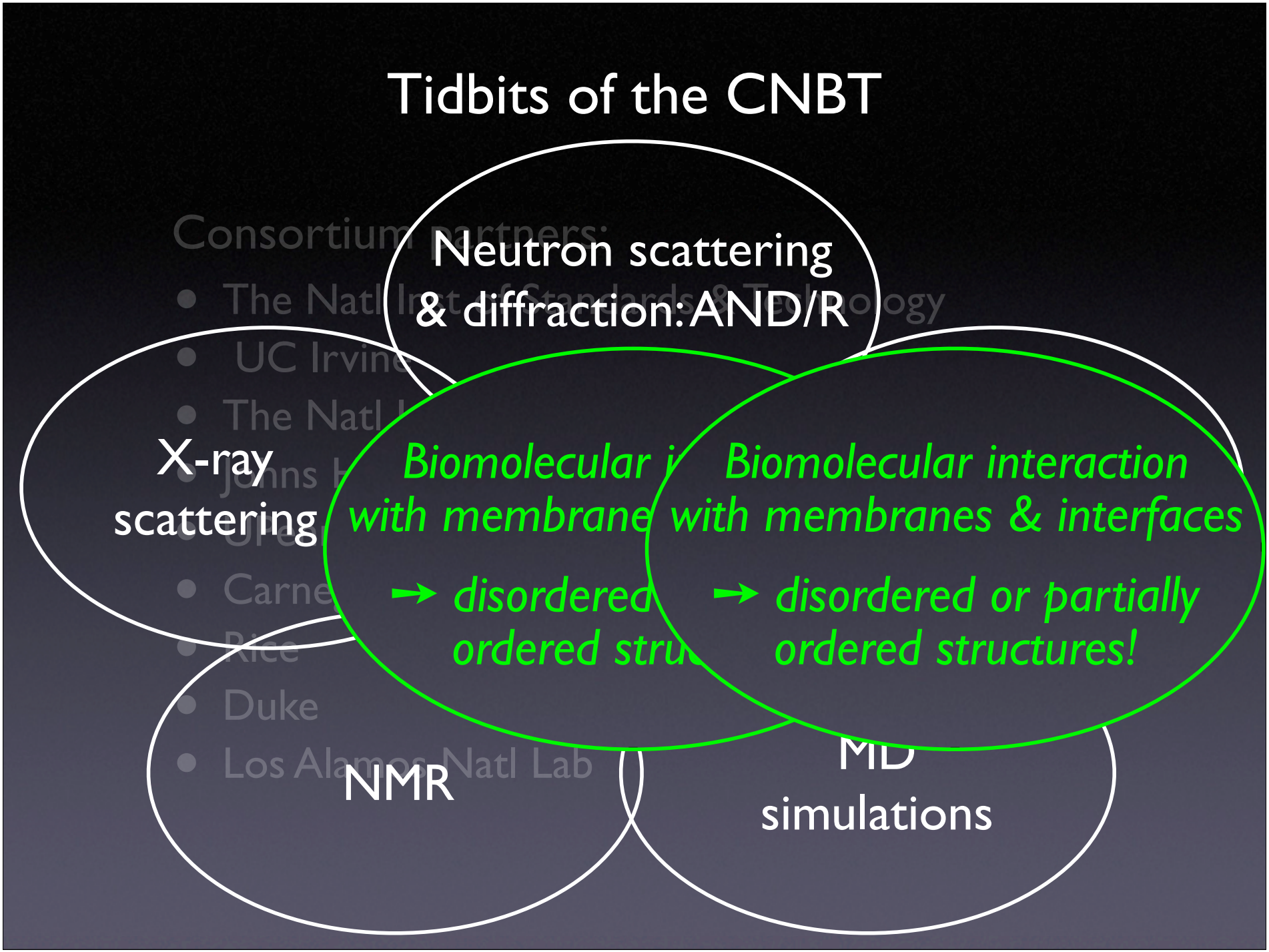
Characterization of Functionalized Biomimetic Membranes: The CNBT and AND/R at NCNR

- The *CNBT* at the *NIST Center for Neutron Research*: A research partnership in nanotechnology
- Tidbits of the CNBT: The consortium
  - Neutron scattering/diffraction: The *Advanced Neutron Diffractometer and Reflectometer* (*AND/R*)
  - MD simulations
  - NMR spectroscopy
  - X-ray scattering
- Technology focus: Membrane biophysics and beyond

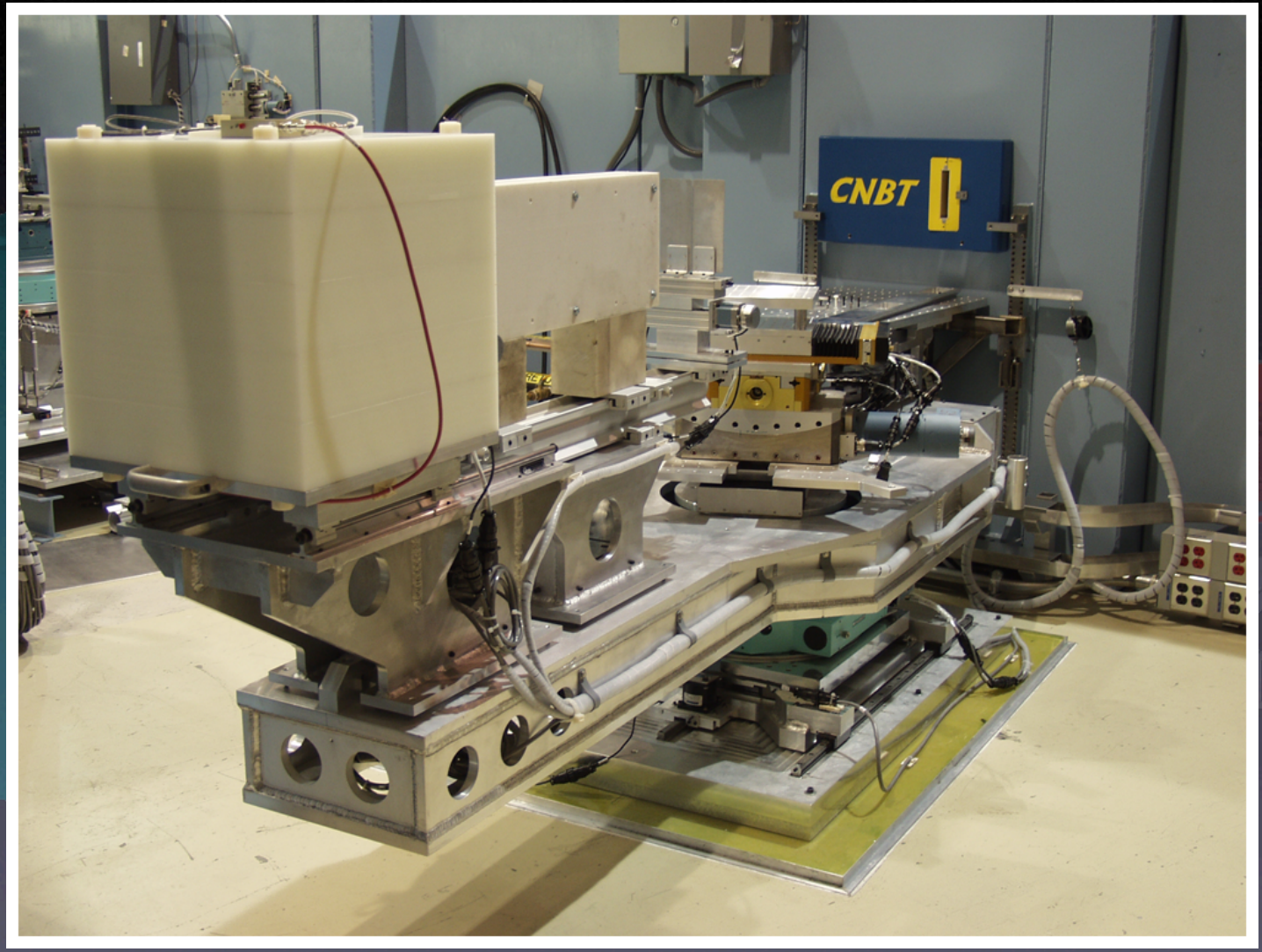
CNBT Cold Neutrons for Biology and Technology

funded by the NIH (1RO1 RR14812)

Tidbits of the CNBT

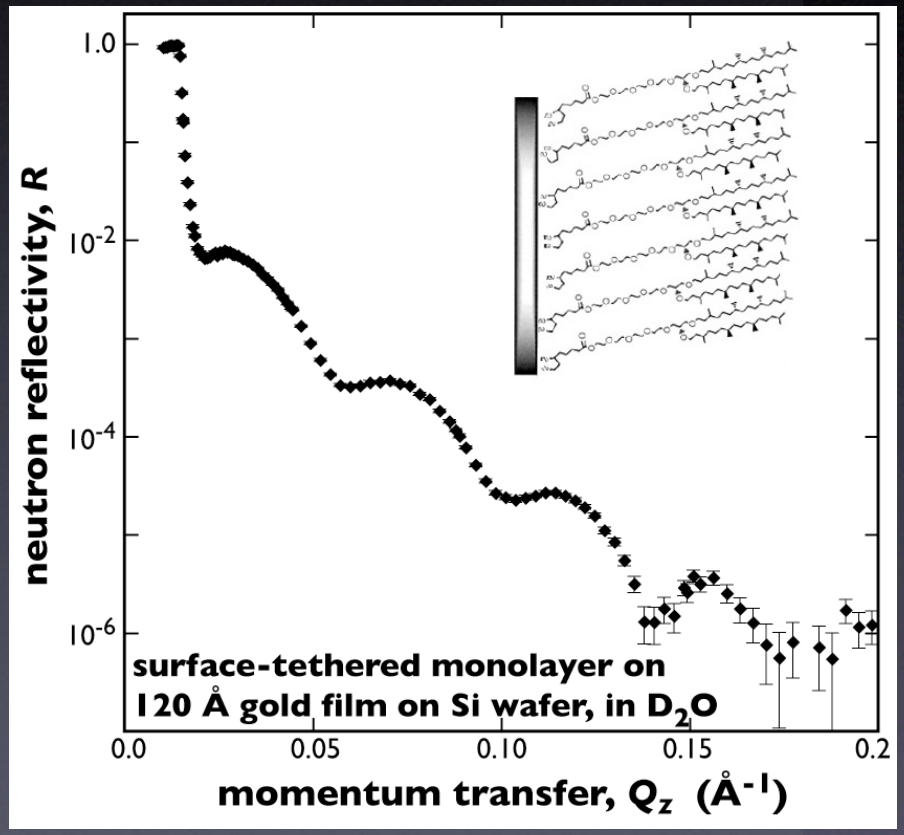


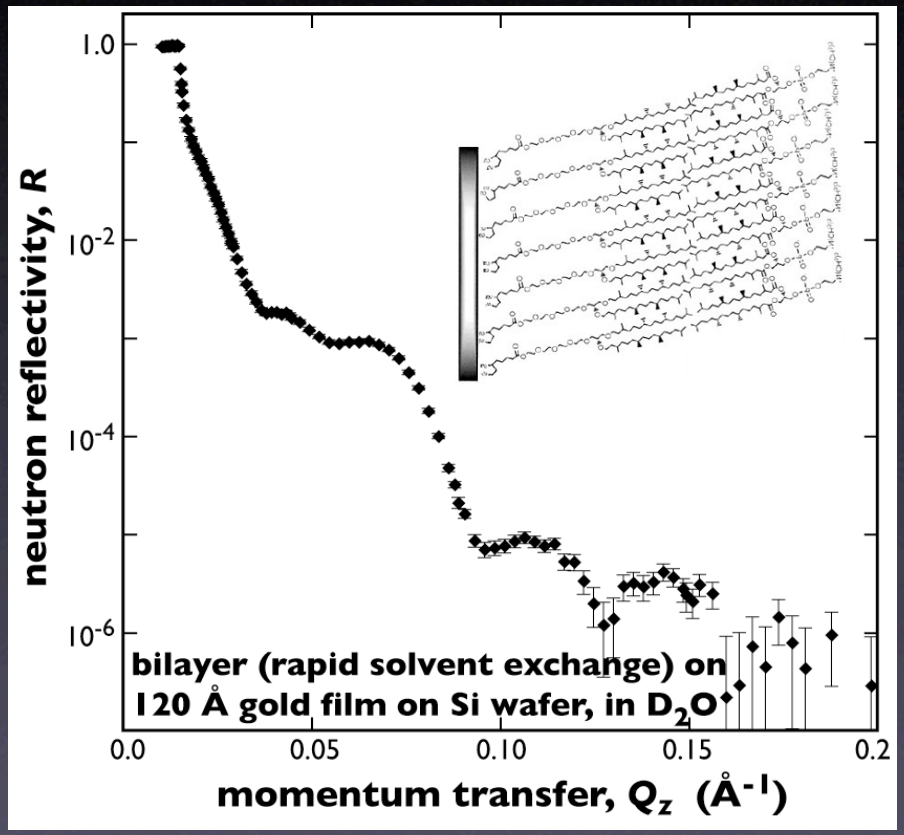
Neutron Scattering and Diffraction



Neutron Scattering and Diffraction

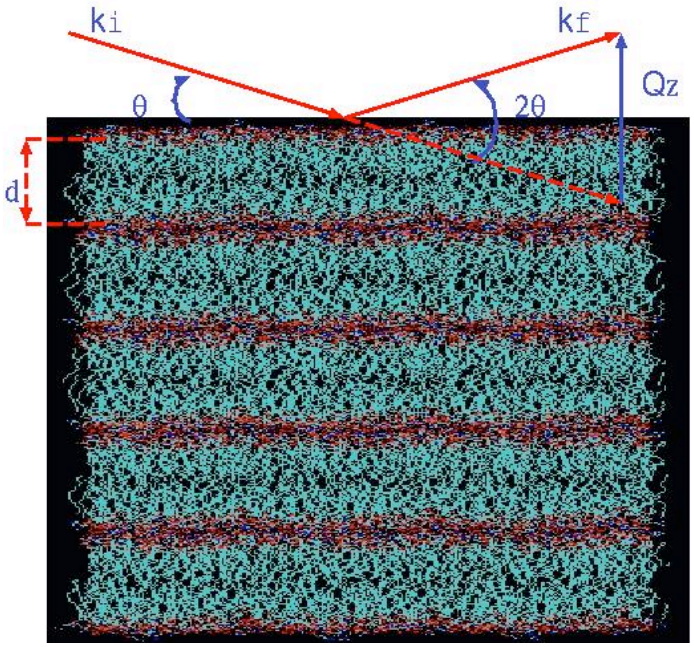
tethered membrane systems – representative reflection results:

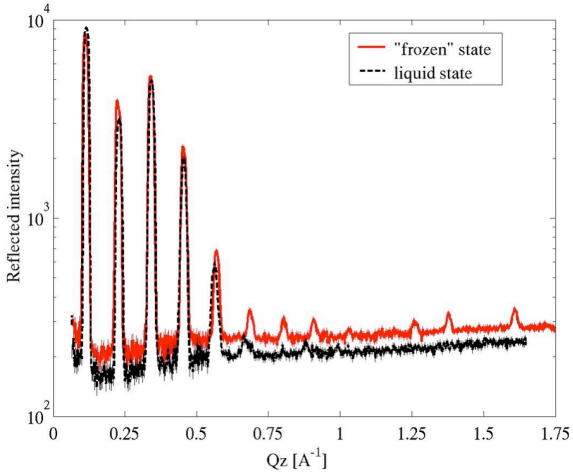


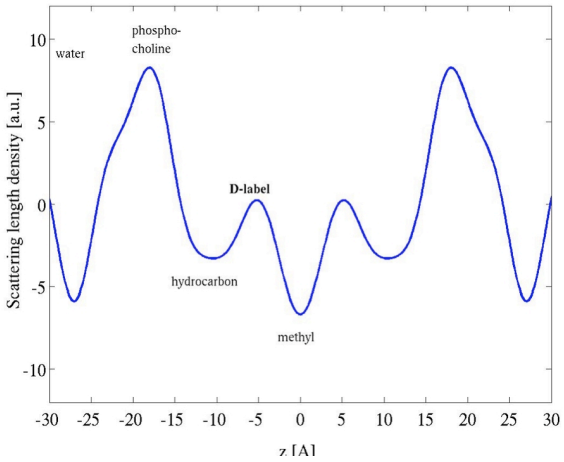


(collaboration with I. Köper, J.J. Kasianowicz in NSF-NIRT program)

Neutron Scattering and Diffraction



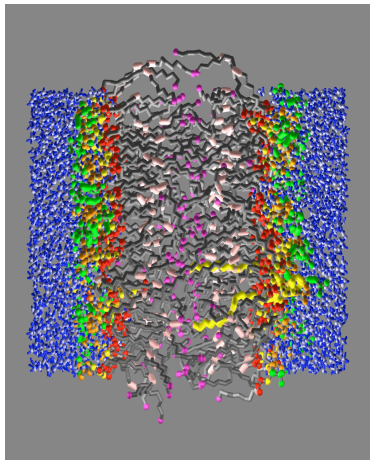




1D diffraction from multi-bilayer samples

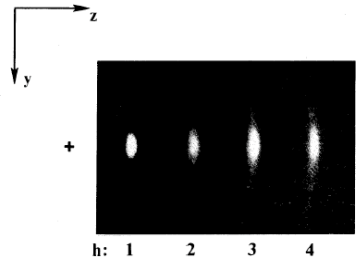
Molecular Dynamics Simulations

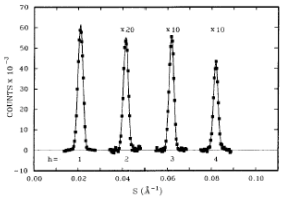
MD simulations & diffraction experiments:
teaming up to refine disordered structures in 3D



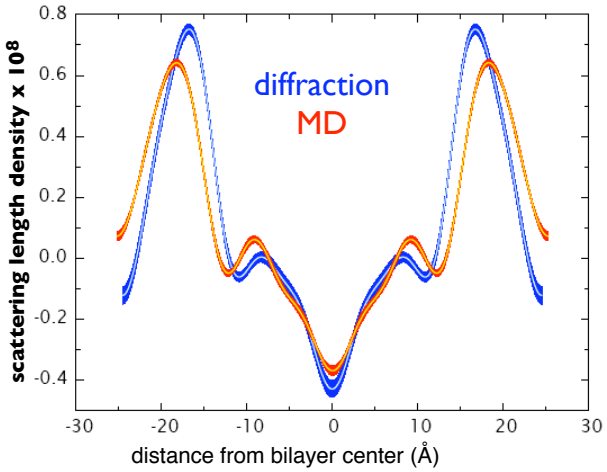
MD simulations:
all-atom phase trajectories

$$\rho(z) = \rho_0 + \frac{2}{d}\sum_{h=1}^{h_{max}} F(h)\cos\left(\frac{2\pi h z}{d}\right)$$





diffraction:
structure factor amplitudes

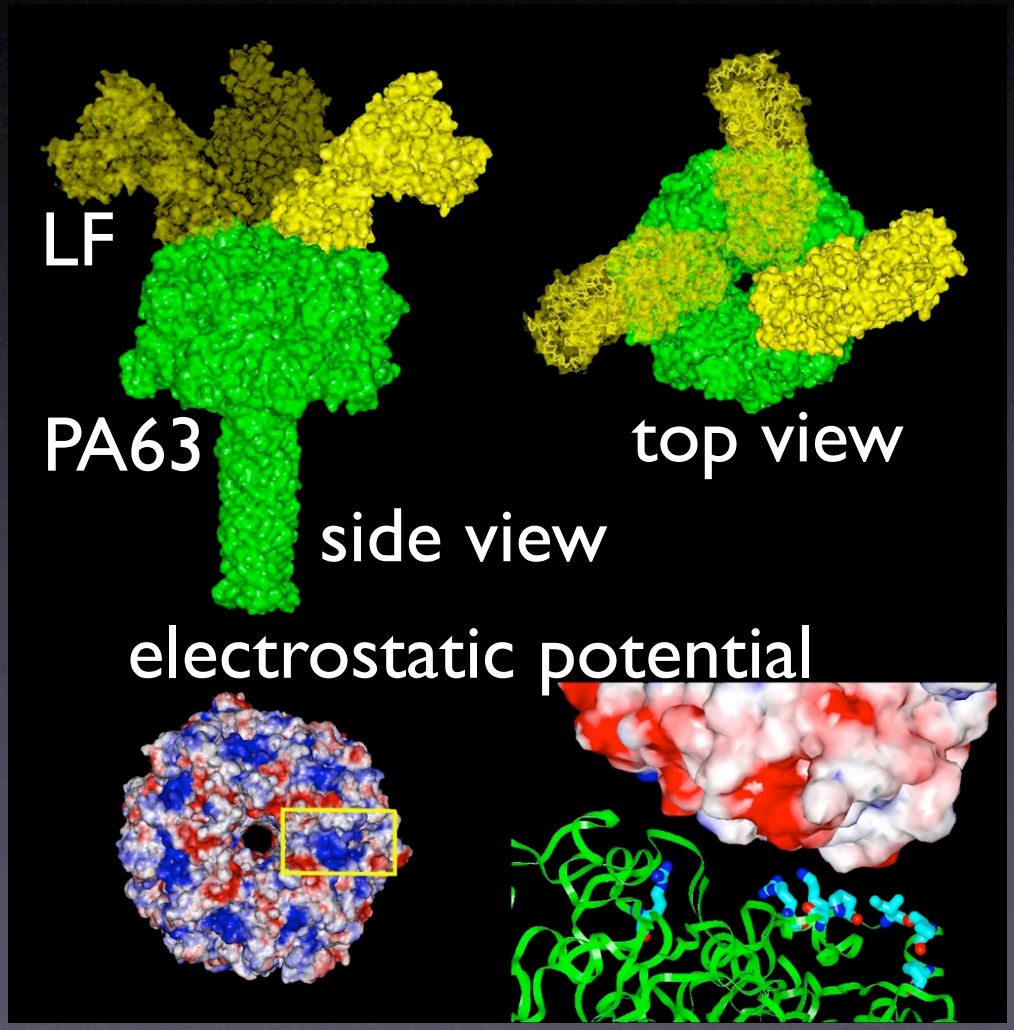


- 3D details to 1D structure
- predictions stimulate new experiments

- validation & refinement of simulation methods
- data for restraint potentials

Benz, Castro-Roman, Tobias & White, BJ (2005)

Characterization of protein membrane pores
(J.J. Kasianowicz)



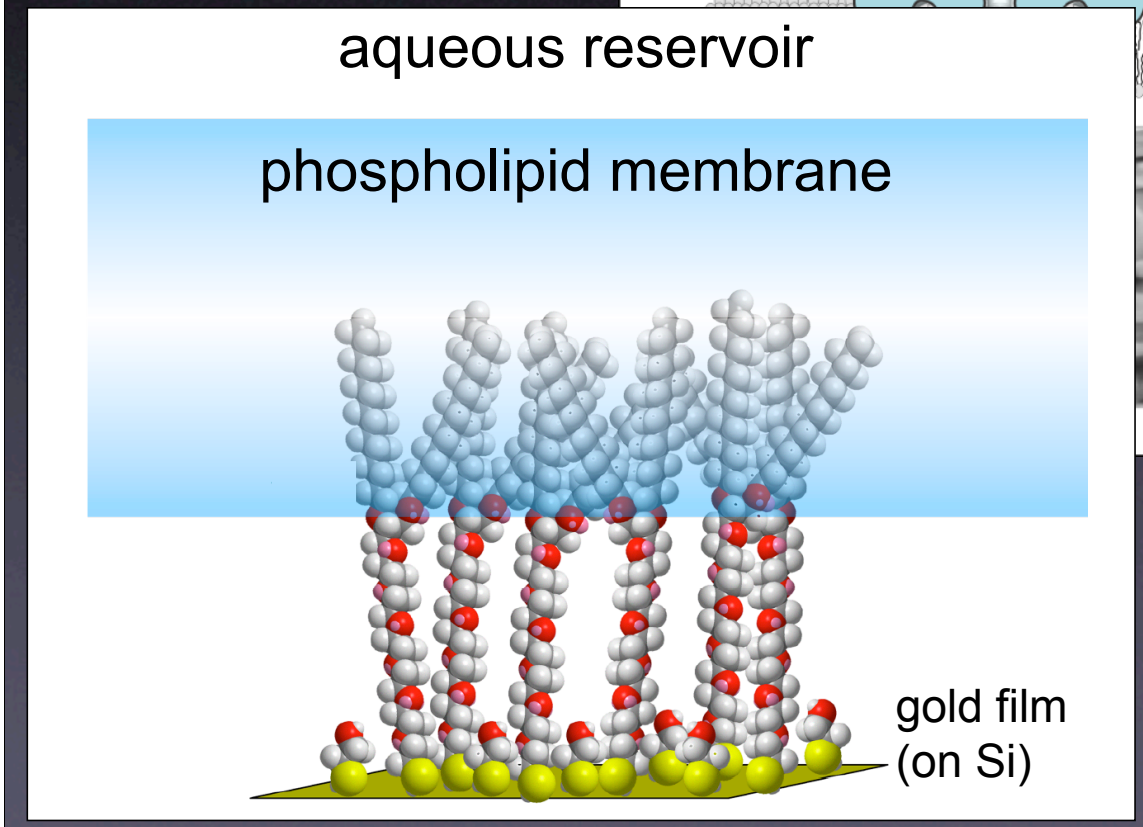
Halverson, Panchal, Nguyen, Gussio, Little, Misakian, Bavari & Kasianowicz, submitted to *PNAS*

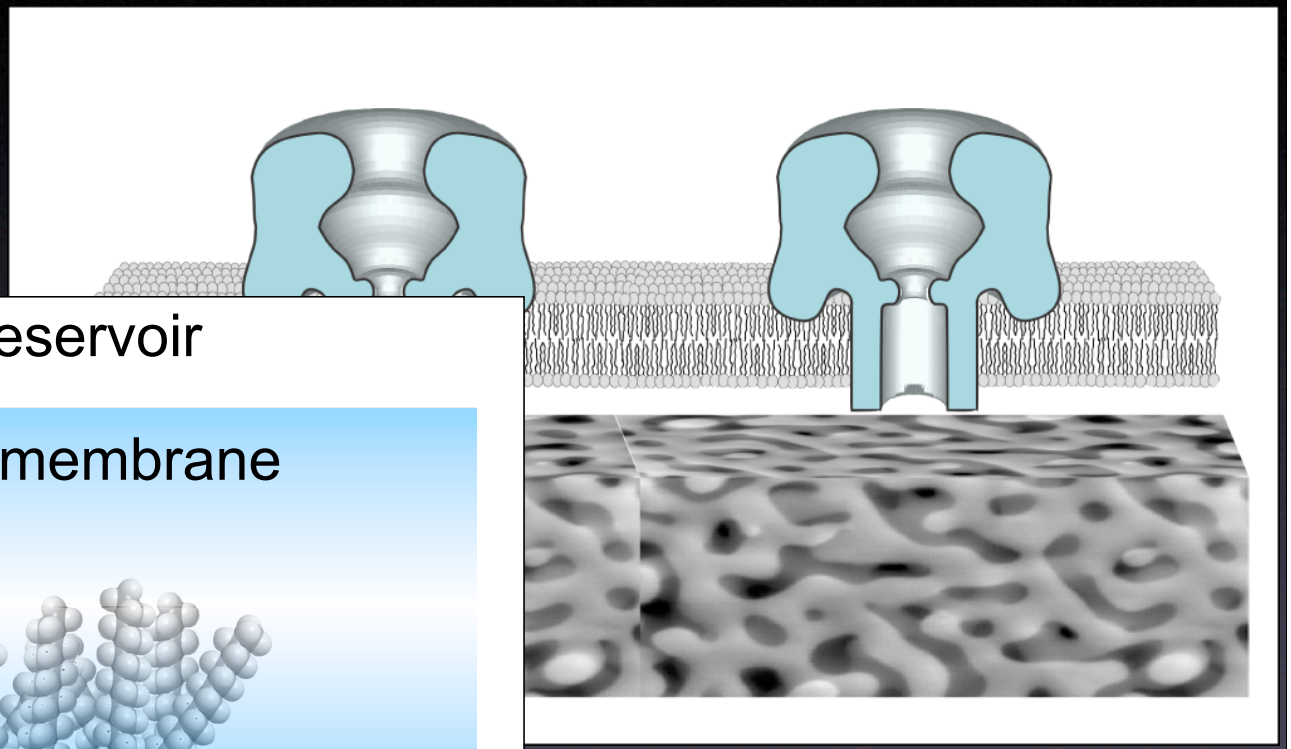
goal:

incorporation into stabilized membrane systems as a basis for

- molecular sensor systems
- pharmaceutical screening

Tethered membrane systems for protein incorporation

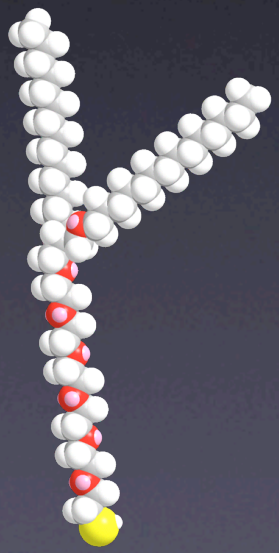




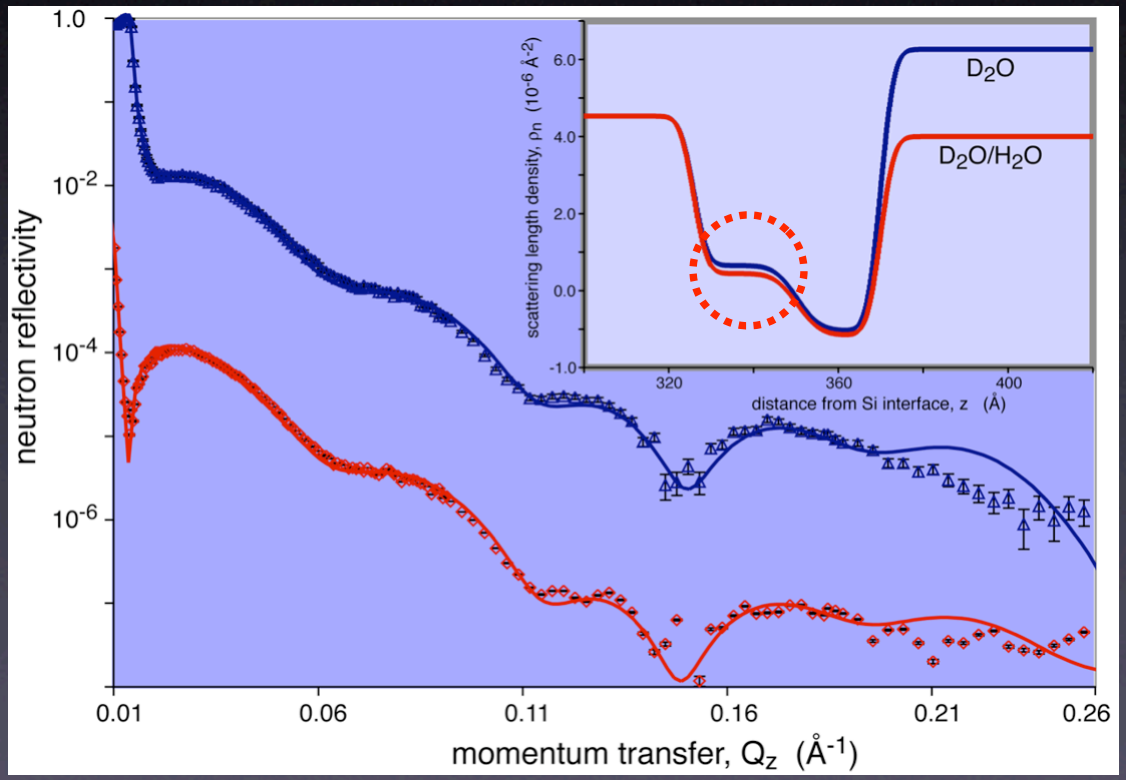
porous gold:
collaboration with J. Erlebacher (Johns Hopkins) in NSF-NIRT

WC14:

A thiolated oligo-EG dialkane for grafting on Au surfaces (synthesis: Vanderah et al.)



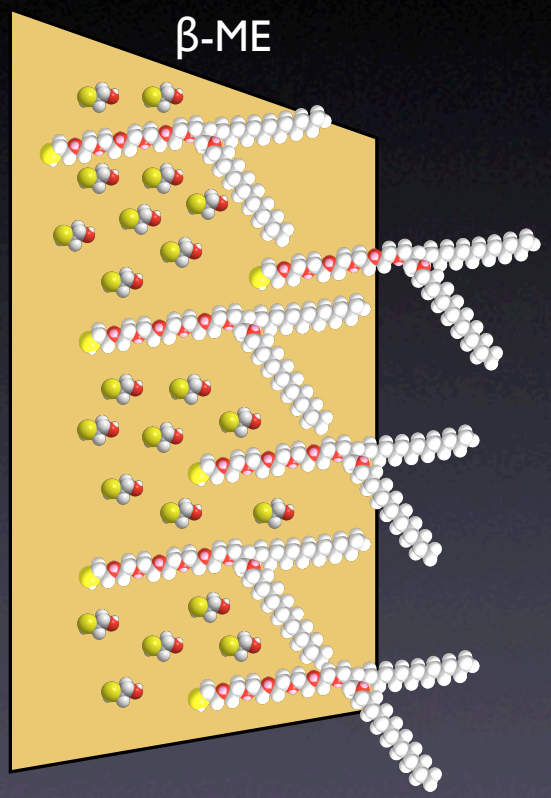
WC14 monolayer on Au (Si) under water

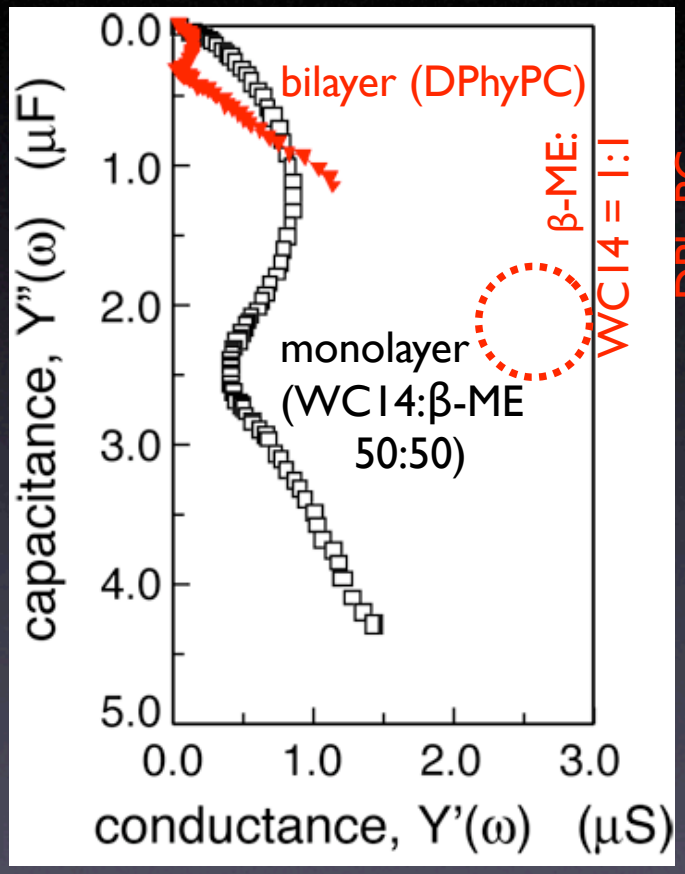


extremely dense alkane packing

< 5 vol% solvent in proximal space

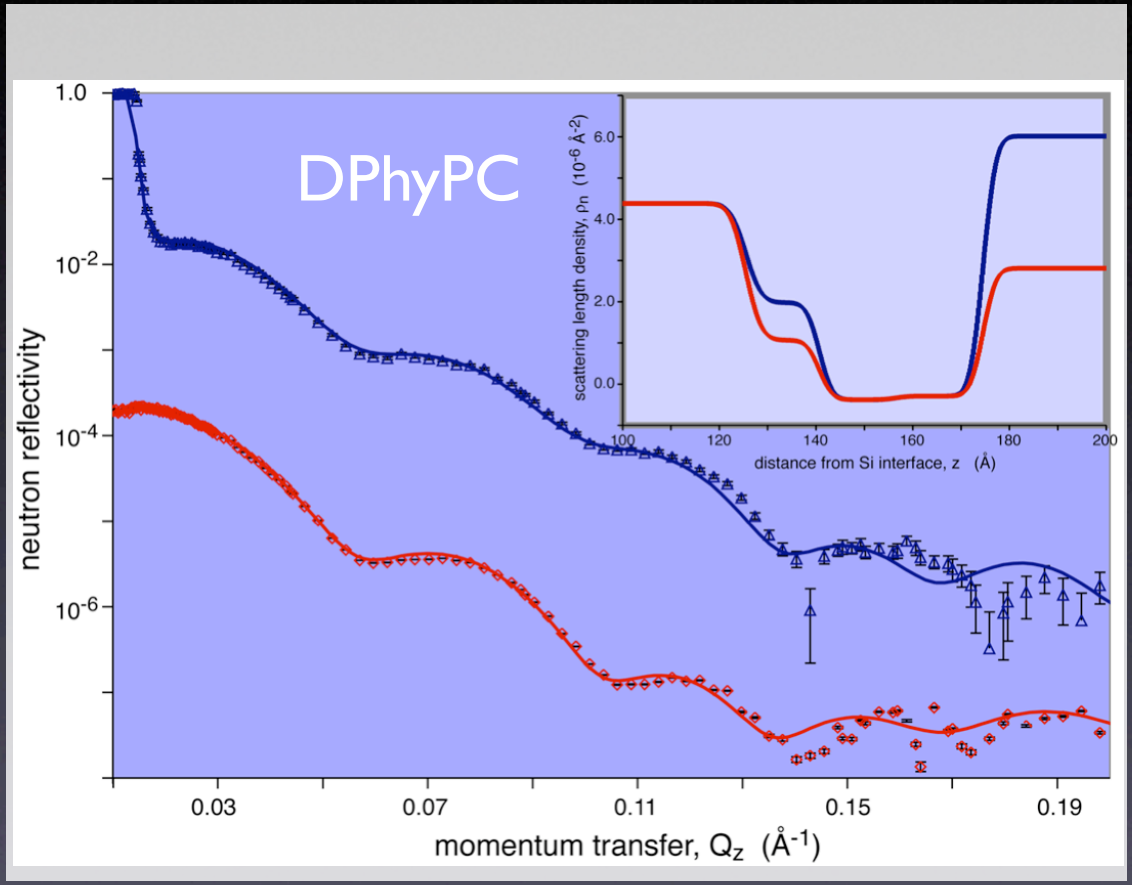
Backfilling with Mercaptoethanol





- Y',Y" of mixed monolayer >> pure WC14
- Y',Y" of bilayer (DPhyPC) based on mixed monolayer ~ as for pure WC14
- β-ME introduces solvent in proximal space

Backfilling with Mercaptoethanol



Conclusions

- Bionanotechnology – just as other areas of nanotechnology – requires multidisciplinary approach
- Central facility promotes collaboration synergies
- Neutrons indispensible tool for bio-derived nanomaterials
- New versatile instrument available at NCNR, the *AND/R*
- Artificial membrane environments will impact future sensing/ screening applications