

# Center For Hierarchical Materials (CHEM)

## Planning Meeting

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University of Cincinnati

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August 3-4, 2020

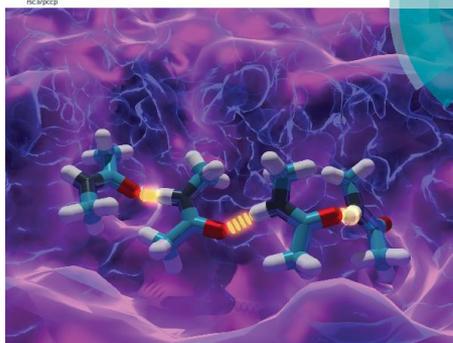


# Introduction

Volume 19 | Number 38 | 14 October 2017 | Pages 25799–26444

## PCCP

Physical Chemistry Chemical Physics  
rsc.li/pccp



ISSN 1463-9076

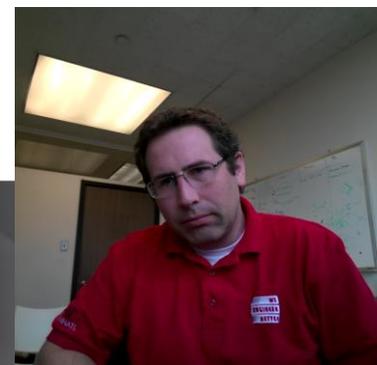
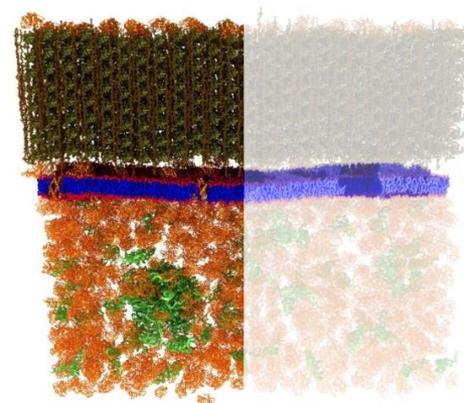
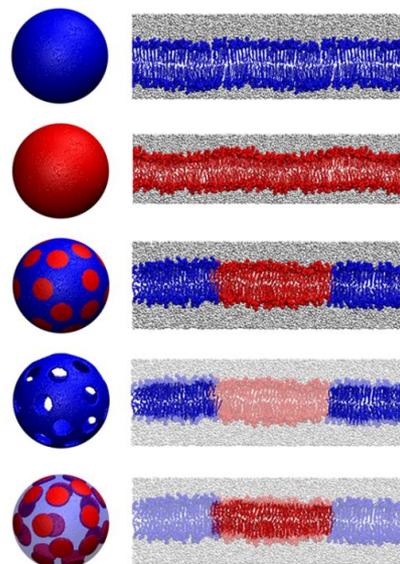


PAPER  
Serena Fucini, Jonathan D. Nickles et al.  
Structural relaxation, viscosity, and network connectivity in a hydrogen bonding liquid



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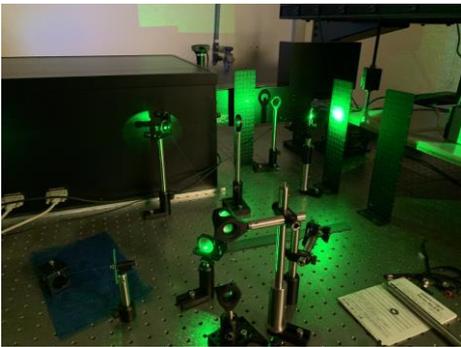
# Tools



Inelastic Scattering / Dynamics  
Direct / Backscattering / Neutron Spin Echo



Elastic Scattering / Structure  
SANS/SAXS



Inelastic Light Scattering



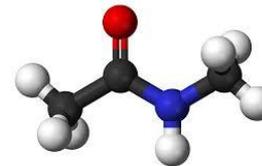
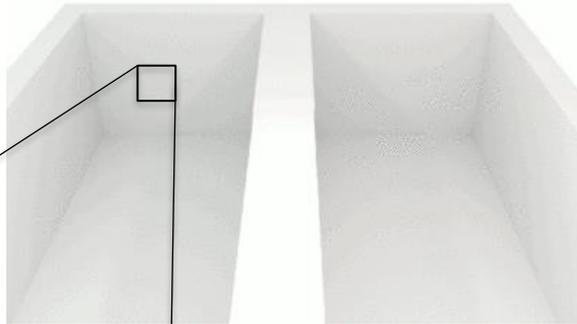
Fluorescence / FRET / Polarization



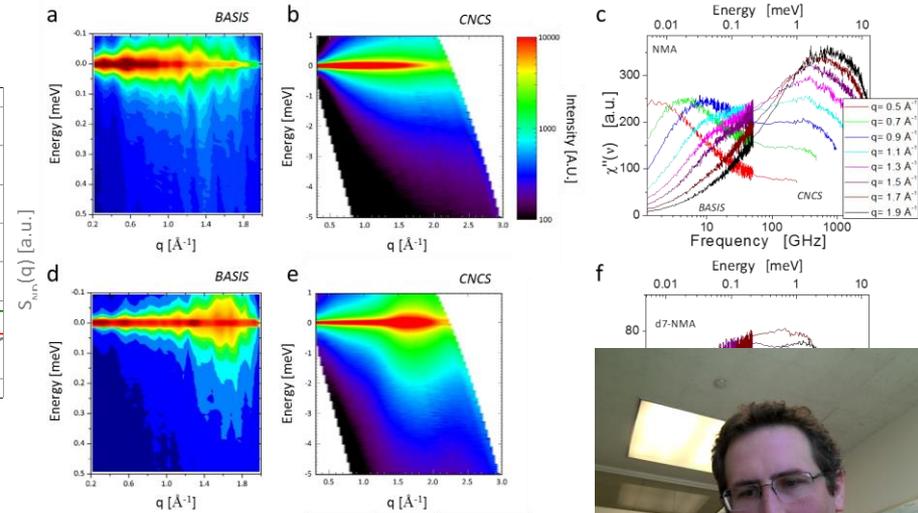
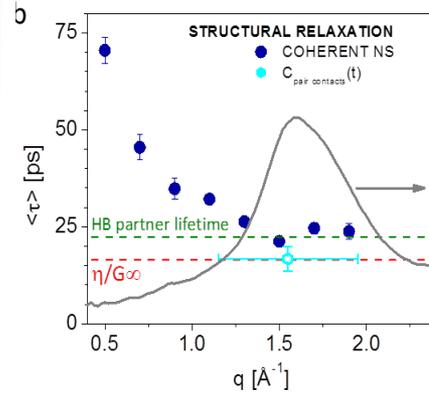
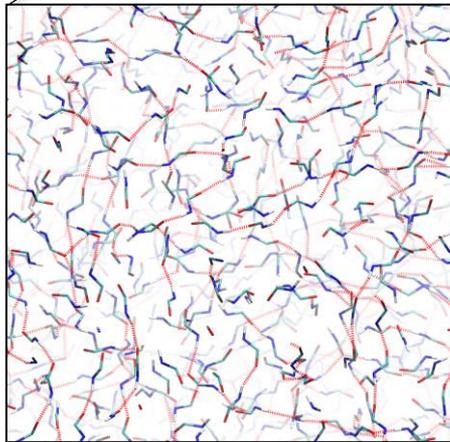
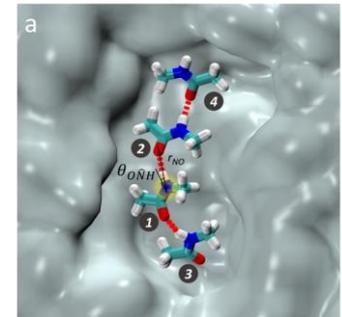
GPU Accelerator  
Small S



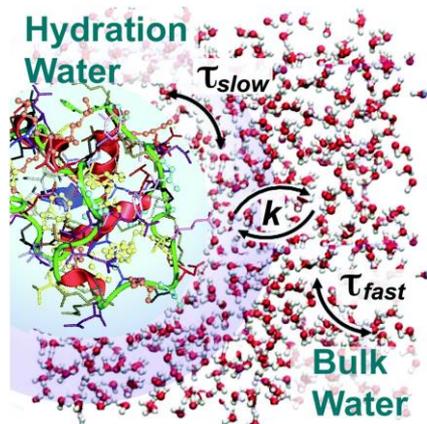
# Small to Big



N-methylacetamide



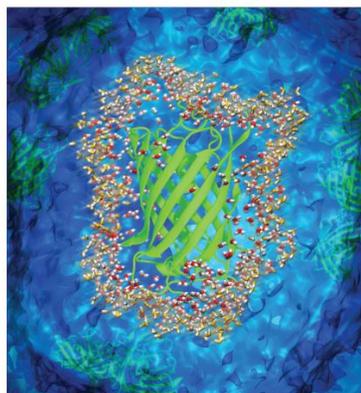
# Small to Big



Comez et al Soft Matter 2016

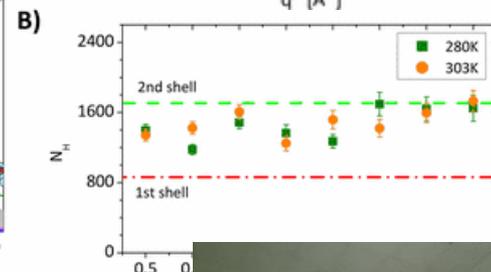
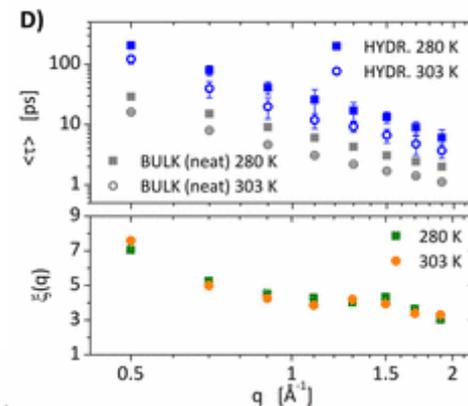
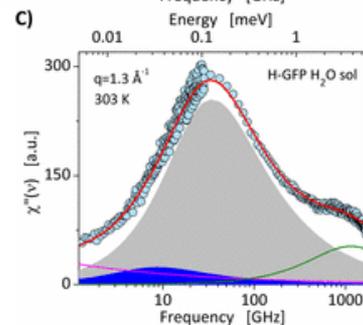
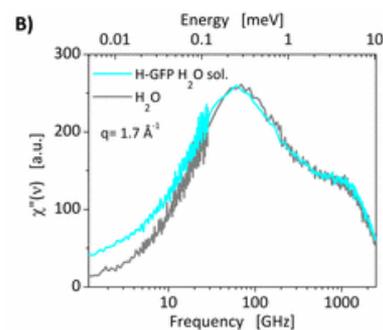
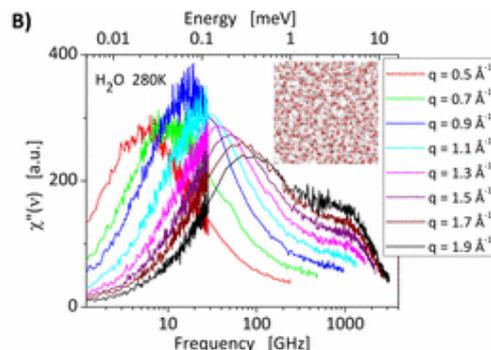
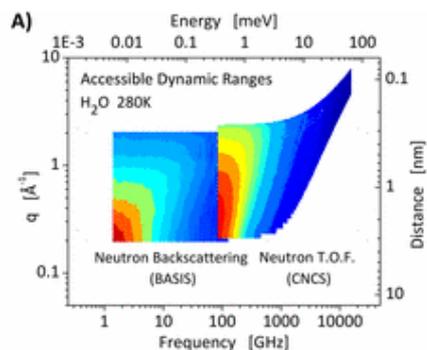
January 25, 2017  
Volume 139  
Number 2  
jacs.org/ACS

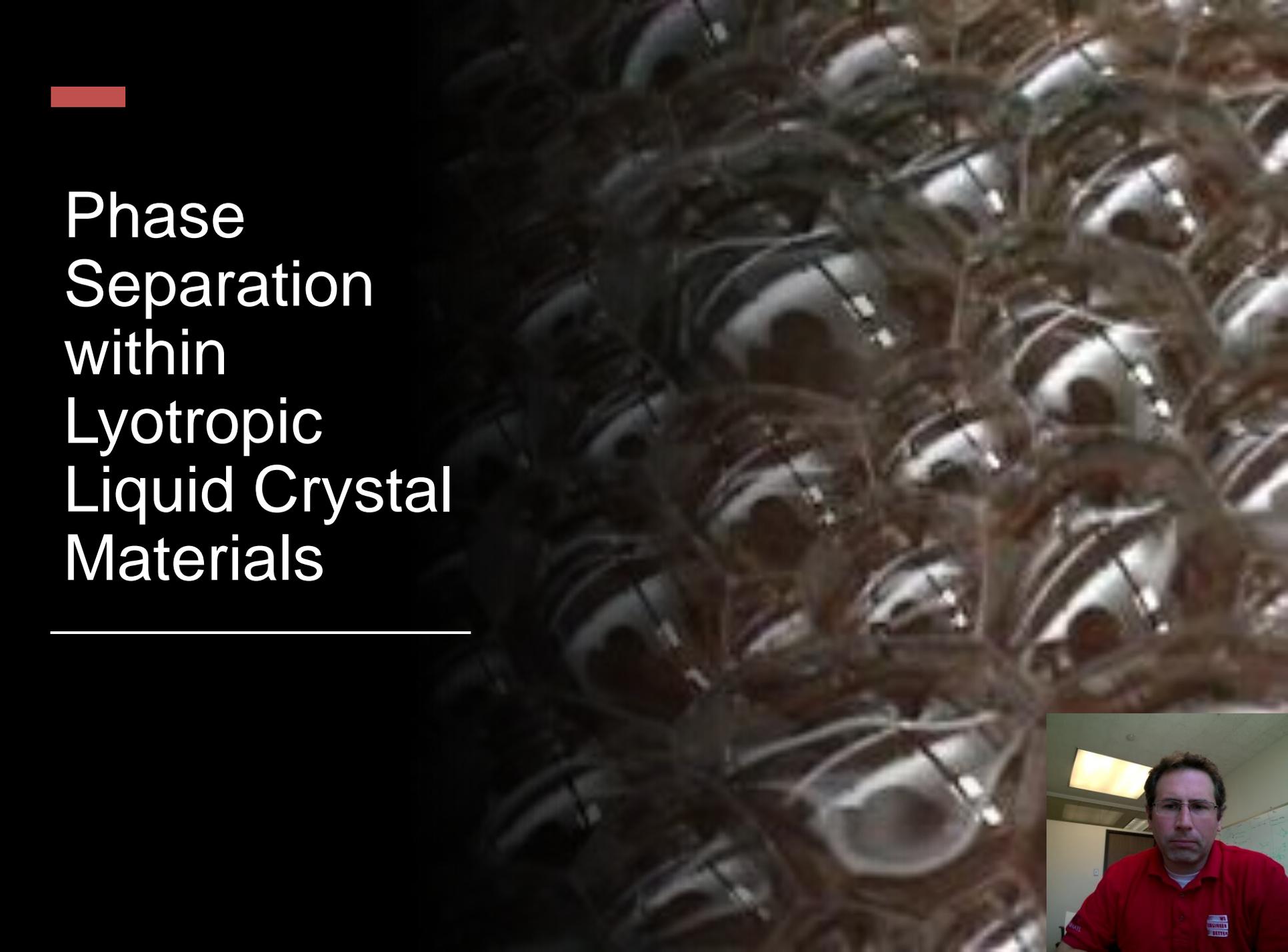
**J | A | C | S**  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY



ACS Publications  
Max Planck Society

Peticaroli et al. JACS 2017.



A large, dark, textured background image showing a complex, repeating pattern of light and dark regions, characteristic of phase separation in lyotropic liquid crystals. The pattern consists of interconnected, somewhat circular and elongated structures, creating a dense, woven appearance. A small red horizontal bar is located in the top left corner of the slide.

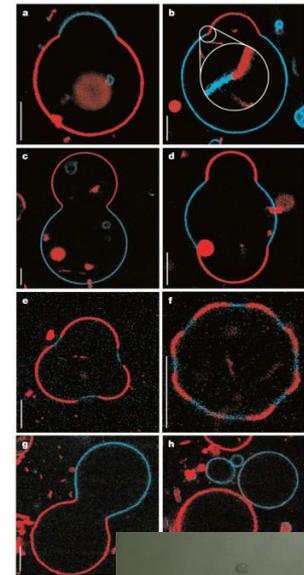
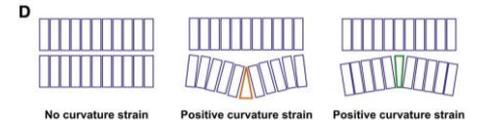
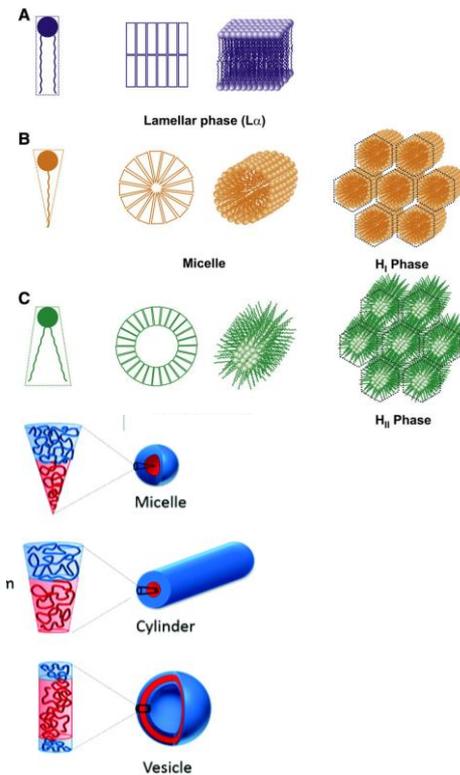
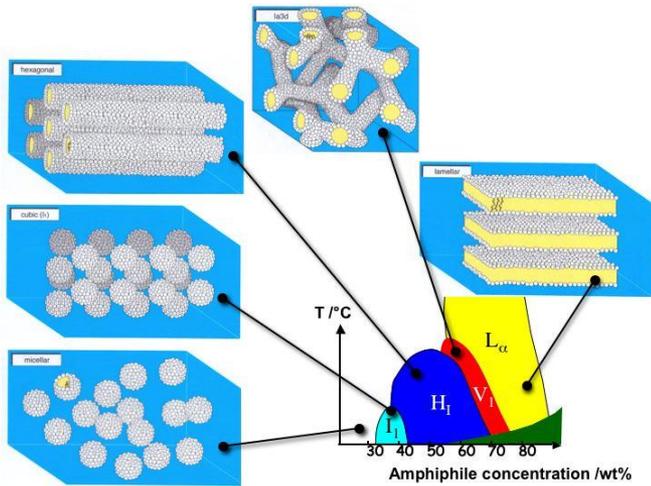
Phase  
Separation  
within  
Lyotropic  
Liquid Crystal  
Materials

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# Lyotropic Liquid Crystal Phases

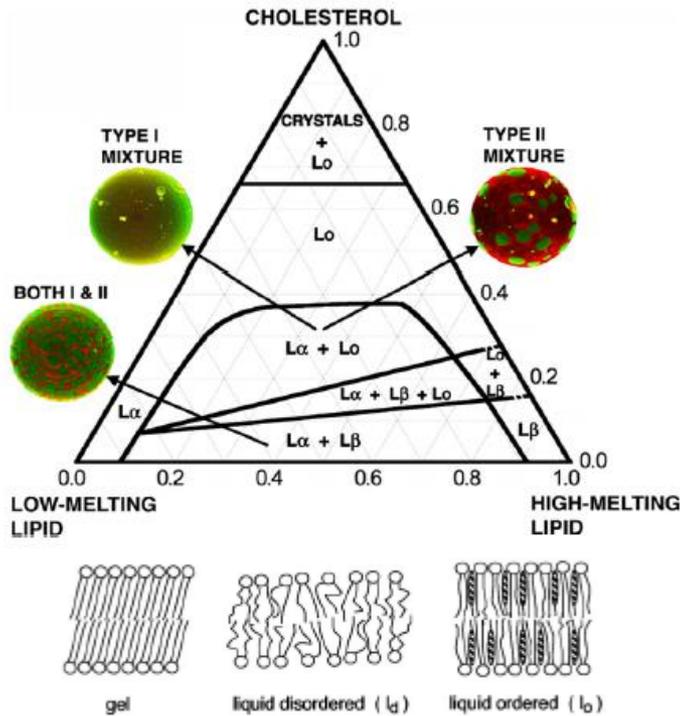
Solvent dispersed liquid crystals with 1D or quasi 1D order



Baumga  
Webb N



# Phase behavior in mammalian model membrane mimics



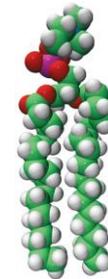
Phase diagrams and lipid domains in multicomponent lipid bilayer mixtures

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

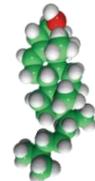
POPC



DSPC

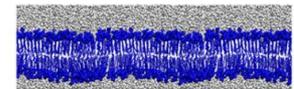


Cholesterol

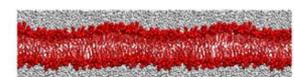


DSPC, POPC, and Chol, in a 39/39/22 ratio

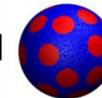
Lo



Ld



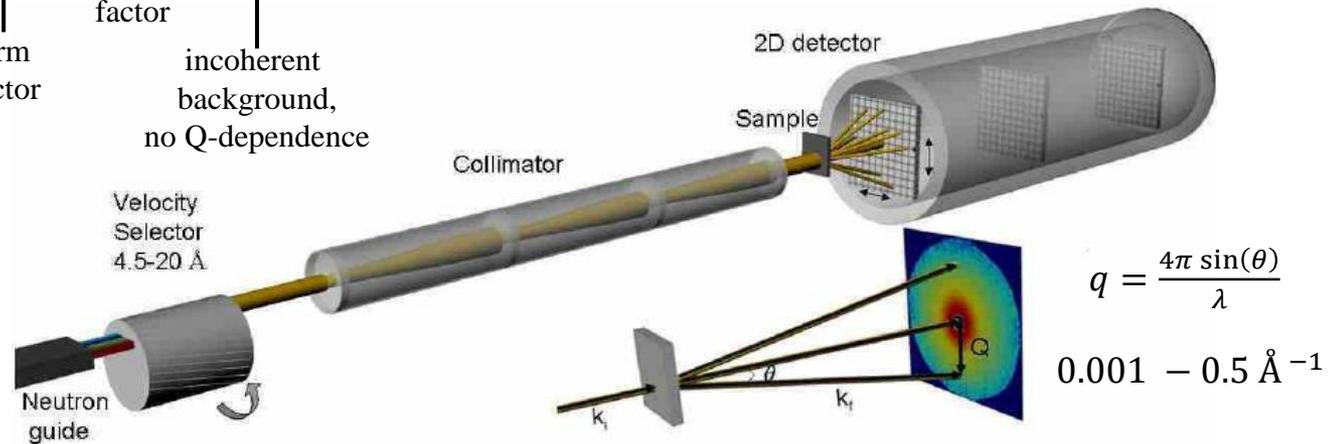
Co-existing Lo/Ld



# 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  
 $\Delta \rho$ : neutron contrast  
 $P(q)$ : form factor  
 $S(q)$ : structure factor  
 $B_{inc}$ : incoherent background, no Q-dependence



- 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



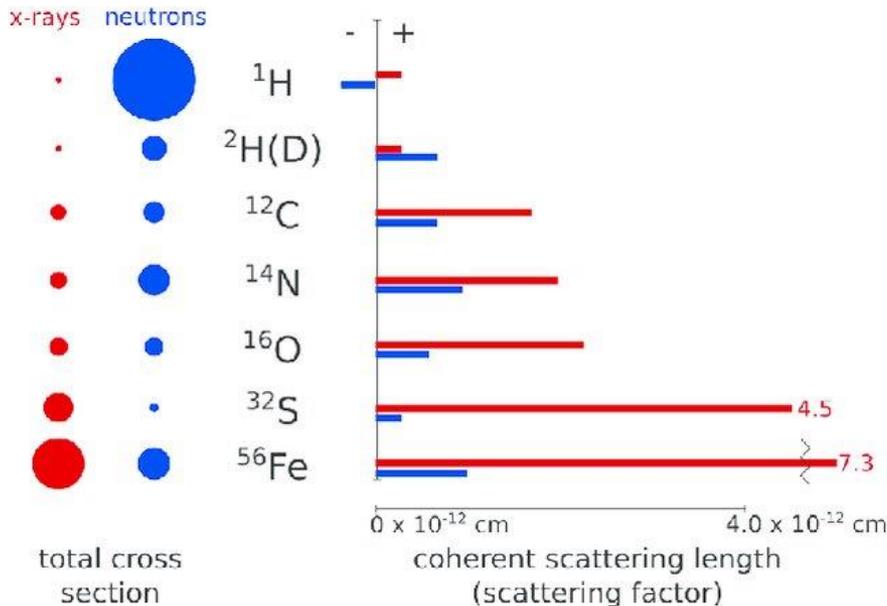
# Neutron Scattering - Contrast

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

neutron  
contrast

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

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

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

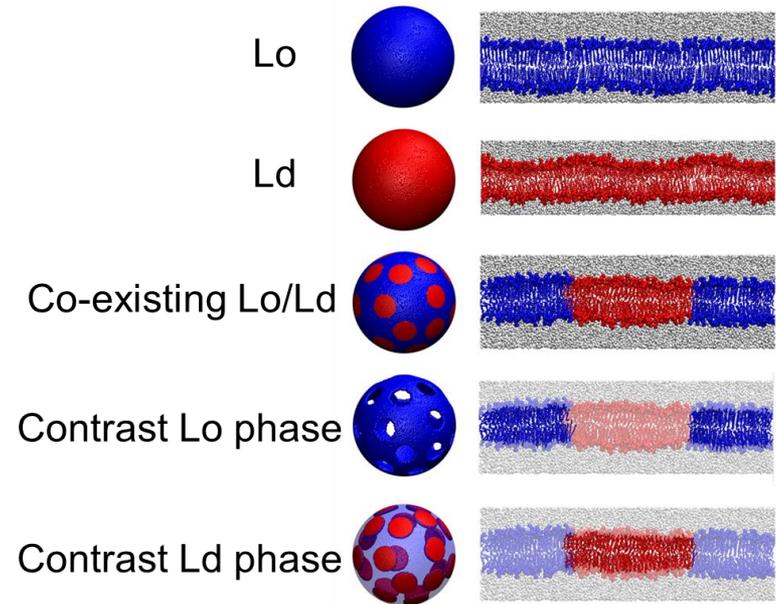
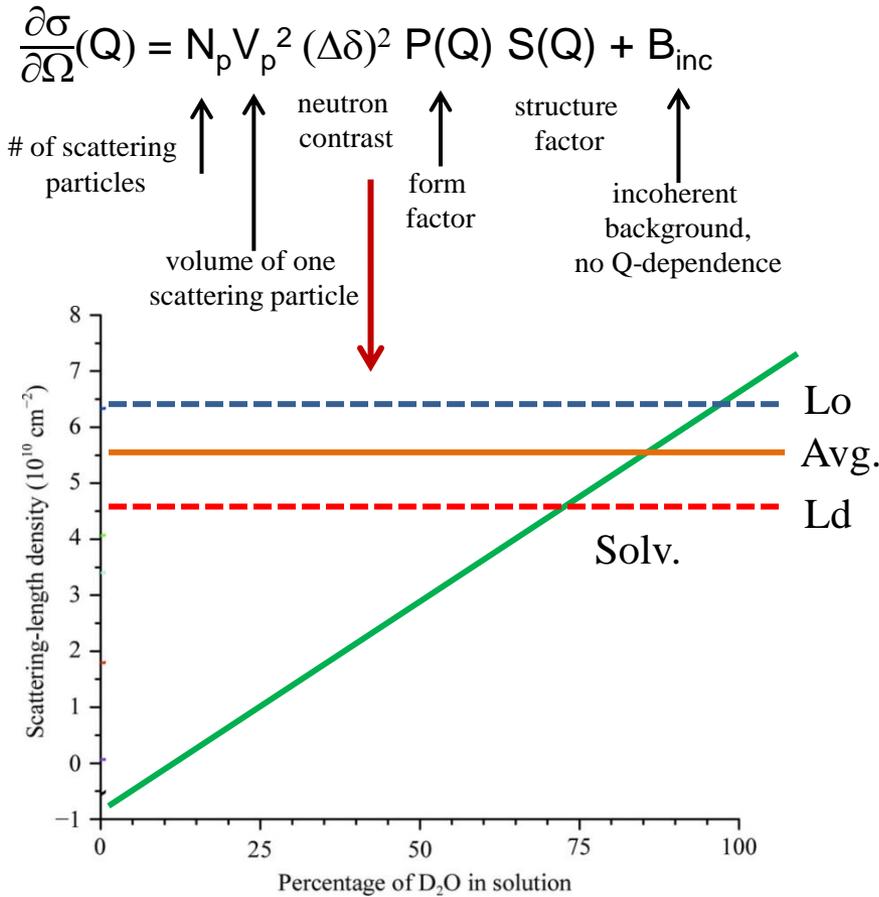
# of scattering particles  $\uparrow$   $\uparrow$  neutron contrast  $\uparrow$  structure factor  $\uparrow$   $B_{inc}$   
 volume of one scattering particle  $\uparrow$  form factor  $\uparrow$  incoherent background, no Q-dependence

$$(\Delta\delta)^2 = (\delta_{lipid} - \delta_{water})^2 = 0 \text{ scattering}$$

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



# Neutrons Scattering - Contrast

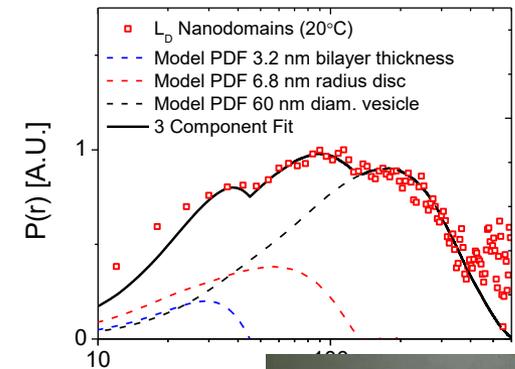
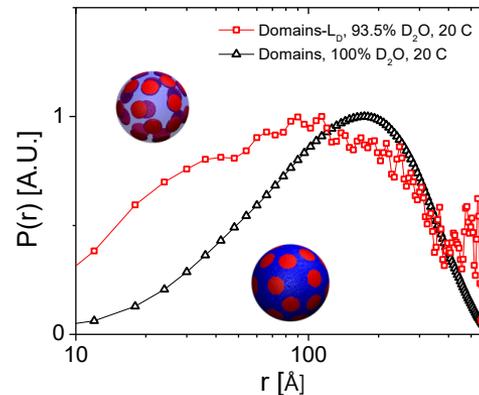
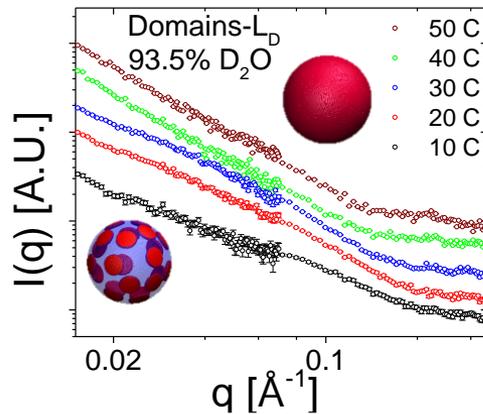
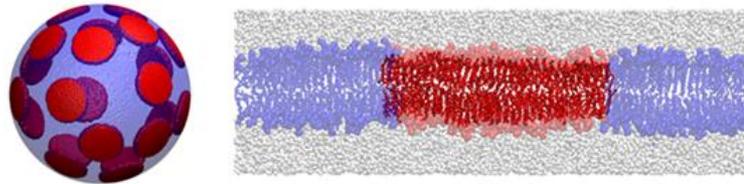


Nickels et al. JAC



# SANS – Structure of Raft-like Features

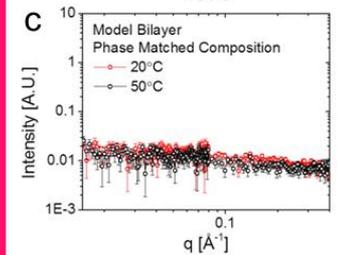
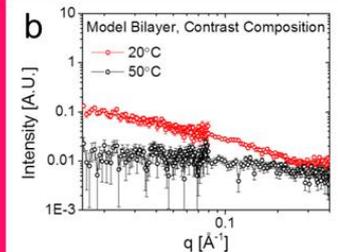
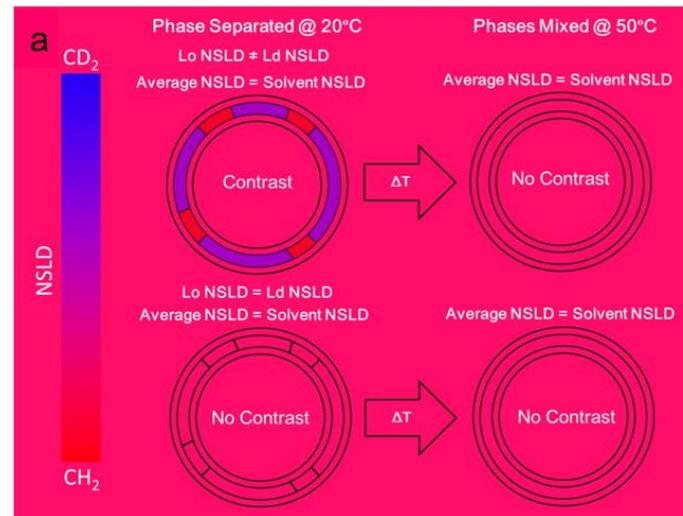
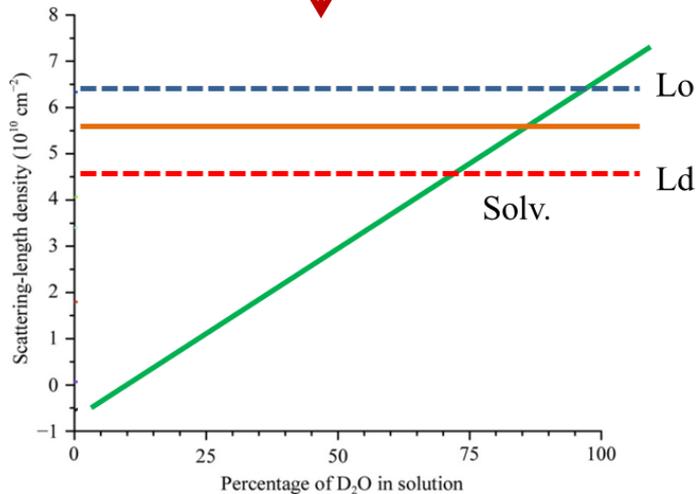
Contrast Ld phase



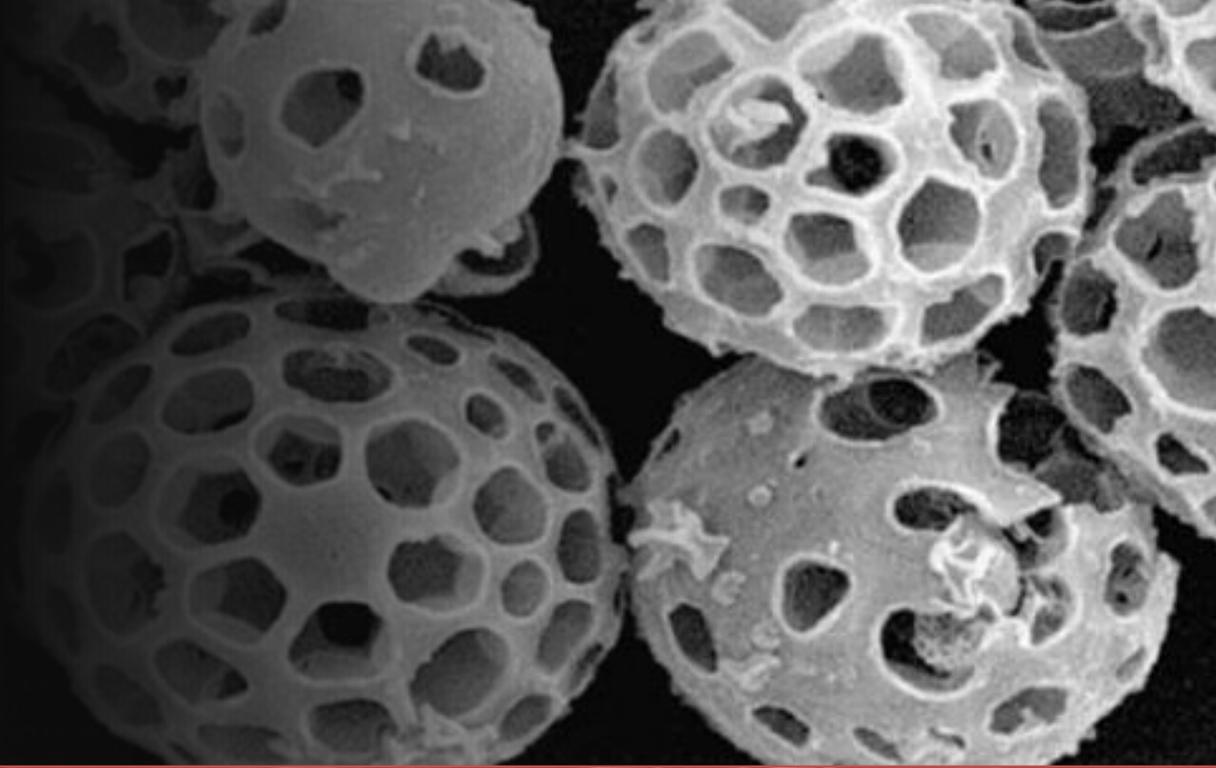
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# Summary



Methods to investigate coexisting lyotropic phases based on scattering contrast.

Lead to new design principles to drive material properties.





Jonathan D. Nickels PhD  
Assistant Professor  
Dept. of Chemical and Environmental Engineering  
University of Cincinnati

A screenshot of the website for The Nickels Lab at the University of Cincinnati. The header includes the lab name and navigation links: Home, Research, Publications, People, Contact, and UC Home. The main banner features a colorful molecular simulation and the text "Nanoscale structure and dynamics Small structures and fast motions have big effects." Below the banner, there is a section titled "We study the structure and dynamics of soft matter and biological materials." followed by a paragraph describing the lab's research approach and a list of topics. Three journal covers are displayed: JACS, PLOS ONE, and PCCP, each with a corresponding title and a brief description of the research.

