acta 1788 (2009) 47–52



DSPC, POPC, and Chol, in a 39/39/22 ratio



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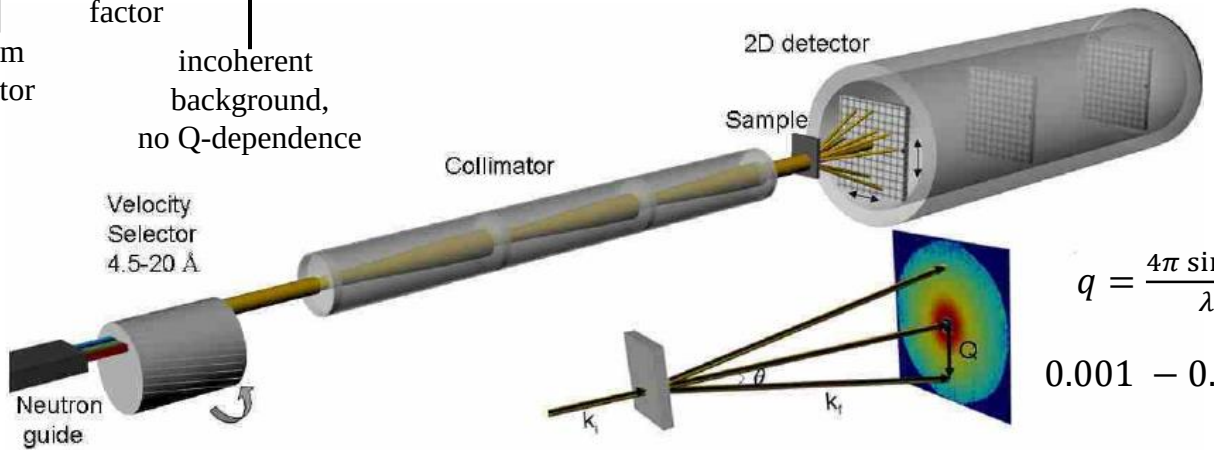
Macromolecular structure - SANS

$$\frac{\partial \sigma}{\partial \Omega}(q) = N_p V_p^2 (\Delta\rho)^2 P(q) S(q) + B_{inc}$$

- N_p: # of scattering particles
- V_p: volume of one scattering particle
- $(\Delta\rho)^2$: neutron contrast
- $P(q)$: form factor
- $S(q)$: structure factor
- B_{inc}: incoherent background, no Q-dependence



$$q = \frac{4\pi \sin(\theta)}{\lambda}$$

$0.001 - 0.5$ Å^{-1}

- Small angle neutron scattering – SANS
  - Observe the angle at which neutrons are scattered from the sample.
  - Scattered intensity is related to the structure and composition of the sample.
  - 100's nm to Å spatial resolution

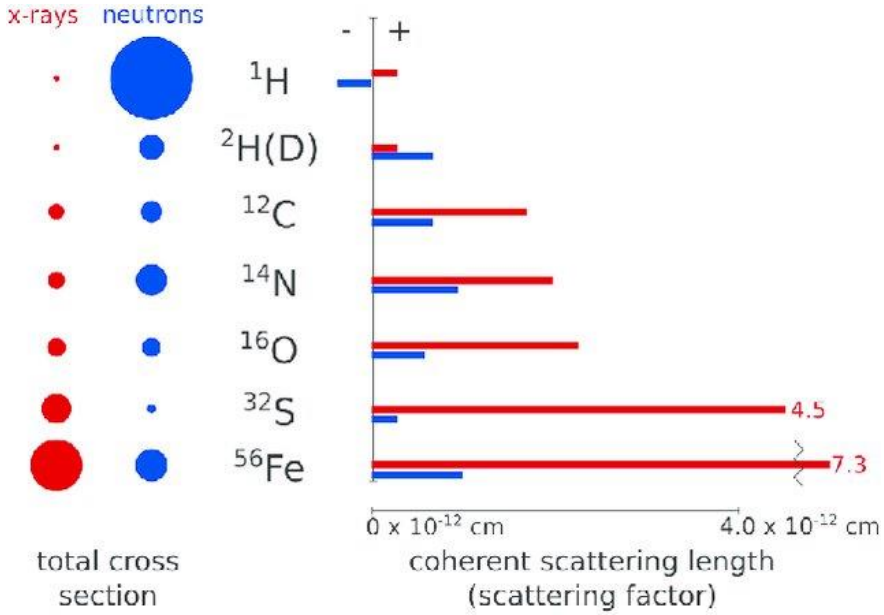
Neutron Scattering - Contrast

$$\frac{\partial\sigma}{\partial\Omega}(Q) = N_p V_p^2 (\Delta\rho)^2 P(Q) S(Q) + B_{inc}$$

neutron contrast

$$\rho = \frac{\sum \boldsymbol{b_i}}{\boldsymbol{V}}$$

Neutron Scattering Length Density



Castellanos et al. Comp. Struct. Bio. (2016)

- Neutron scattering length, *b*, is an atomic property that varies by element and isotope.
- Neutrons are especially sensitive to the isotopes of hydrogen.
- Lipids are hydrogen rich
  - Good internal contrast
  - Available in deuterium

Neutrons Scattering and Contrast Matching

$$\frac{\partial\sigma}{\partial\Omega}(Q) = N_p V_p^2 (\Delta\delta)^2 P(Q) S(Q) + B_{inc}$$

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$(\Delta\delta)^2 = (\delta_{lipid} - \delta_{water})^2 = 0$ scattering
$(\Delta\delta)^2 = (\delta_{lipid} - \delta_{water})^2 = 0$ no scattering

Neutrons Scattering - Contrast

$$\frac{\partial\sigma}{\partial\Omega}(Q) = N_p V_p^2 (\Delta\delta)^2 P(Q) S(Q) + B_{inc}$$

# of scattering particles

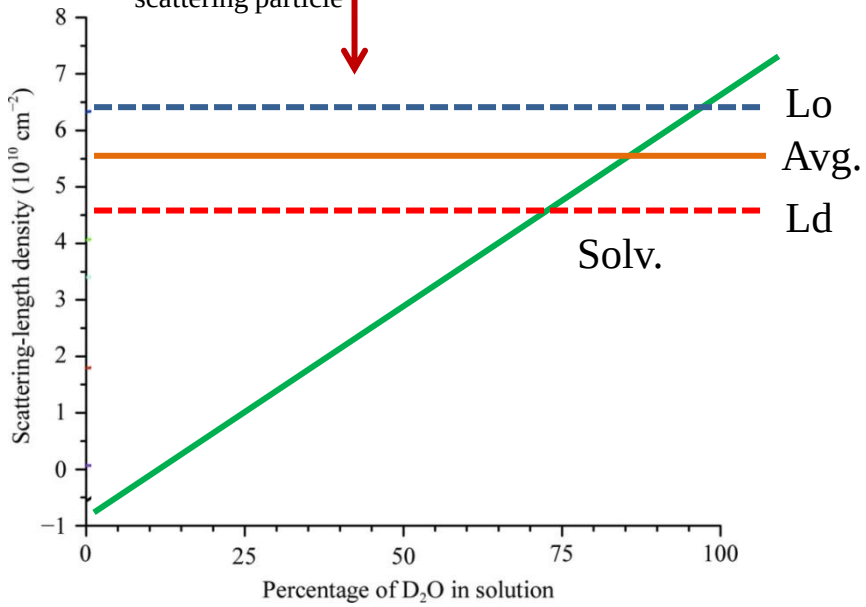
volume of one scattering particle

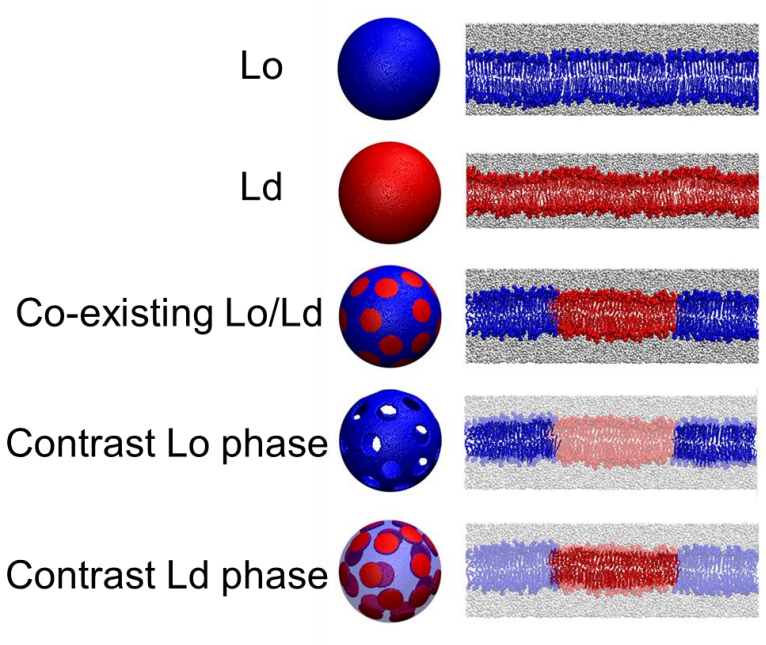
neutron contrast

form factor

structure factor

incoherent background, no Q-dependence

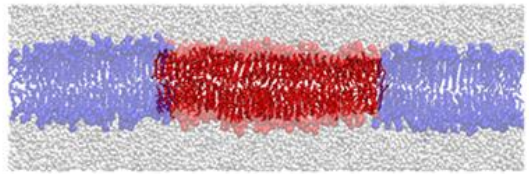


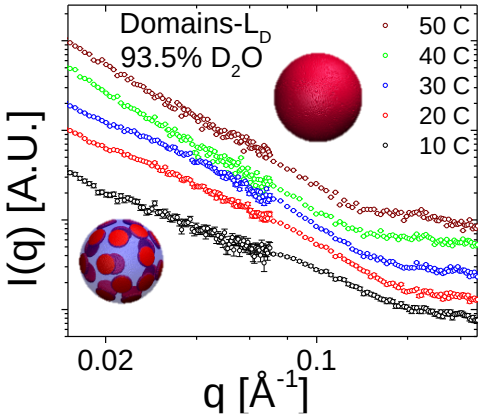


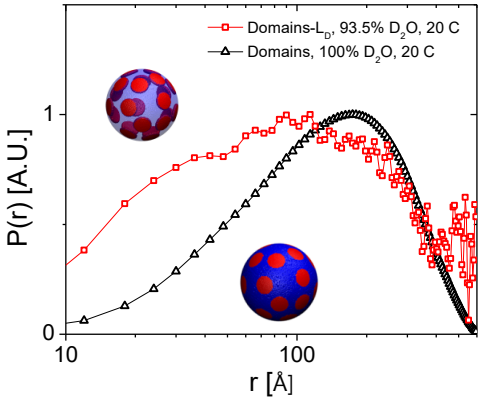
Nickels et al. JAC

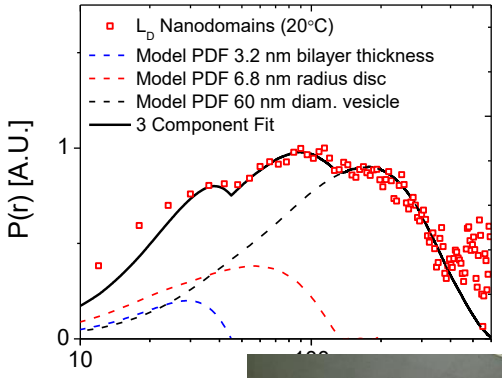
SANS – Structure of Raft-like Features

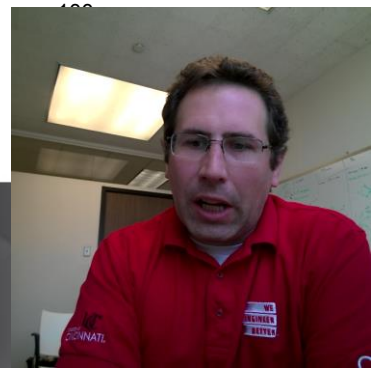
Contrast Ld phase











Neutrons Scattering - Contrast

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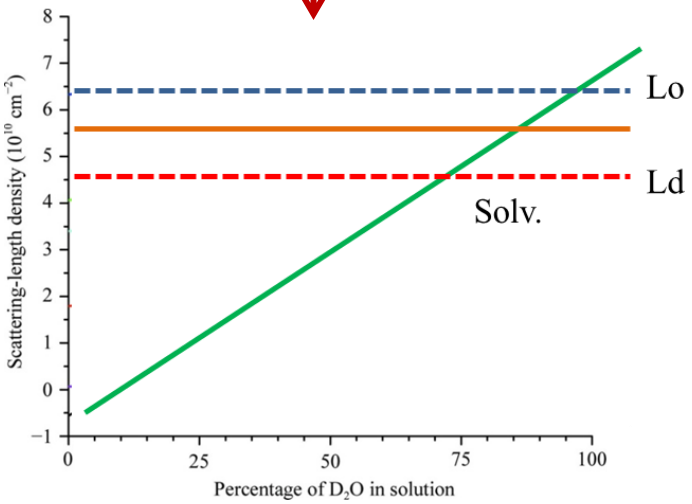
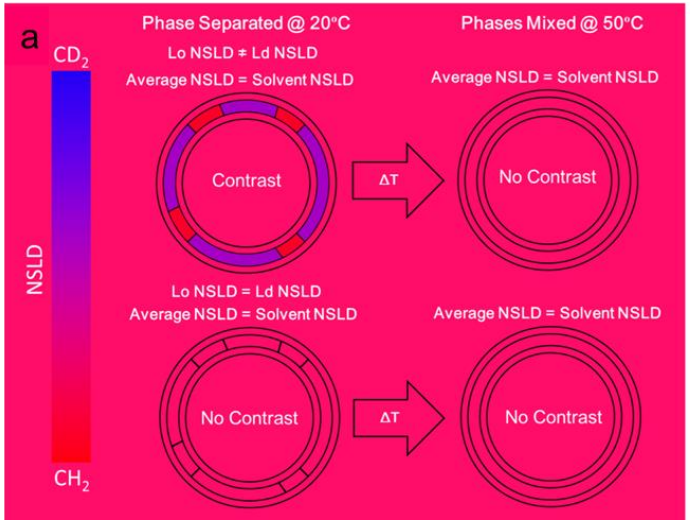
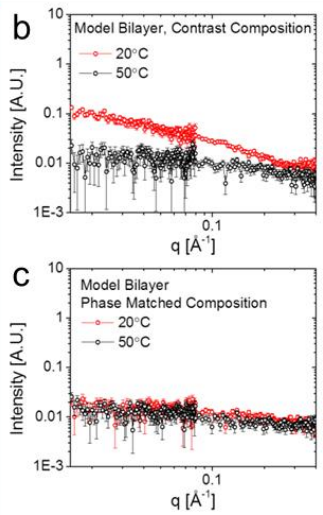


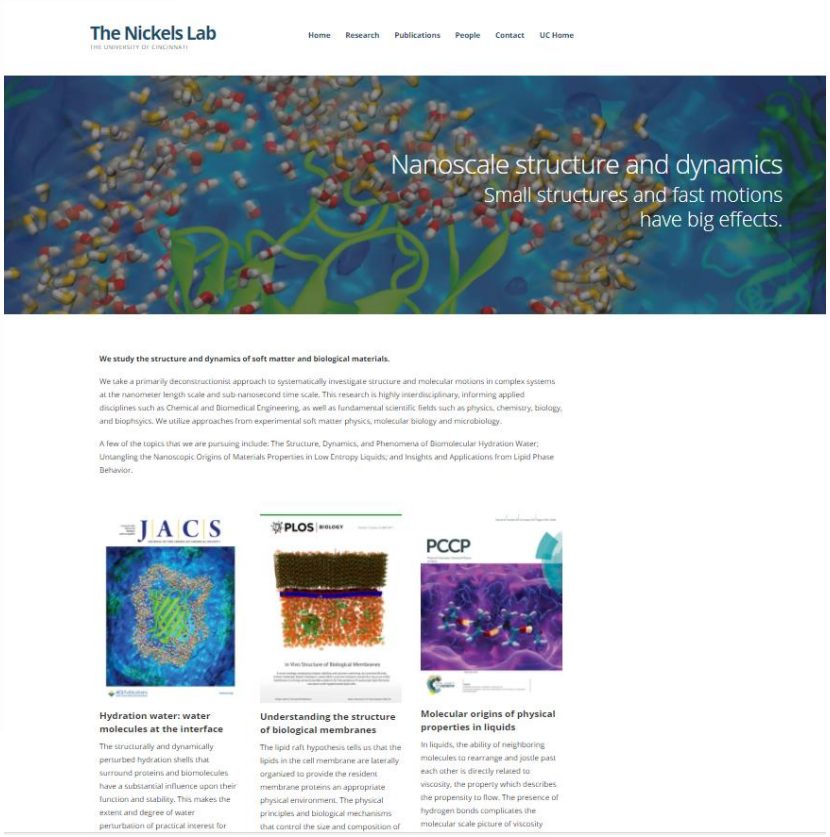




Summary

Methods to investigate coexisting lyotropic phases based on scattering contrast.

Lead to new design principles to drive material properties.



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