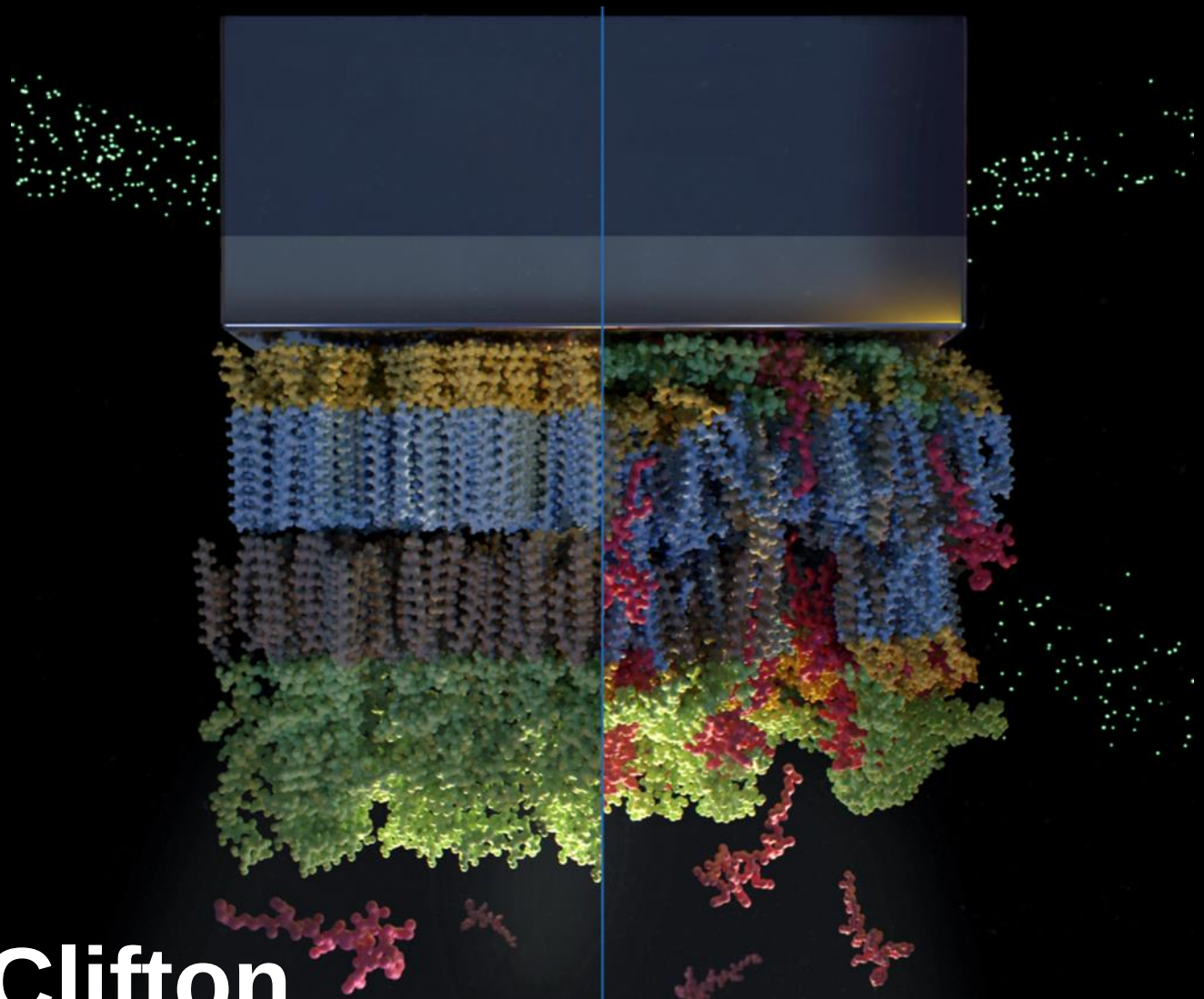
Neutron Reflectometry in Soft Matter Studies



Luke Clifton

This lecture

- **The practicality's of Neutron reflectometry on soft matter systems.**

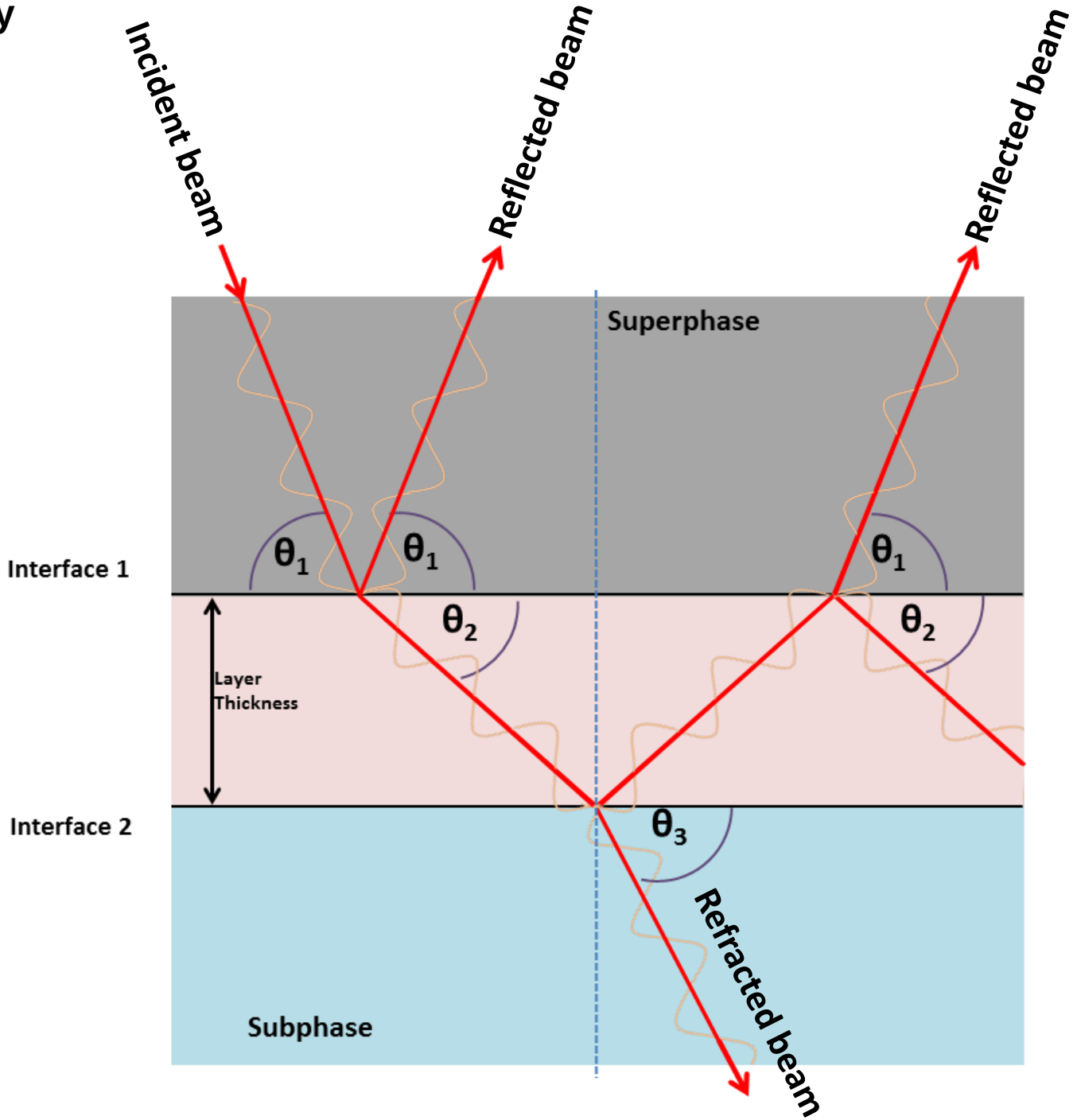
- **Utilisation of hydrogen (protium): deuterium isotopic contrast variation to tailor the information content in NR data.**

- **Examples of soft NR studies discussed with an emphasis on experimental design.**

Neutrons – a tailor-made probe

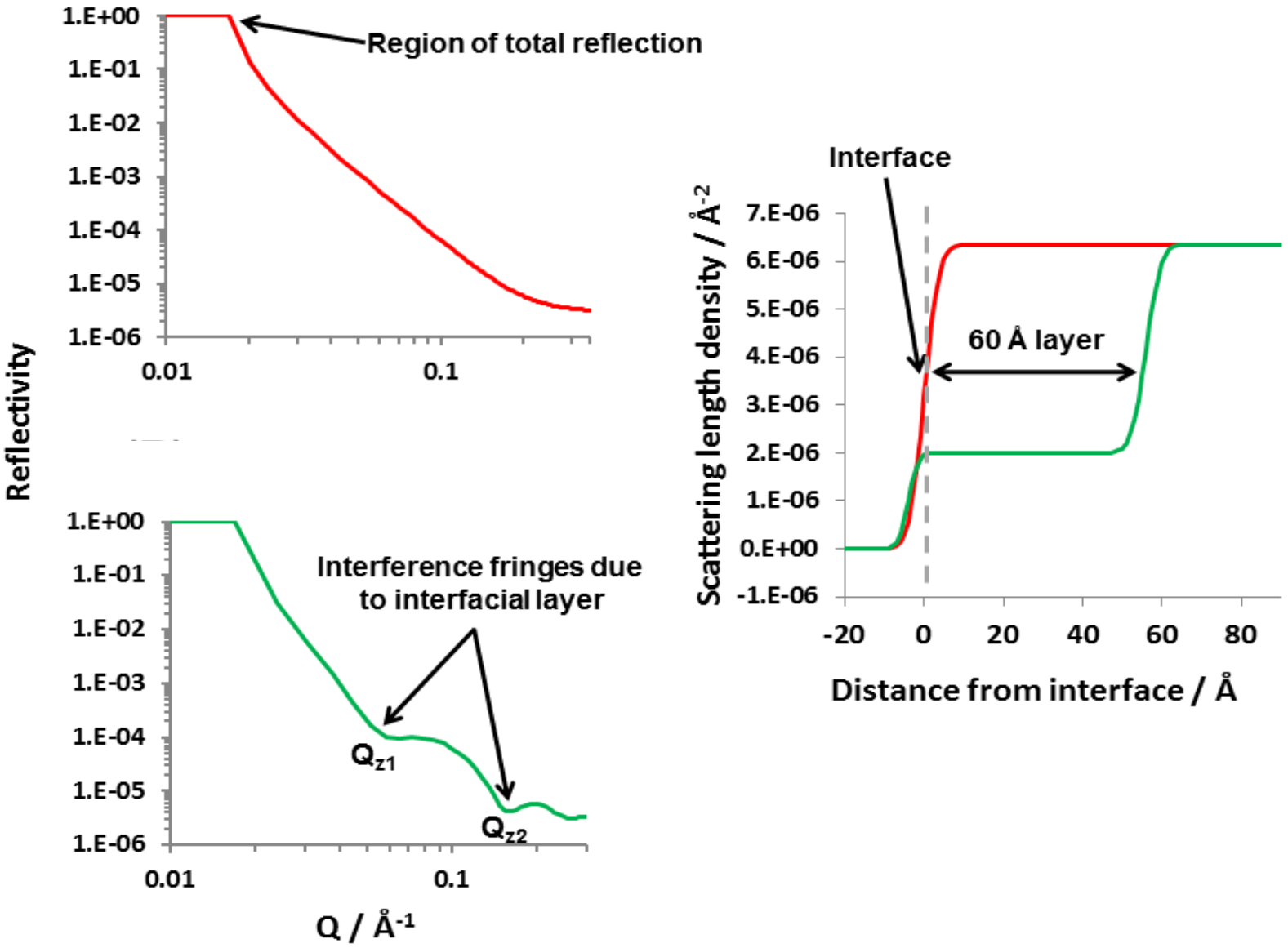
- Neutron wavelength and energy ‘just right’ for condensed matter.
- H / D contrast
- Magnetic Moment
- Highly penetrating
- Non Destructive

Reflectometry

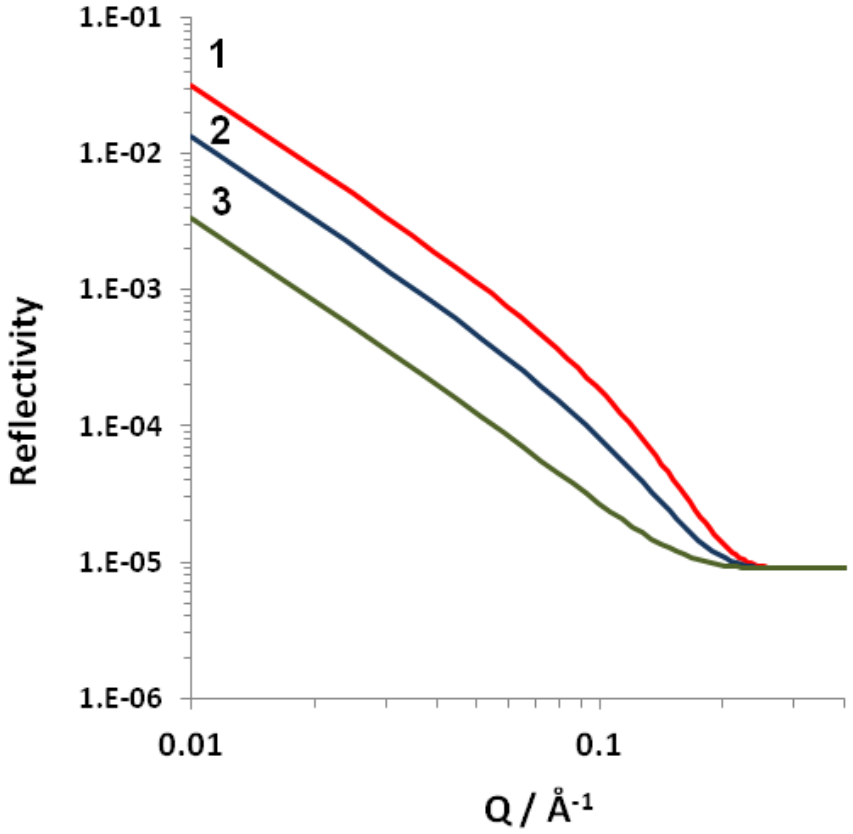


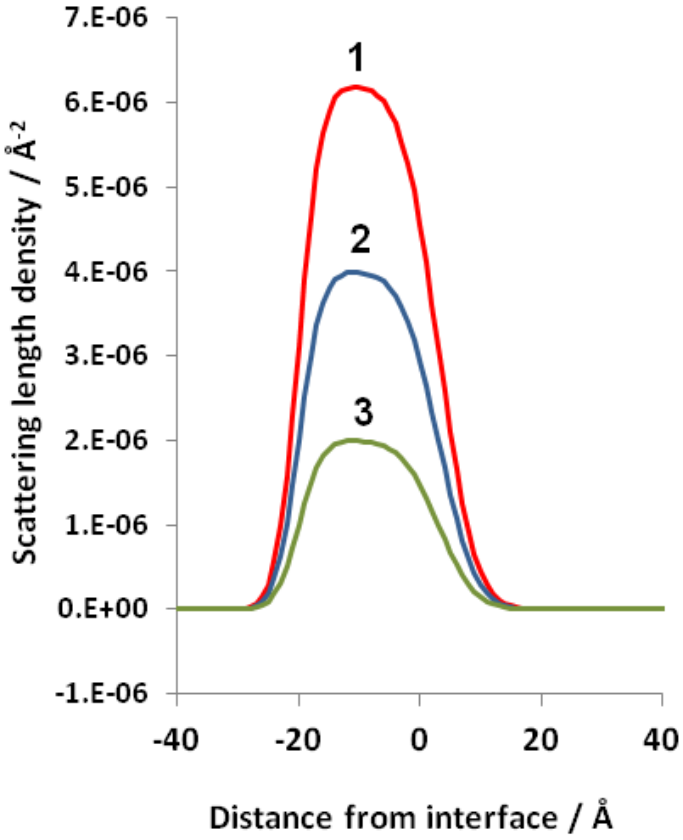
Reflectometry gives you Distances

$$d = \frac{2\pi}{\Delta Q}$$

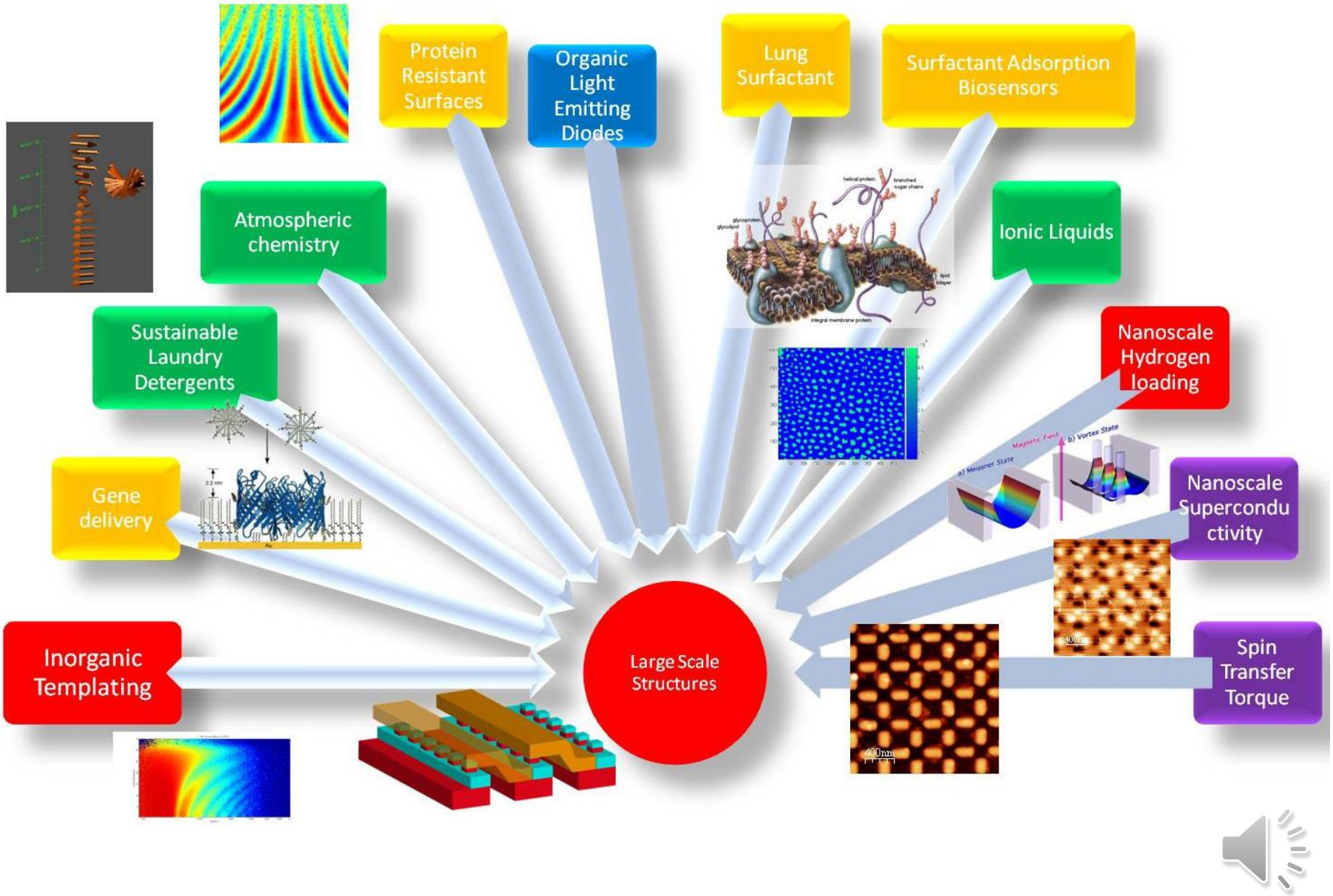


Reflectometry gives you Composition

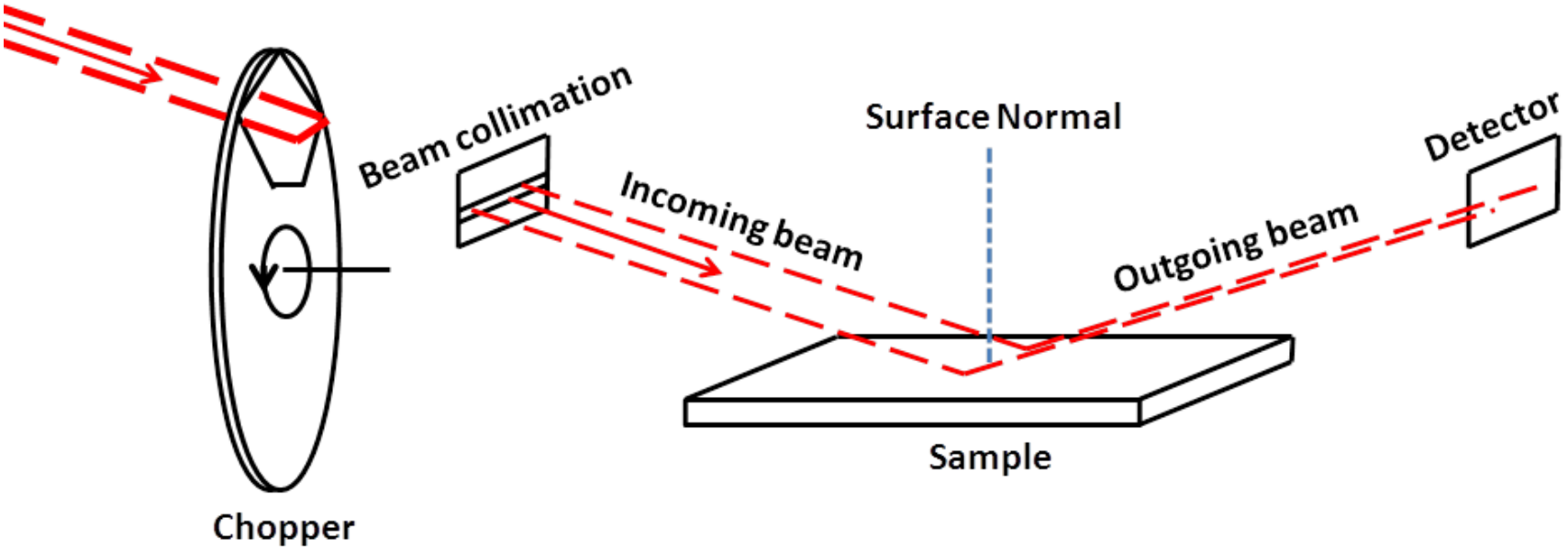


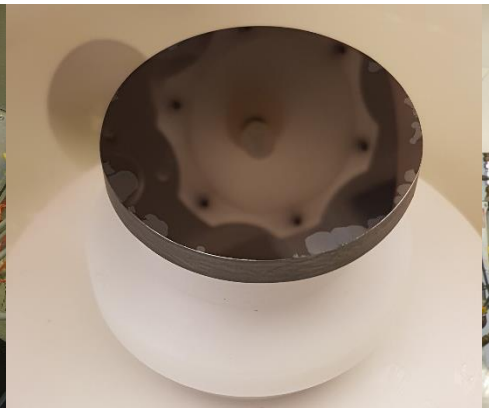


Reflectometry is useful in many areas of science



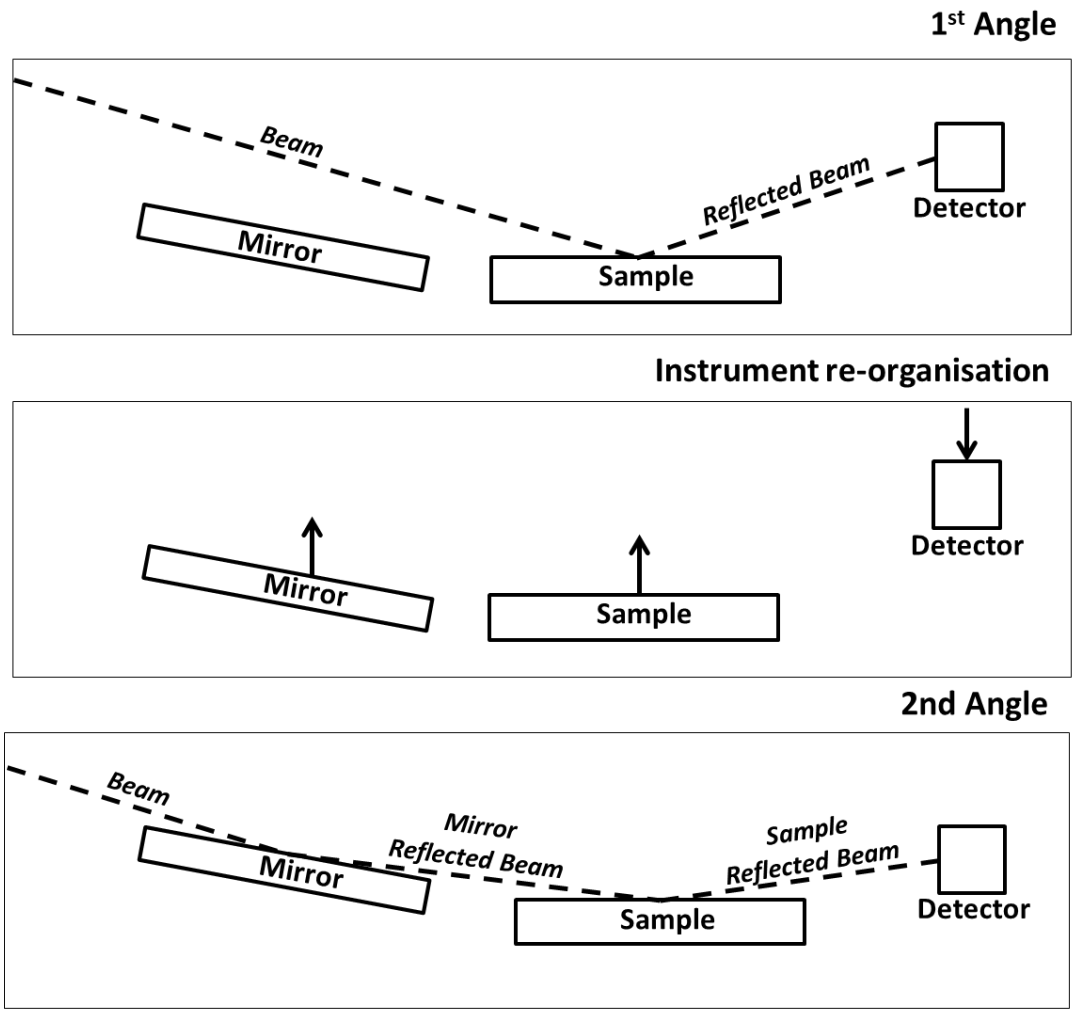
Neutron Reflectometry : Air/Liquid & Solid/Air

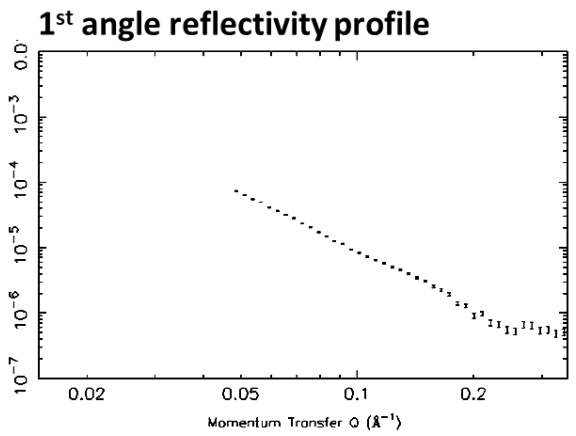


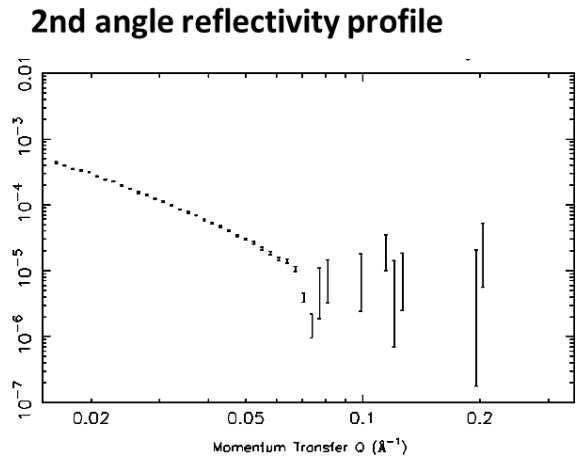



Neutron Reflectometry : Air/Liquid

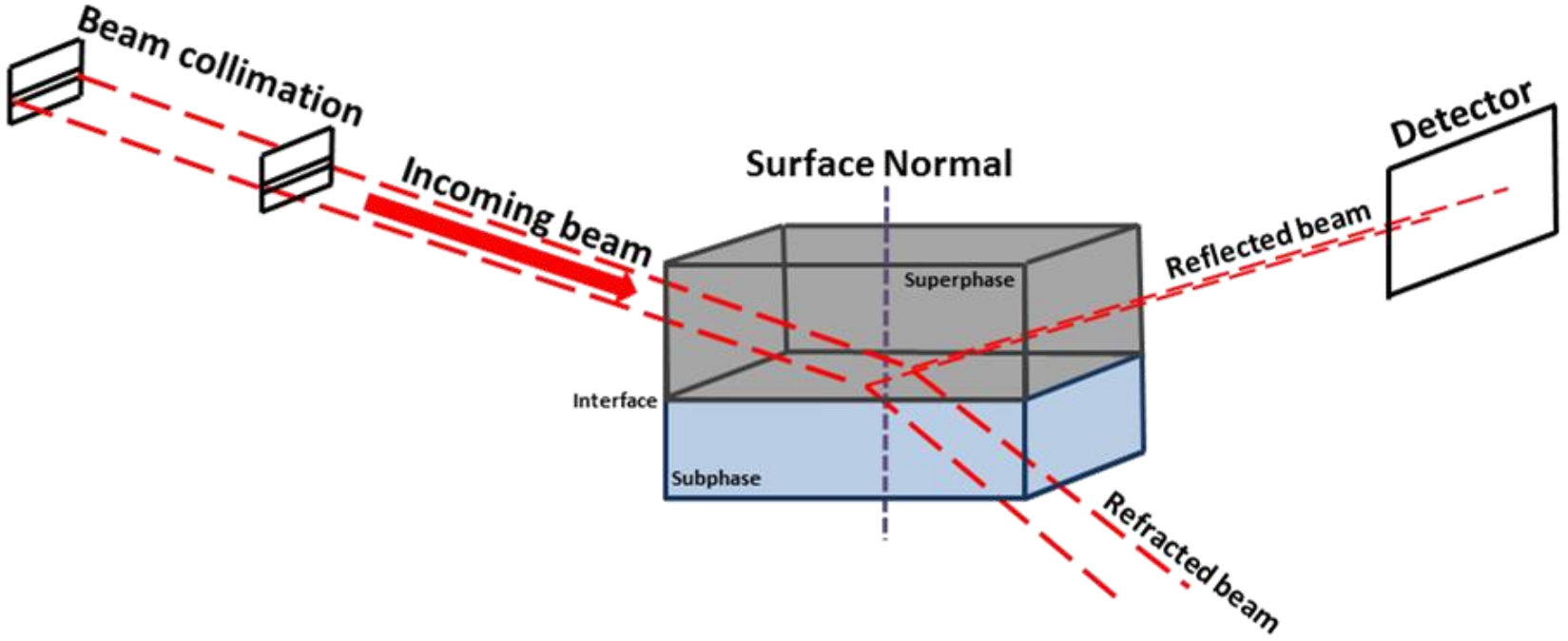
$$Q_z = \frac{4\pi Sin\theta}{\lambda}$$

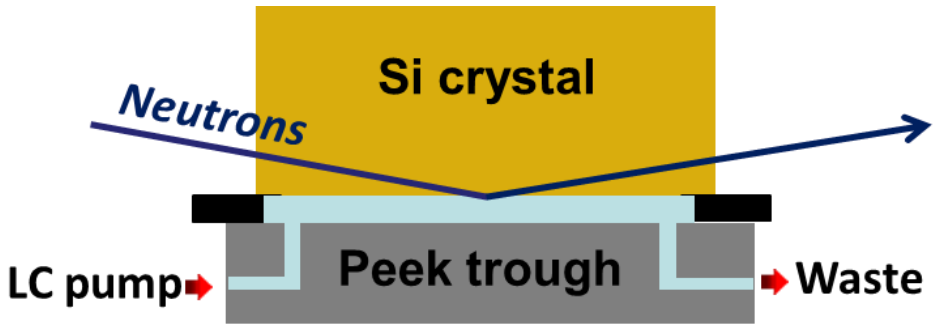


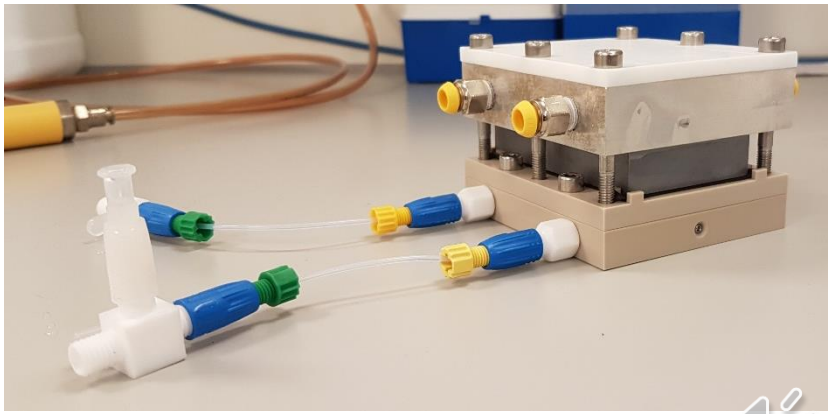




Neutron Reflectometry: Solid-Liquid





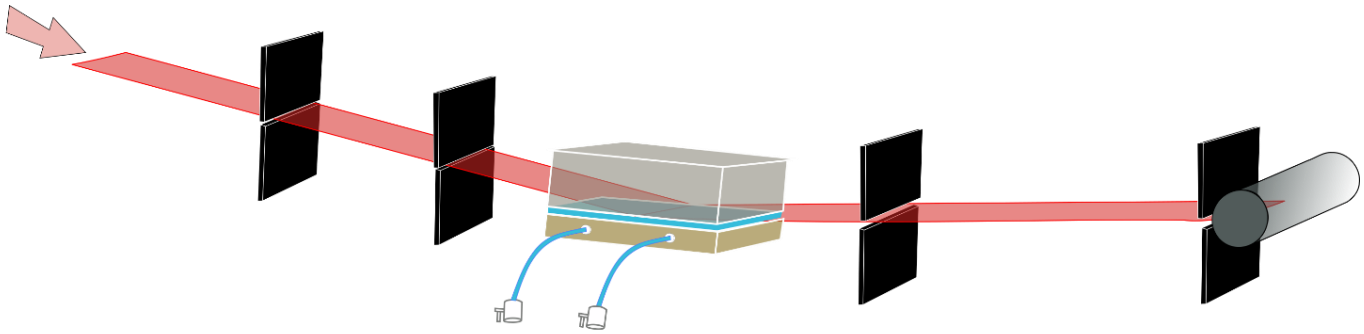


Clifton et al, 2019, Lipid-Protein Interactions, Methods in Molecular Biology, 201-251

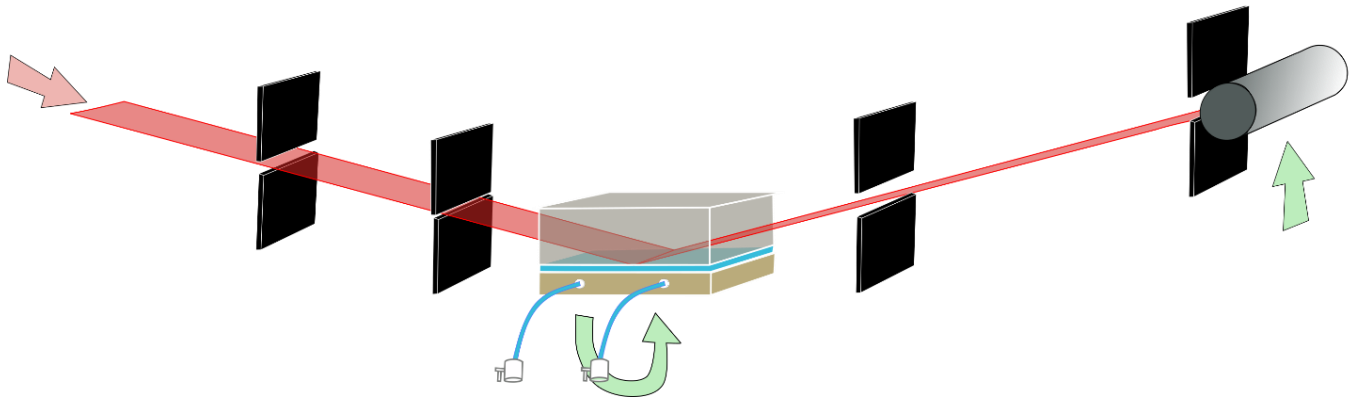
Neutron Reflectometry: Solid-Liquid

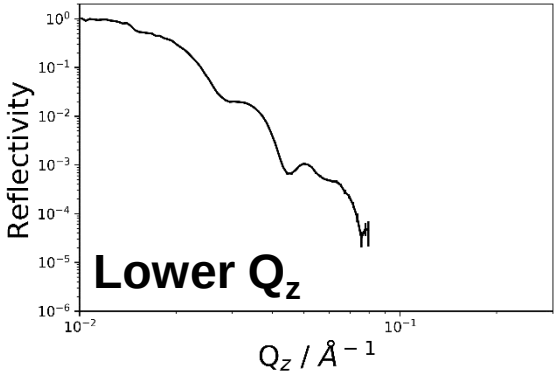
$$Q_z = \frac{4\pi Sin\theta}{\lambda}$$

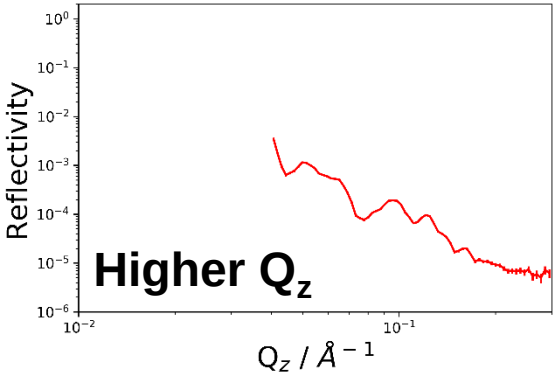
Lower Q_z

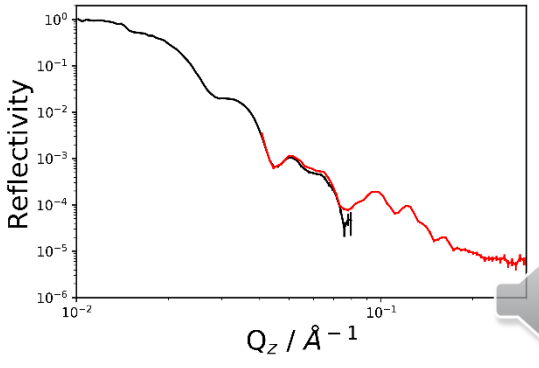


Higher Q_z

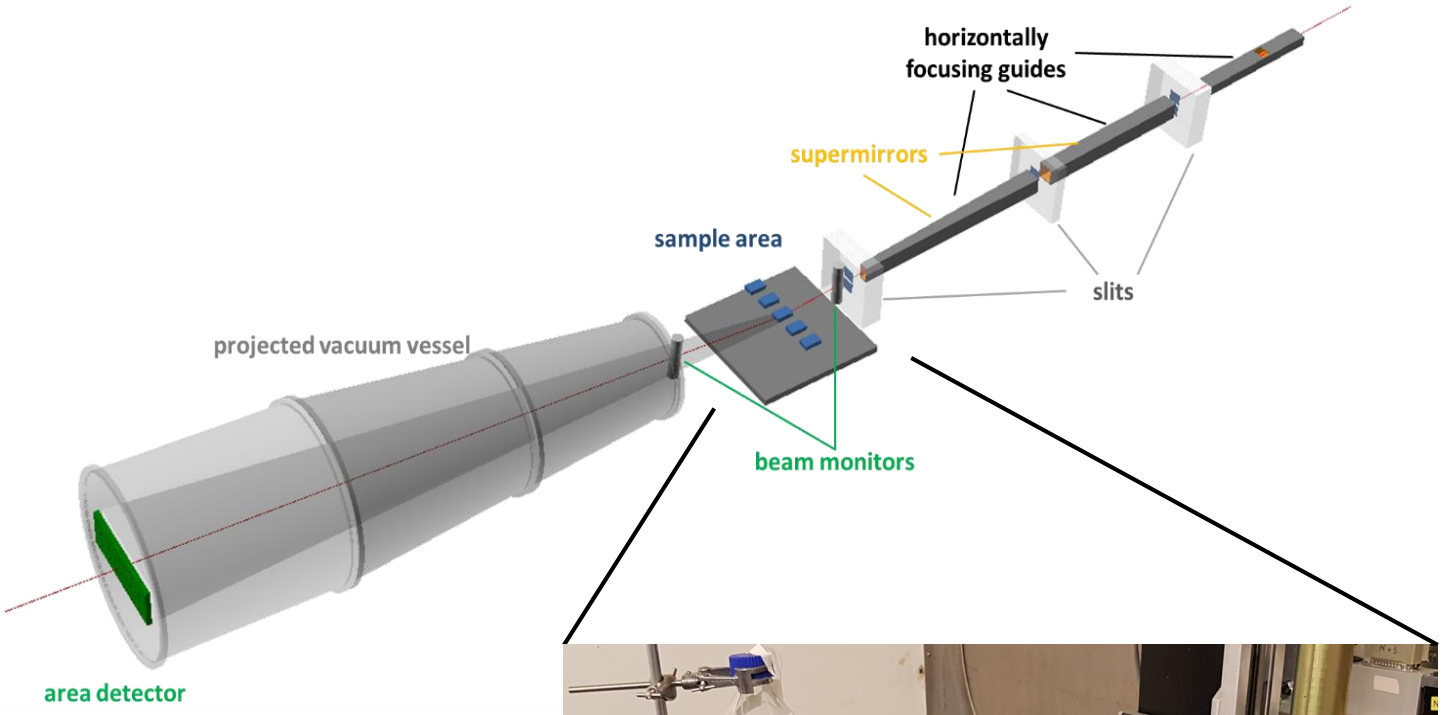


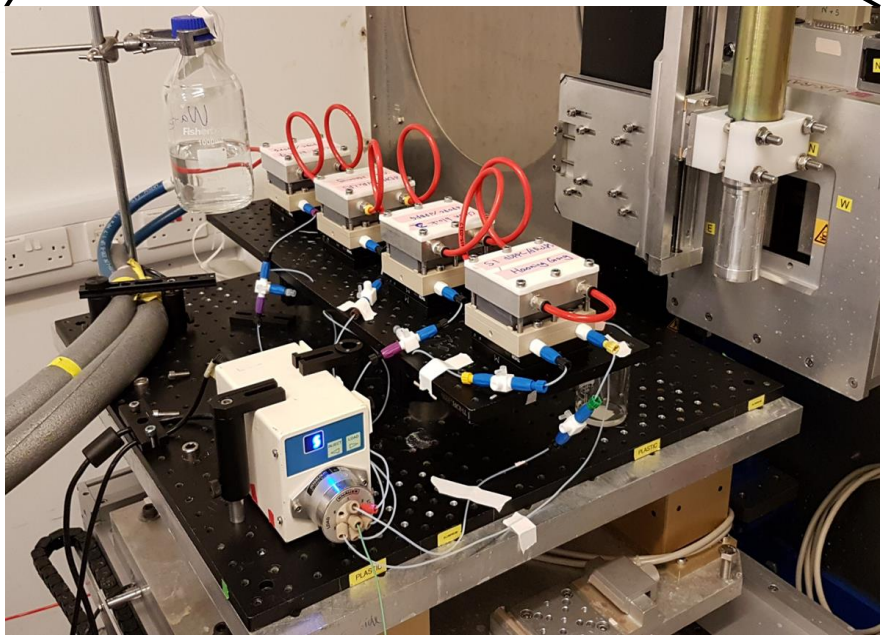


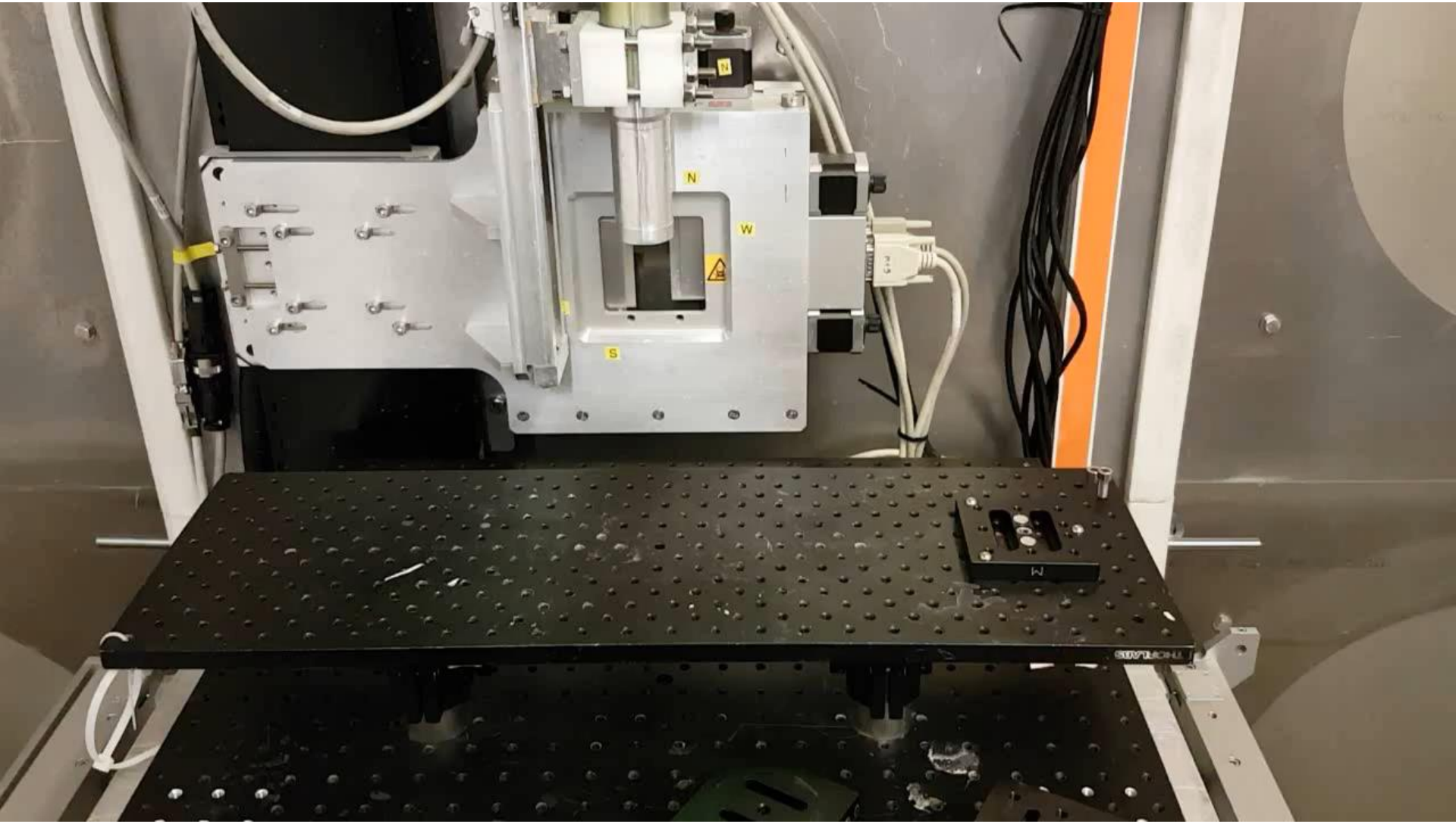




Neutron reflectometry






N
W
S
M

NR ~Describes the Scattering Length Density Profile Across and Interface

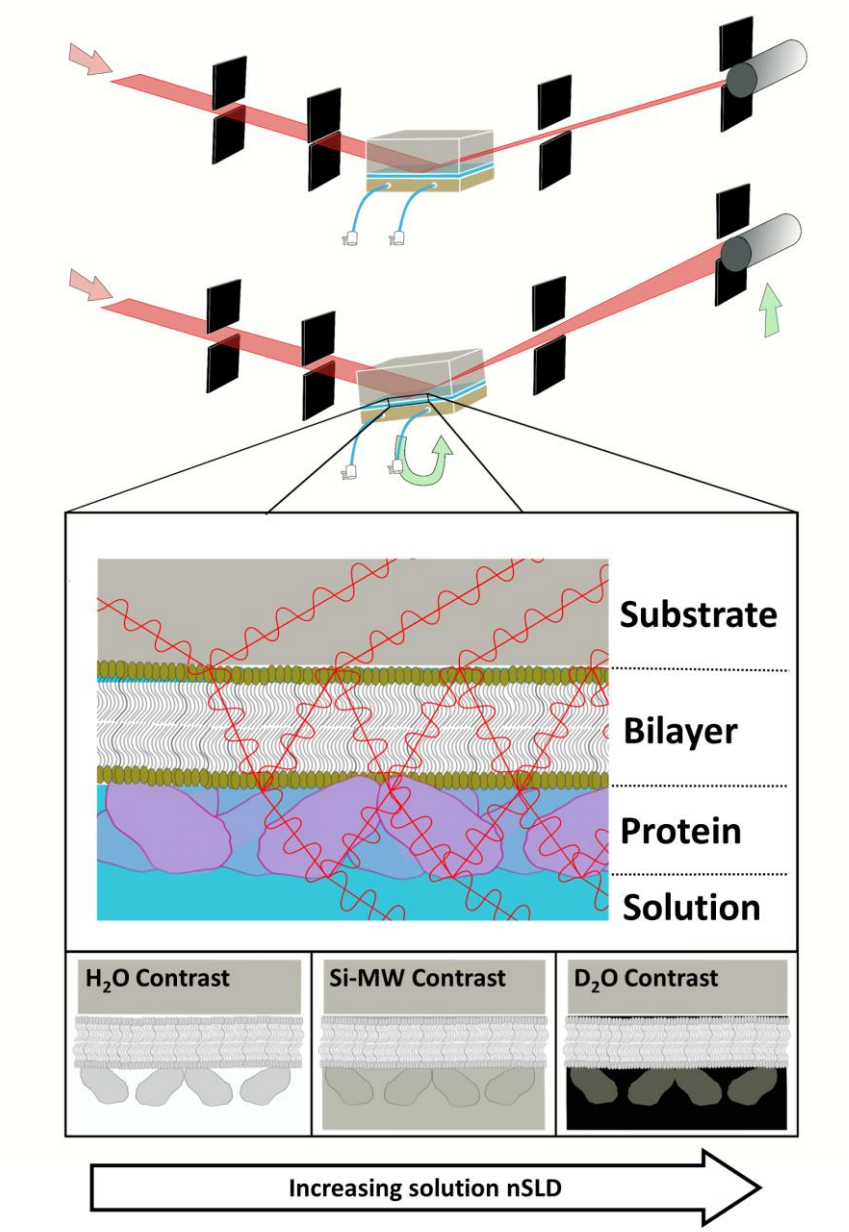
$$R(Q_z) \approx \frac{16\pi^2}{{Q_z}^4} \left| \int_{-\infty}^{+\infty} \rho'(z) exp^{(-izQ_z)} dz \right|^2$$

What you need to resolve your structure:

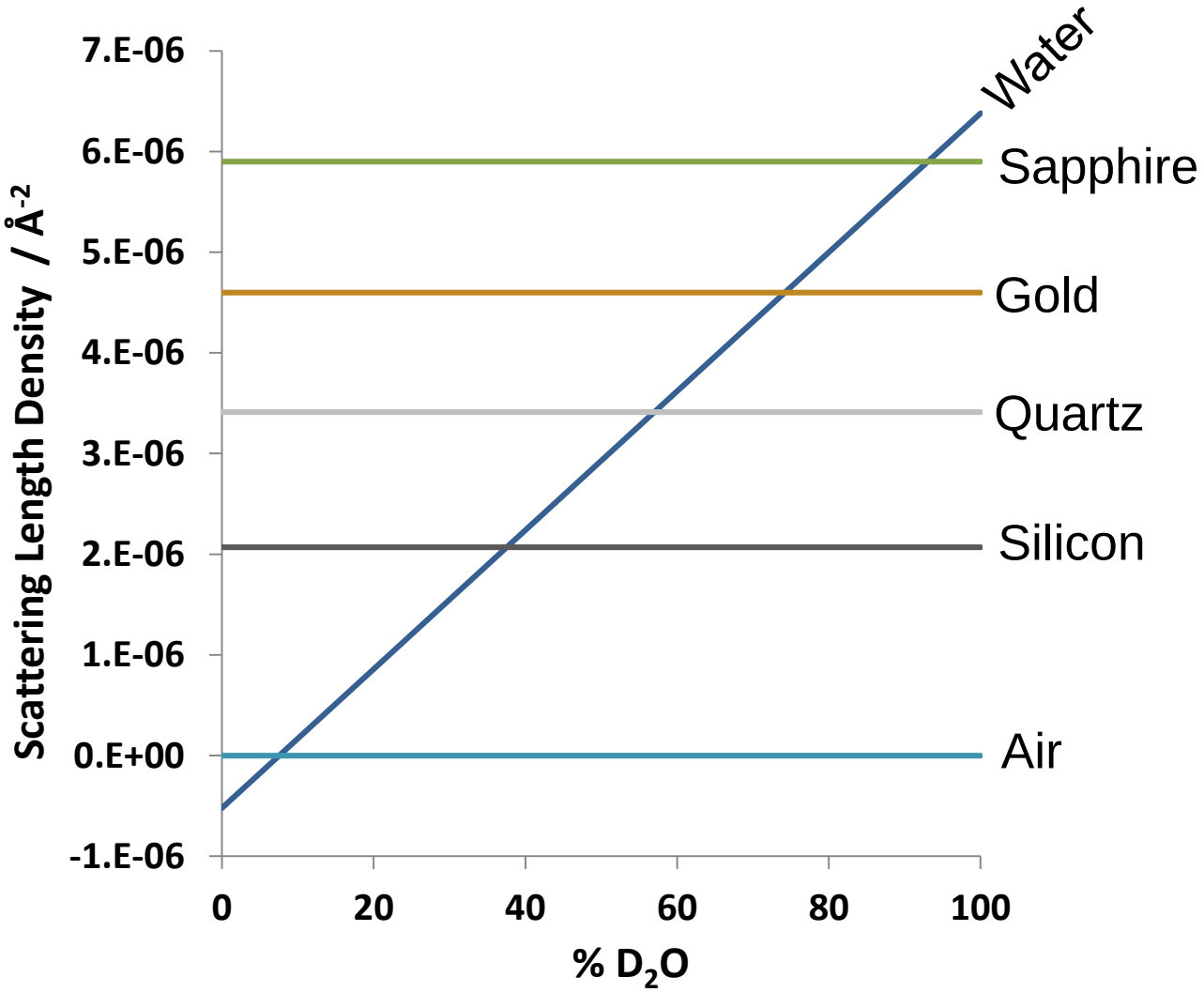
- Priori information:
  - Simplest form knowledge of the superphase and subphase.
  - Knowledge of the neutron scattering length density of the interfacial components:

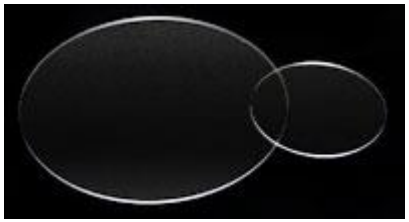
$$\rho = \frac{\sum b}{V}$$

Neutron reflectometry: Isotopic Contrast Variation reveals Complex Structure



Isotopic contrast allows for Individual Components to be Identified amongst Complex Samples Natural Contrast : Substrates





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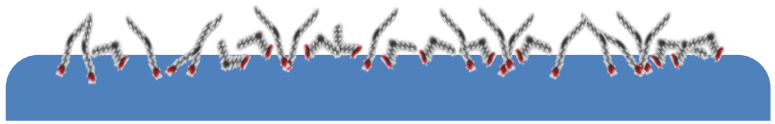
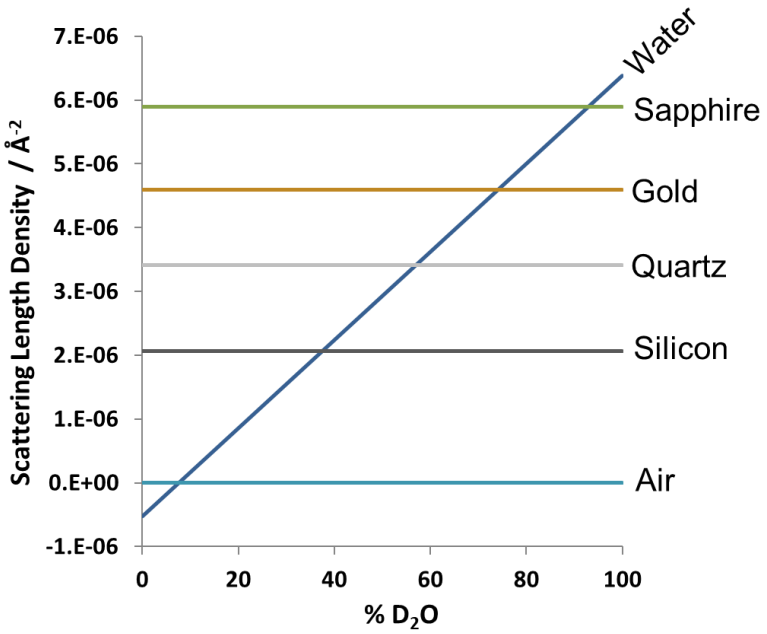
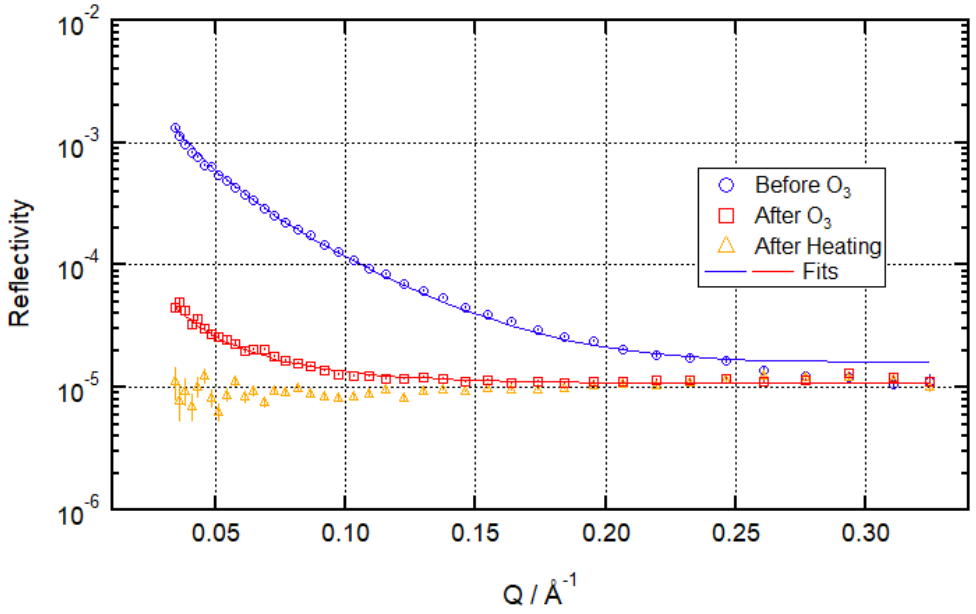


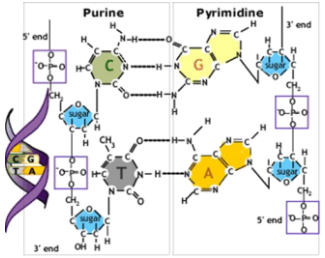




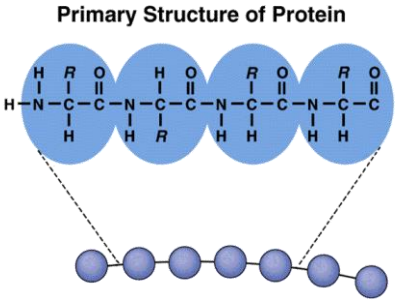
Woden, B.; Skoda, M. W. A. et al. Atmospheric Chemistry and Physics, 2021, 21, 1325.

Isotopic contrast allows for Individual Components to be Identified amongst Complex Samples Natural Contrast : Bio-molecules

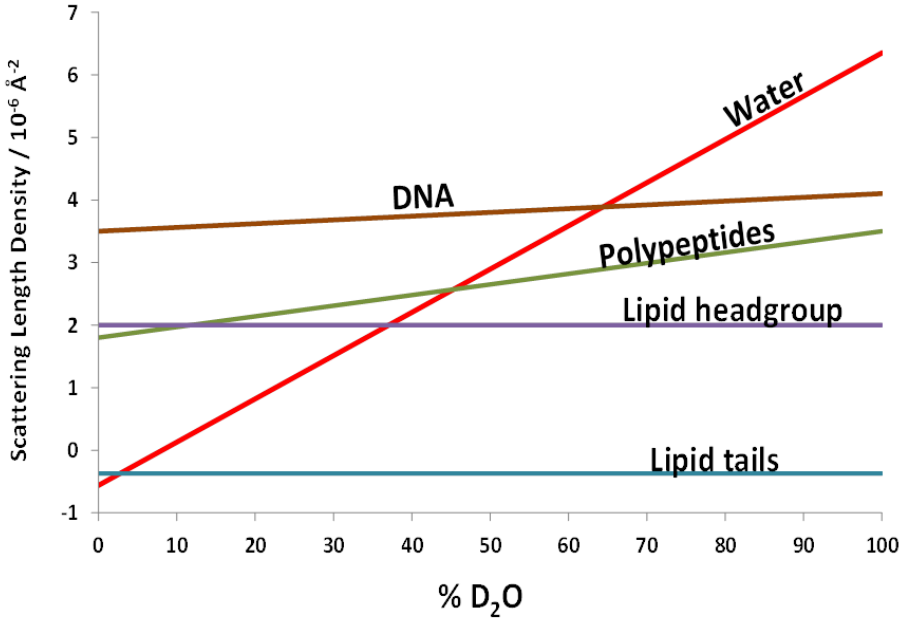
Element	Scattering Length (b)/ 10^{-5} Å
Hydrogen (99.98% protium)	-3.74
Deuterium	6.671
Carbon	6.646
Nitrogen	9.36
Oxygen	5.803
Sulphur	2.847
Phosphorus	5.13

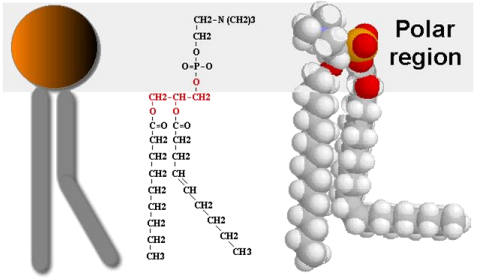


~3.8 × 10^{-6} Å^{-2}



~2.5 × 10^{-6} Å^{-2}

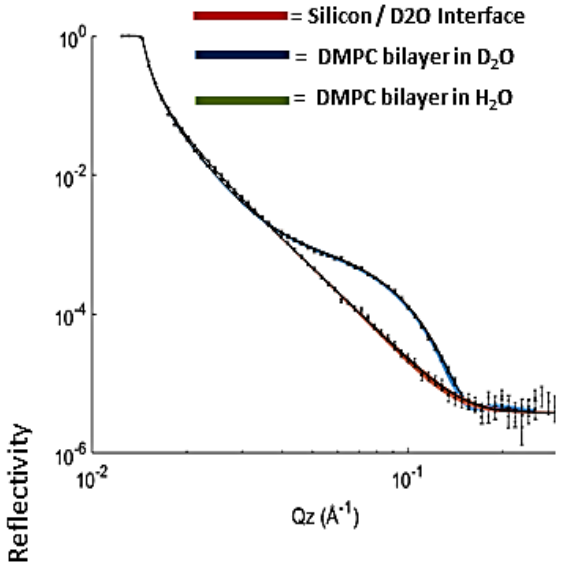


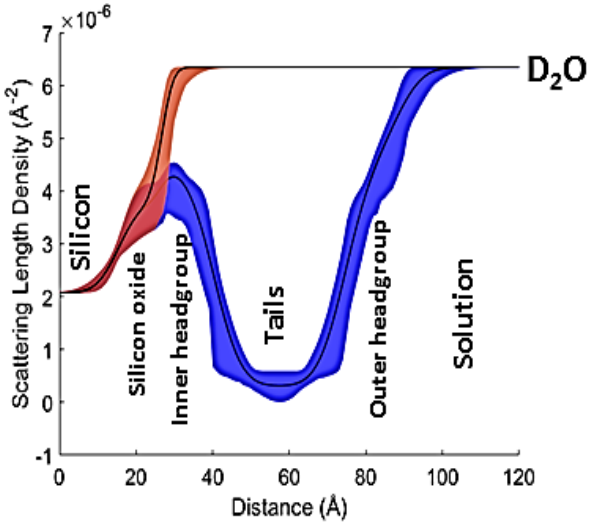


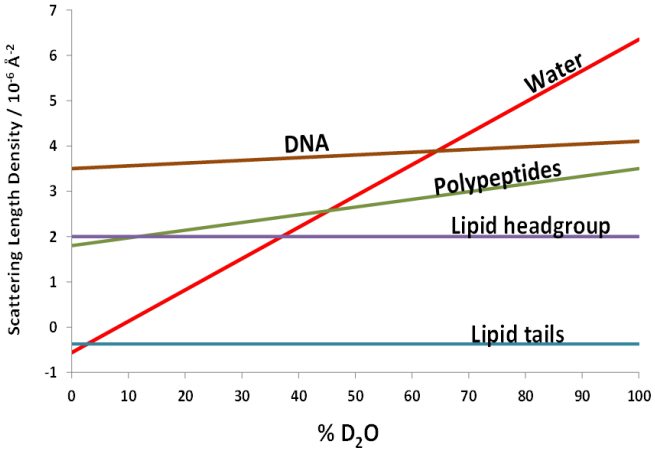
~2 × 10^{-6} Å^{-2}

-0.37 × 10^{-6} Å^{-2}

Isotopic contrast variation – Reducing ambiguity and Resolving Structural Complexity







Clifton et al, 2019, Lipid-Protein Interactions, Methods in Molecular Biology, 201-251

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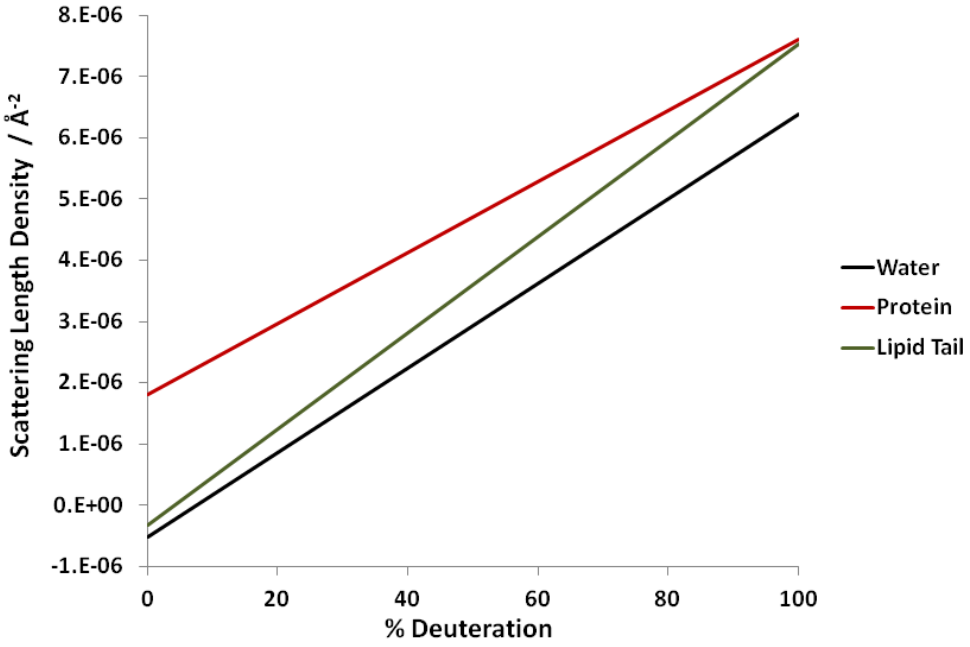
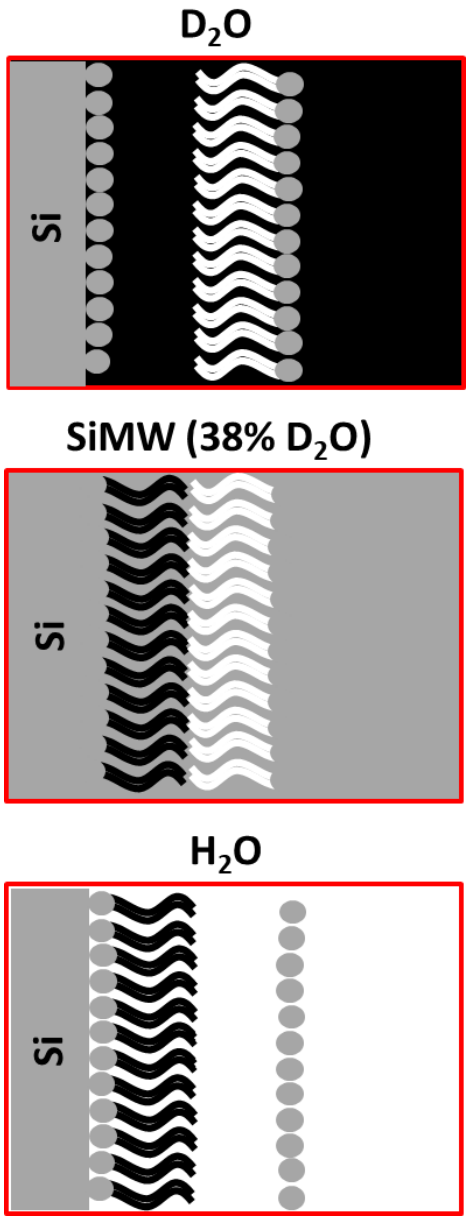
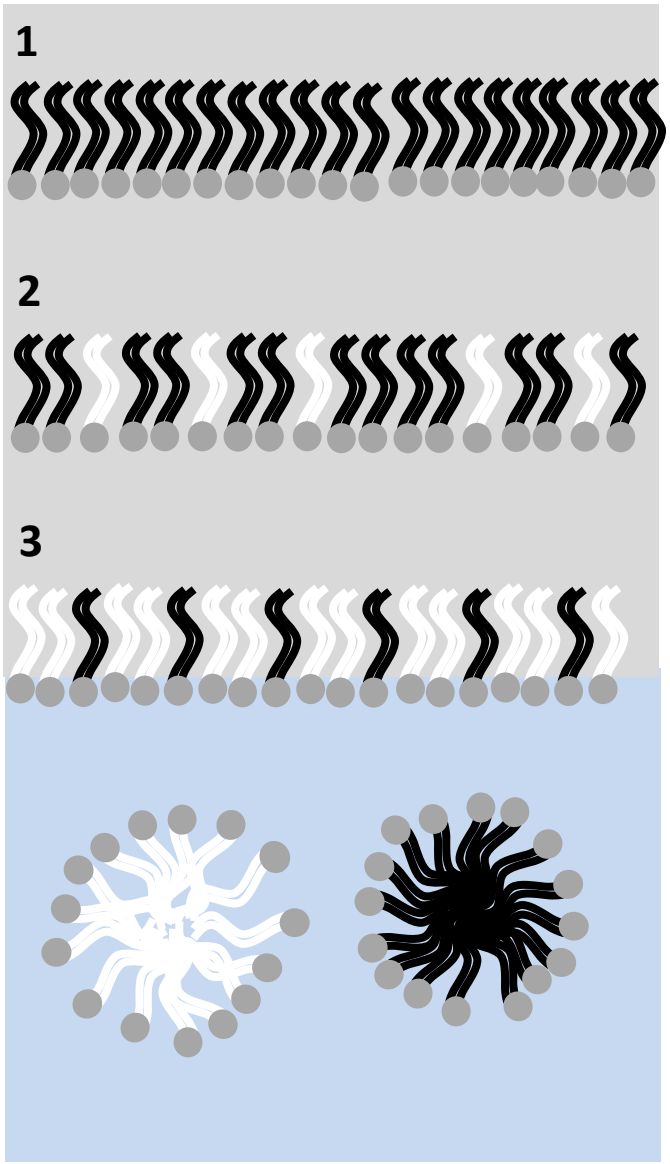
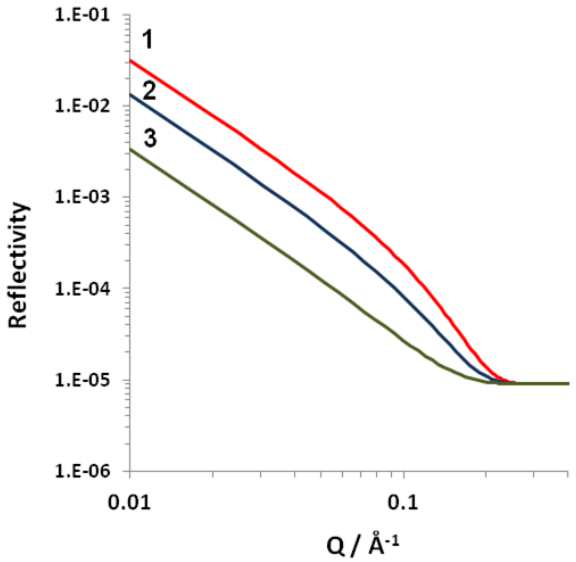
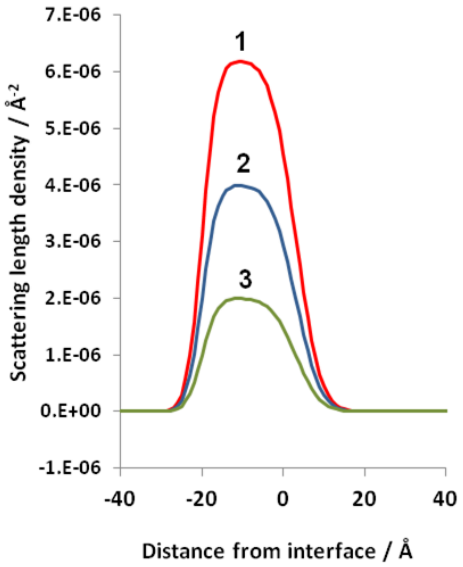


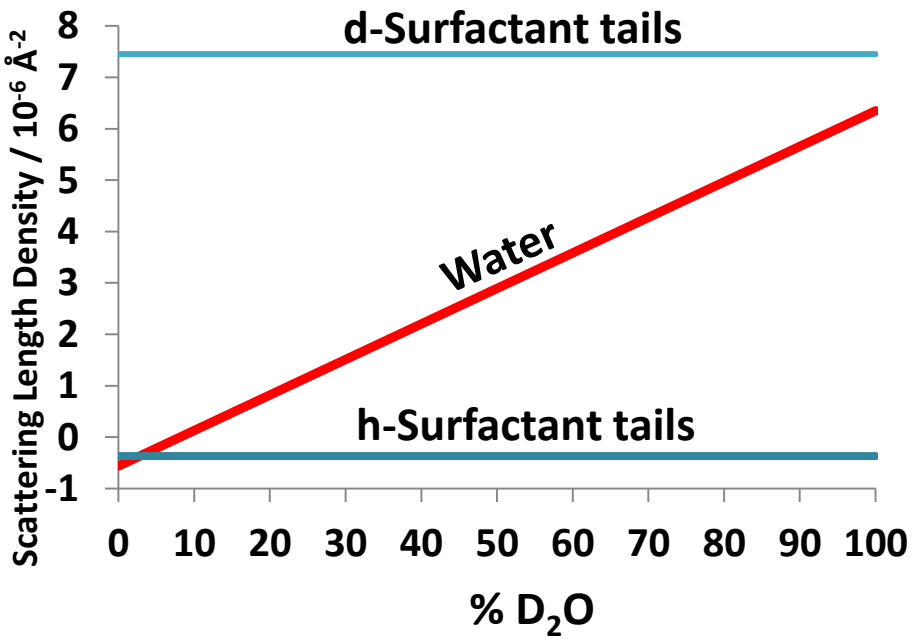


Mixtures of d- and h- labelled materials : Resolving Complexity at the A/L Interface









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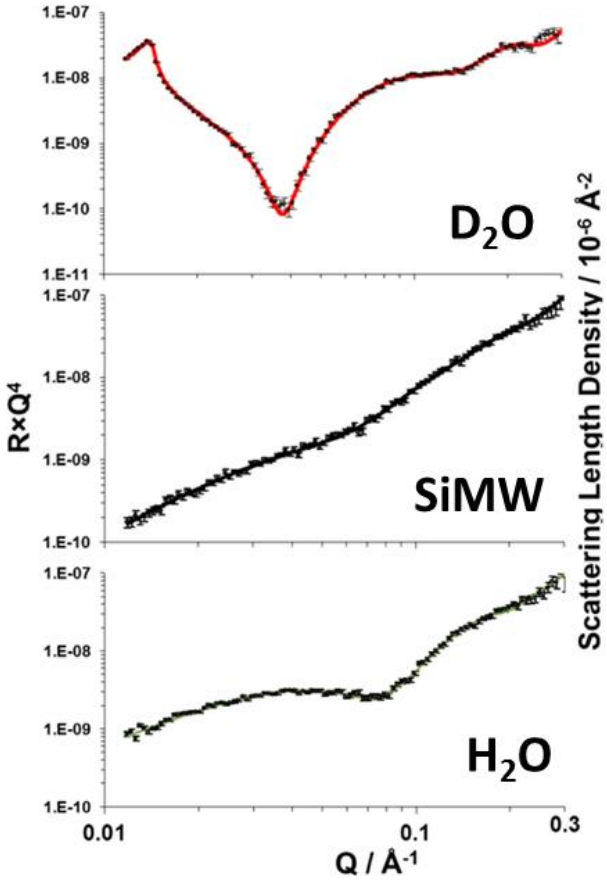
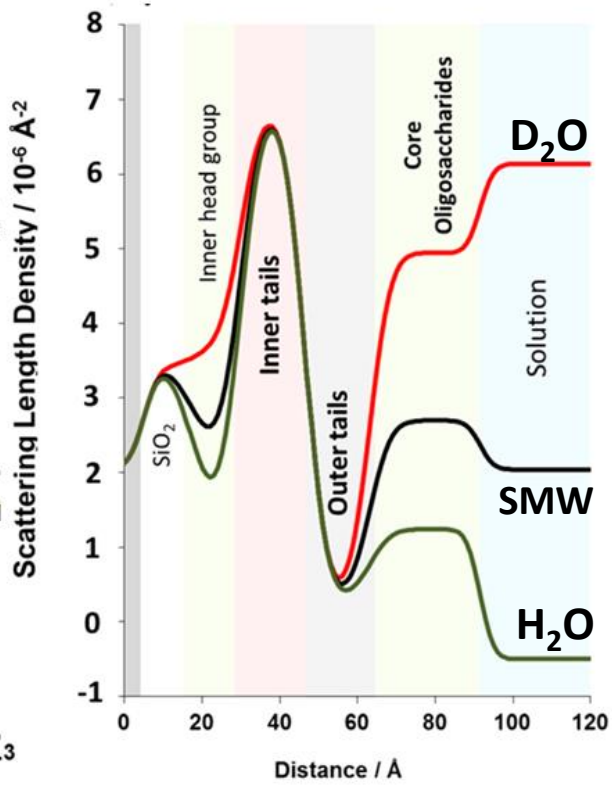
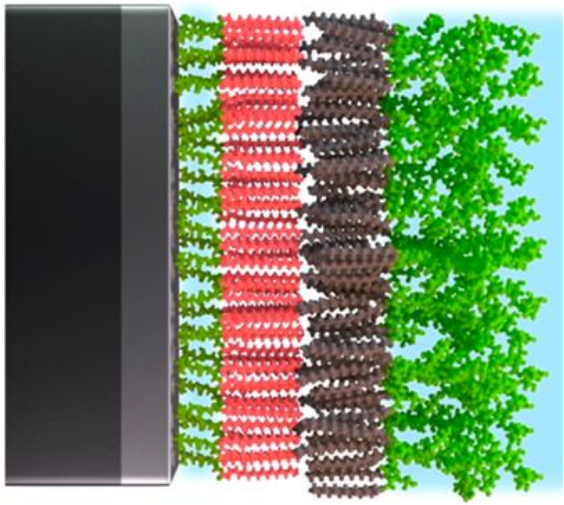
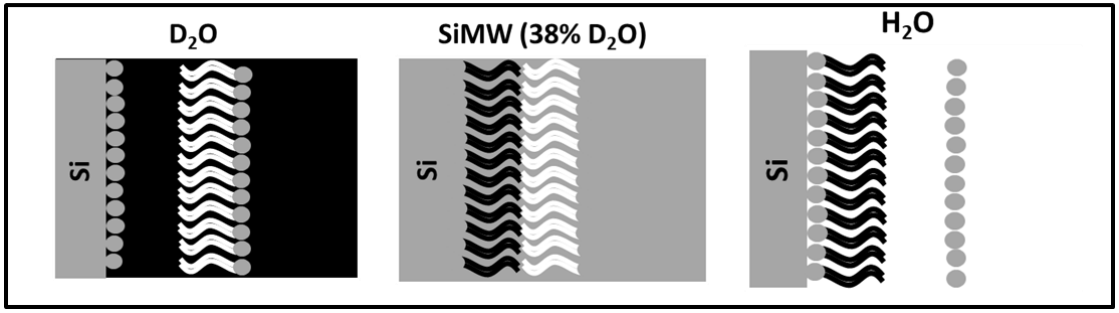


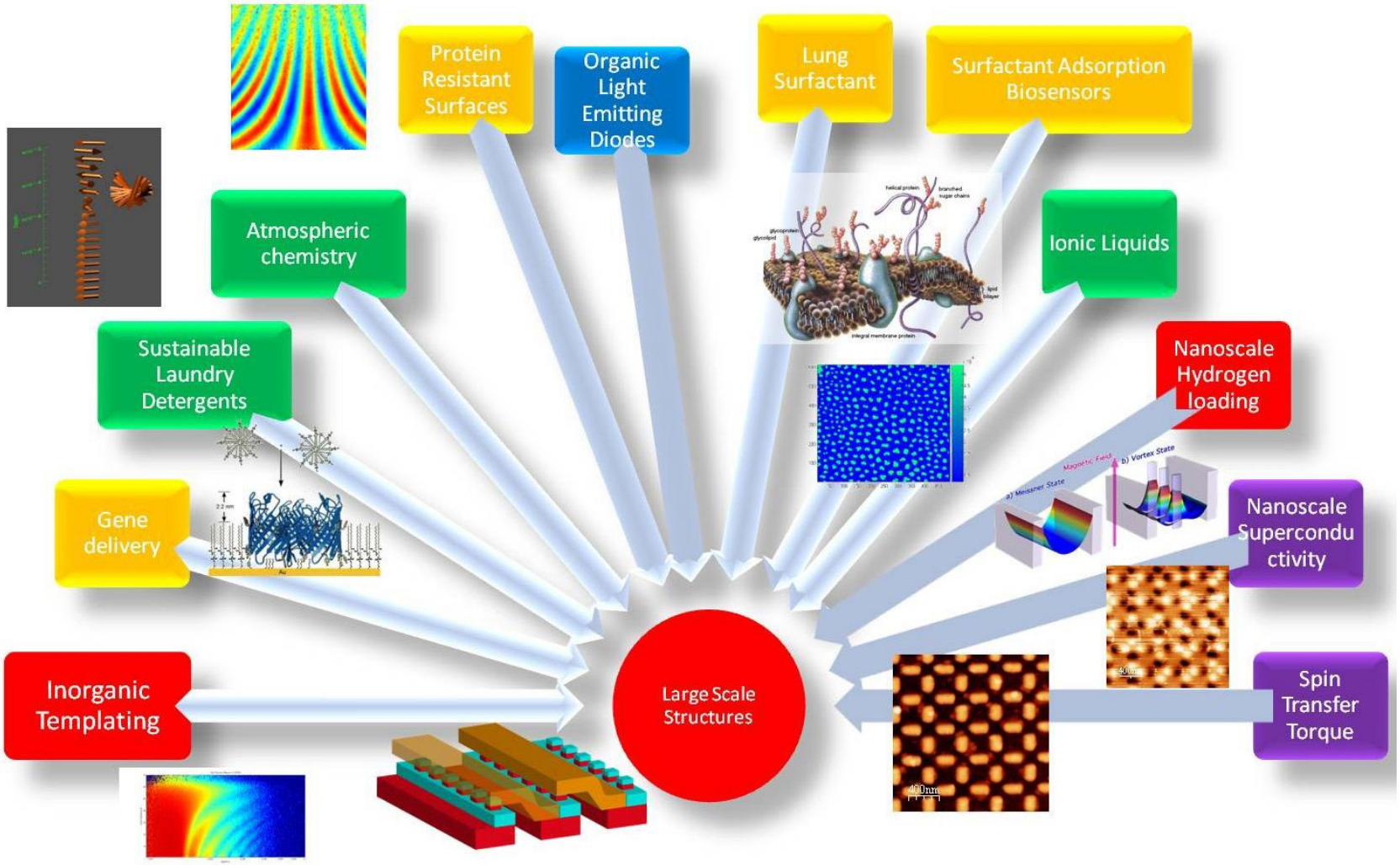




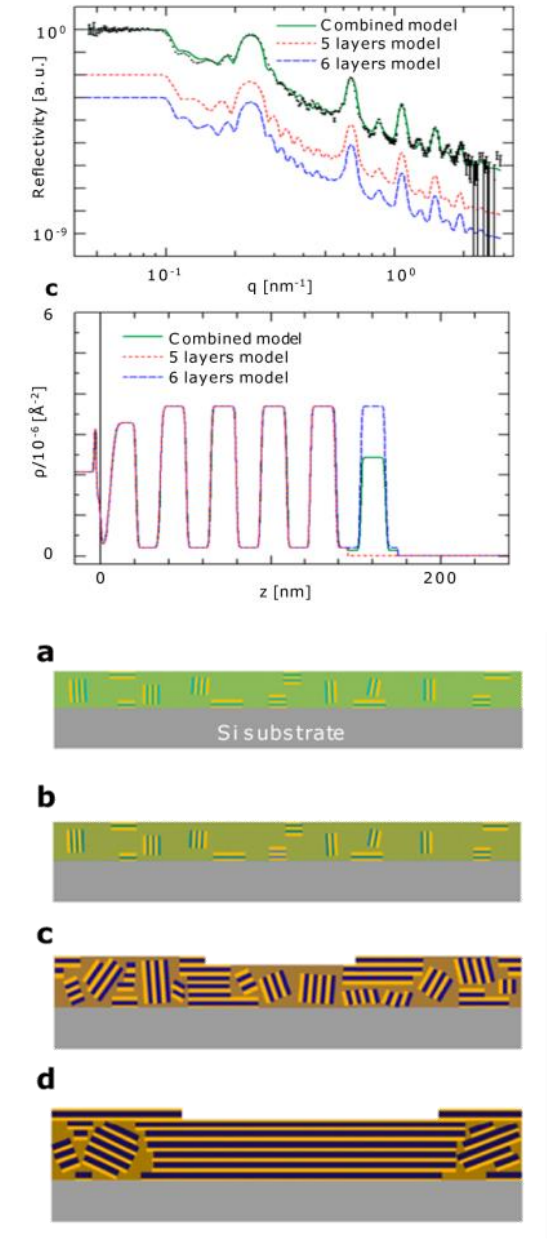


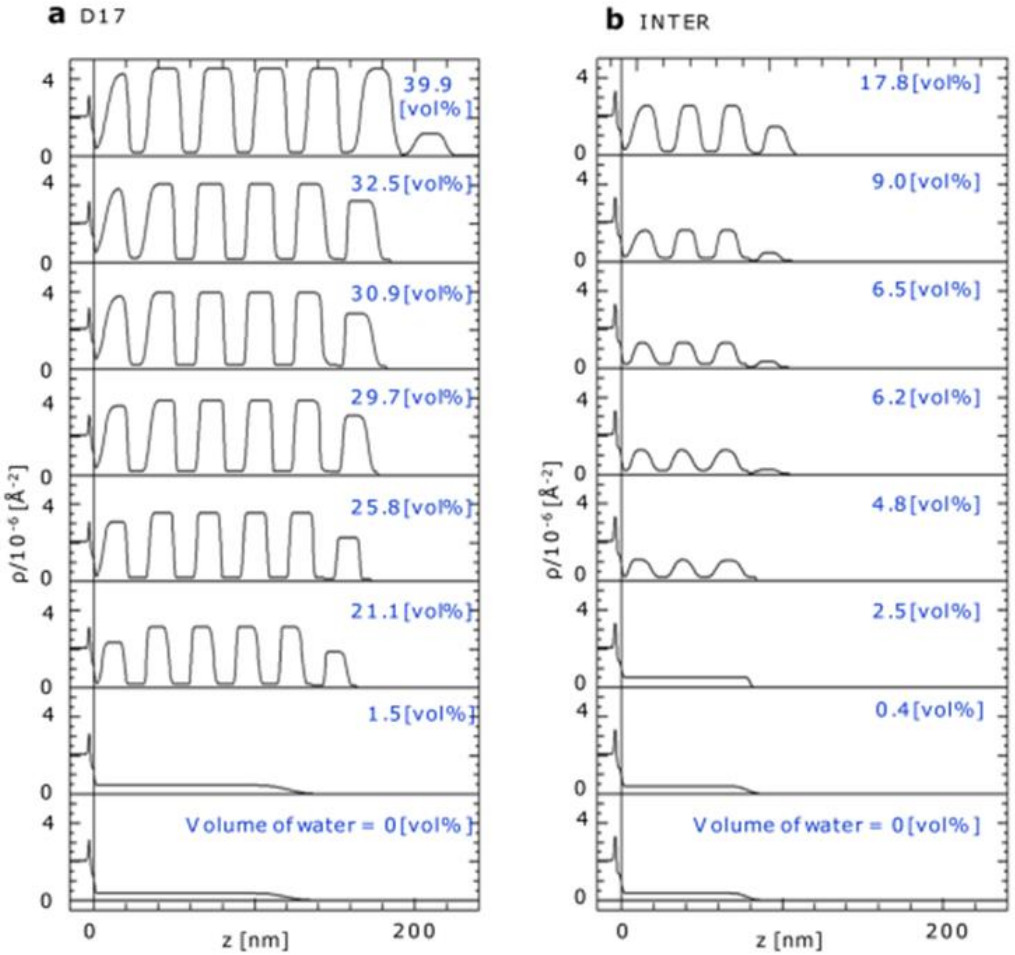
Clifton *et al*, Langmuir, 2015, 31, 1, 404-412.

Examples


Protein Resistant Surfaces
Organic Light Emitting Diodes
Lung Surfactant
Surfactant Adsorption Biosensors
Atmospheric chemistry
Ionic Liquids
Sustainable Laundry Detergents
Nanoscale Hydrogen loading
Gene delivery
Nanoscale Supercondu ctivity
Inorganic Templating
Large Scale Structures
Spin Transfer Torque

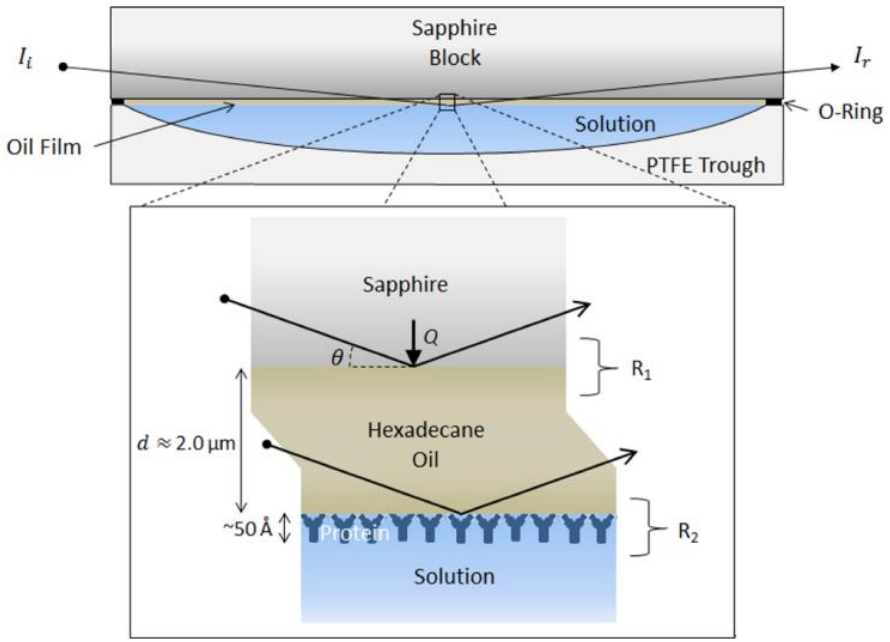
Polymers at the Solid/Air Interface

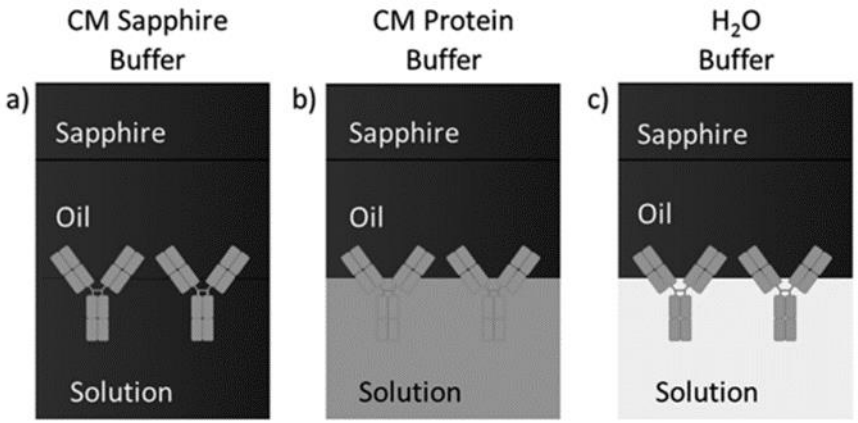


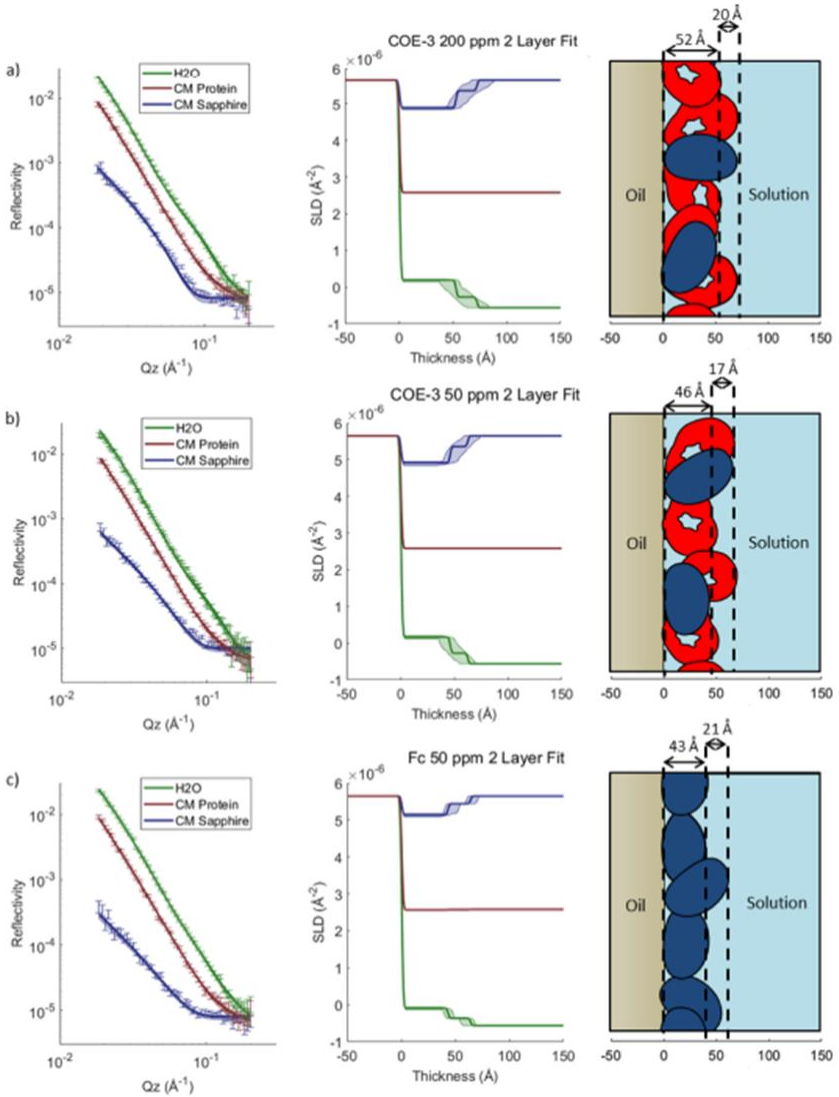


Kamata *et al*, Macromolecules, 2014, 22, 2444-2447

Therapeutics at the Oil-water Interface

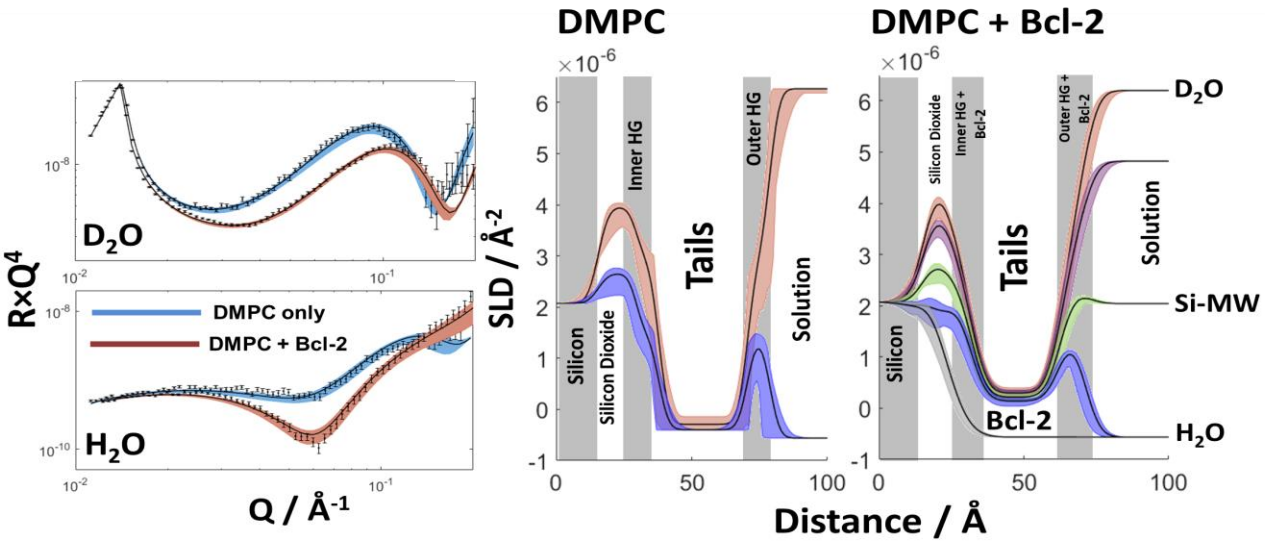






Ruane *et al*, Langmuir, 2019, 34, 13543-13552

Understanding Cell Death



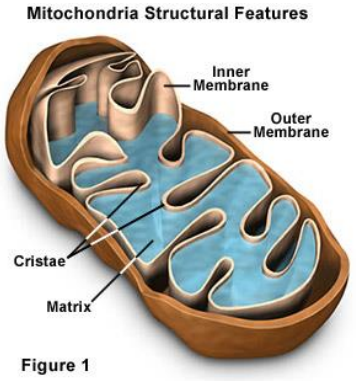
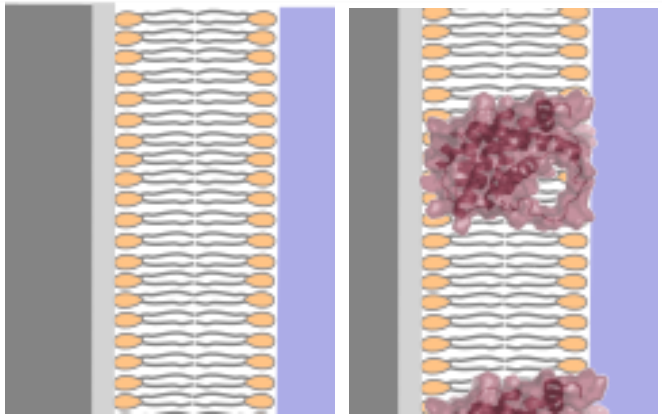
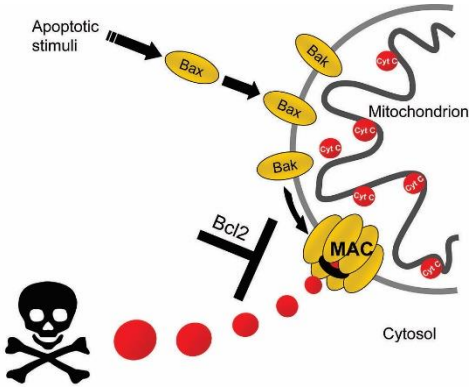


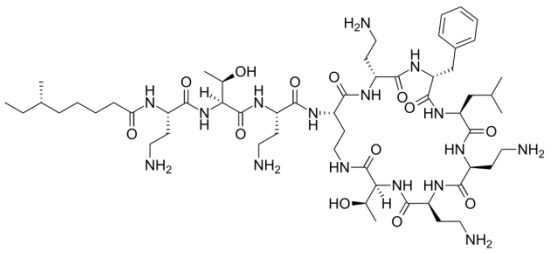
Figure 1

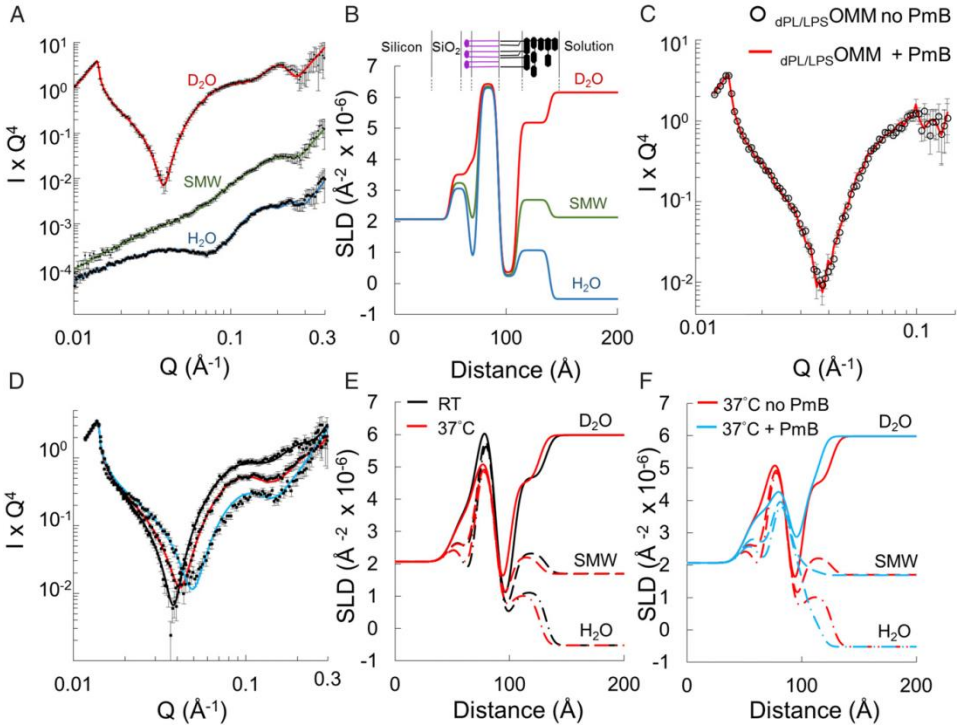


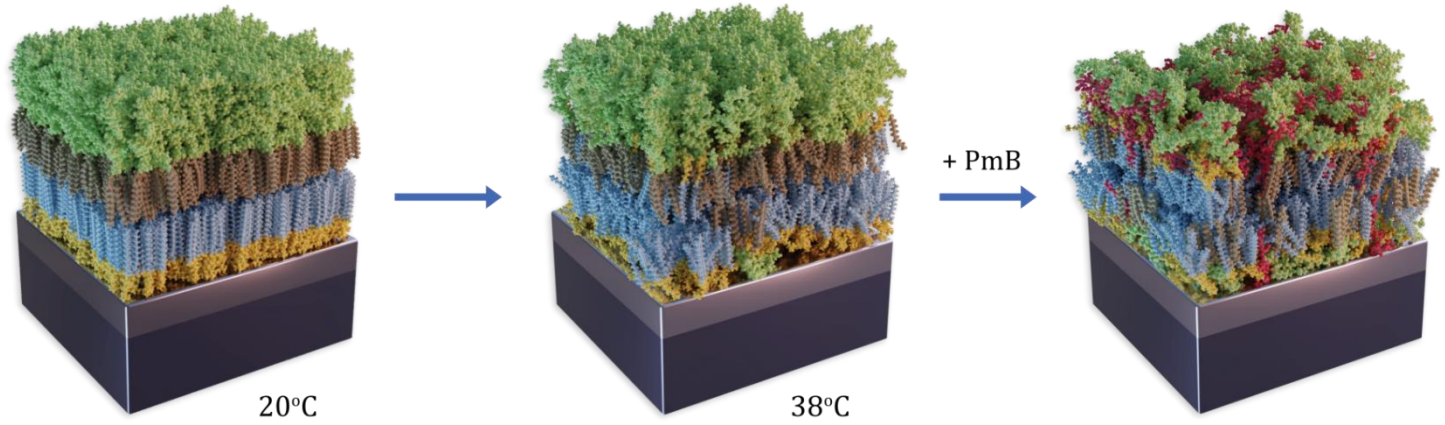


Mushtaq *et al*, Communications Biology, 2021, 4 (1), 1-10

Model Gram Negative Bacterial Membranes : Antibiotic Testing

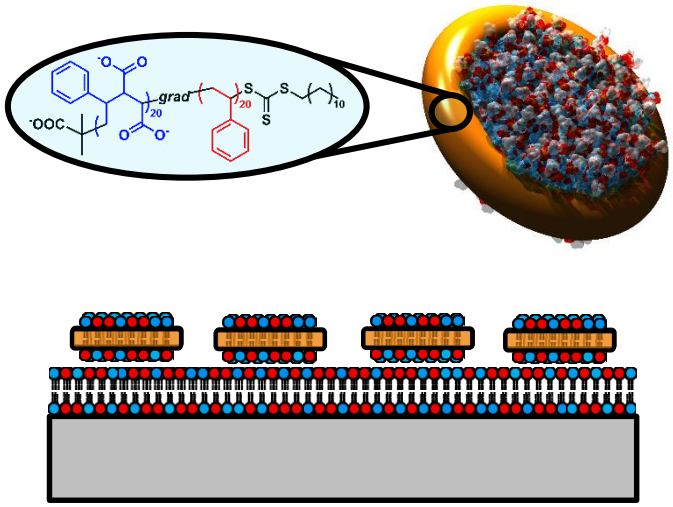


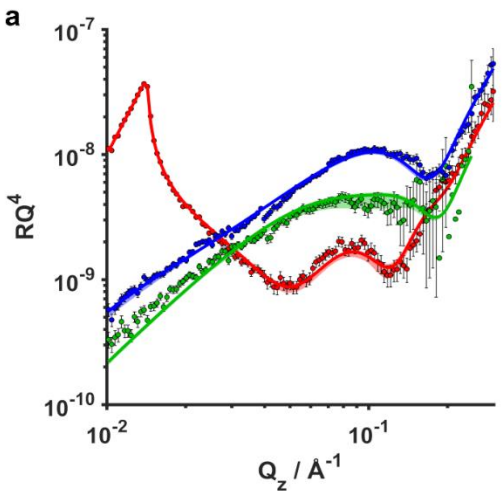


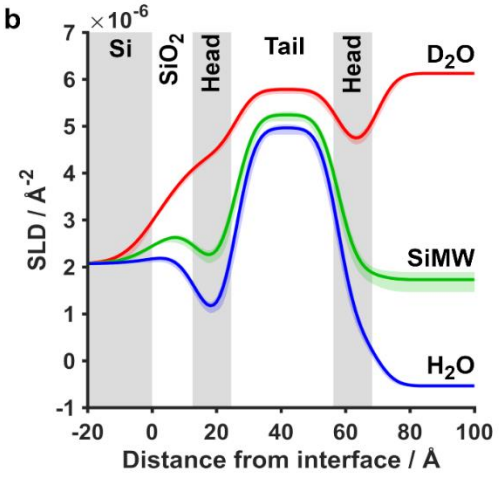


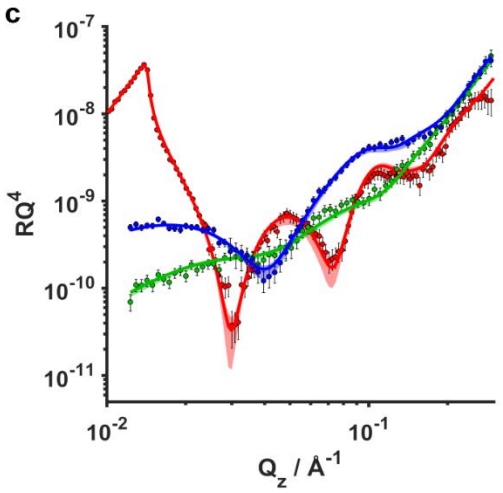
Paracini *et al*, PNAS, 2018, 115 (31), E7587-E7594

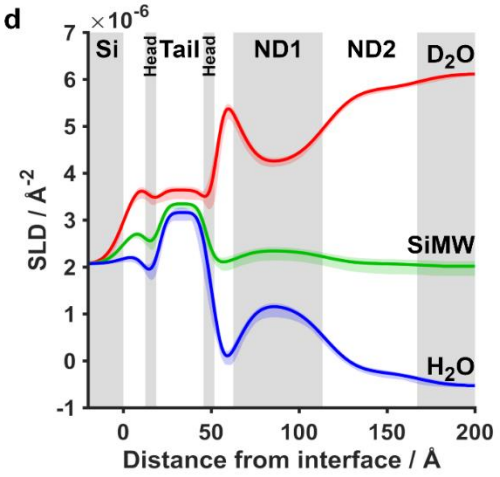
Adsorption of a polymer-stabilised phospholipid nanodisc on a supported lipid bilayer





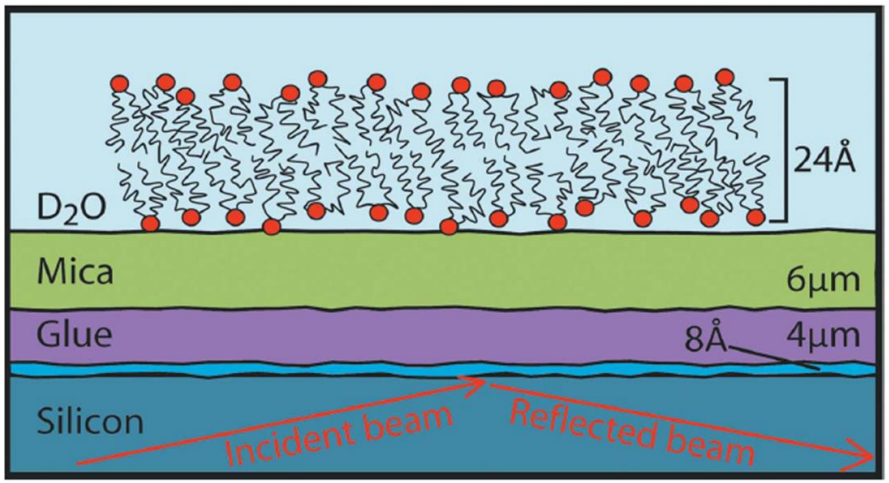


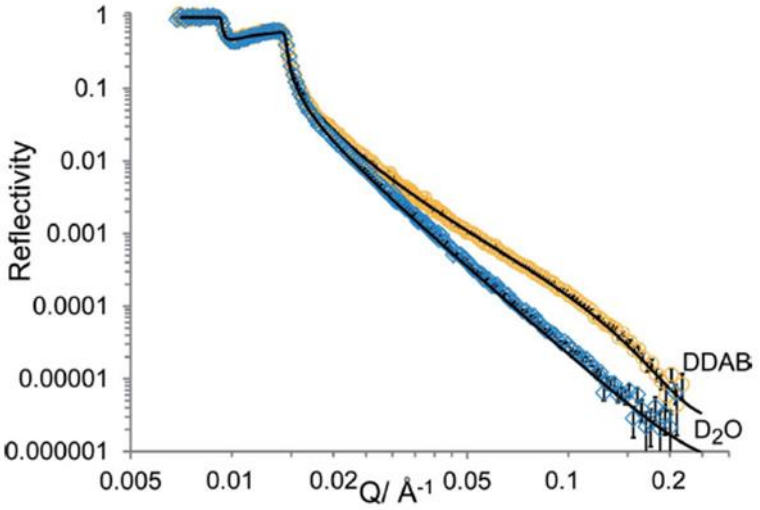




Hall *et al*, JCIS, 2020, 574, 272-284

Examining very buried interfaces

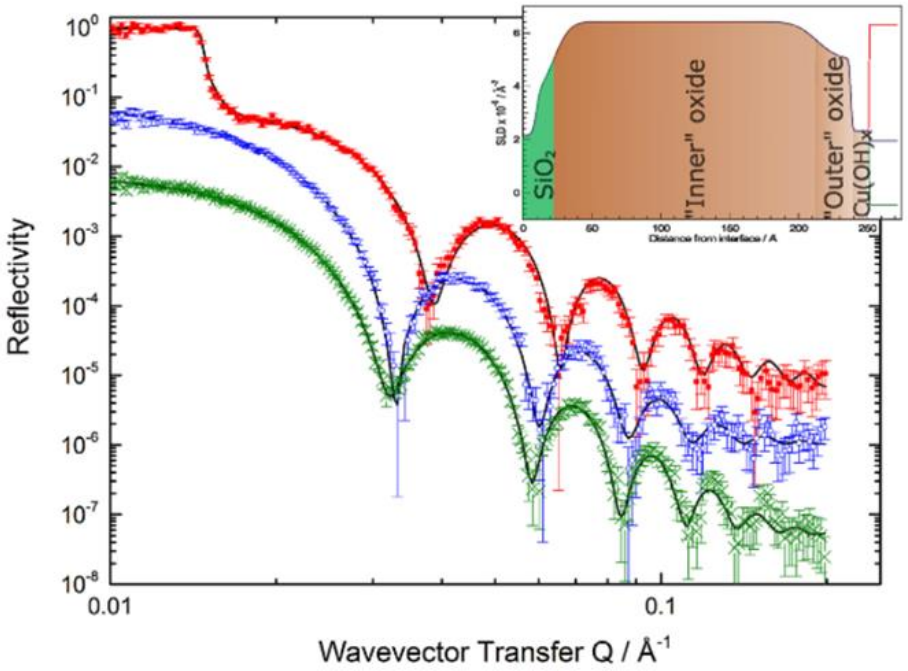


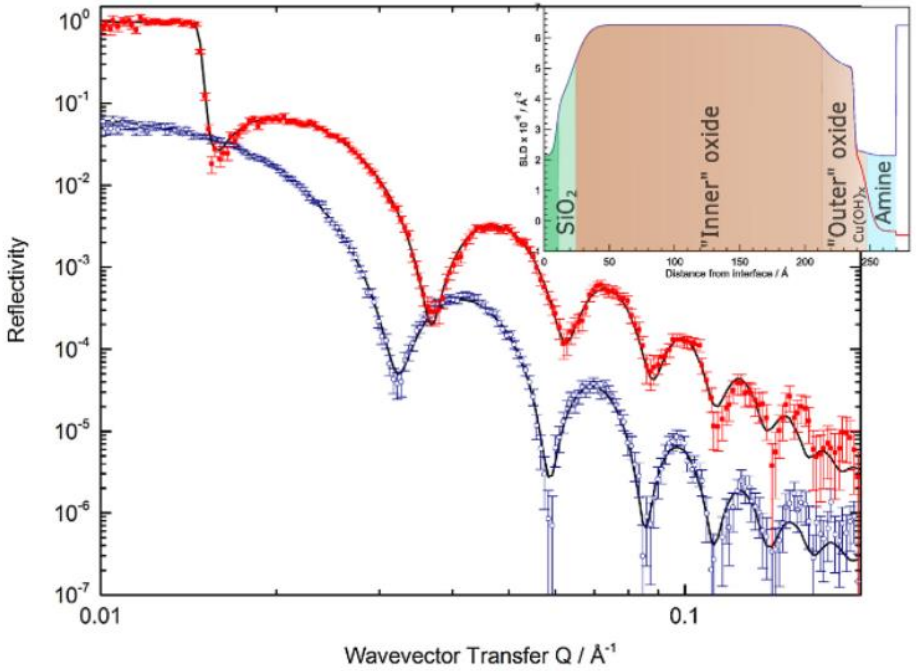


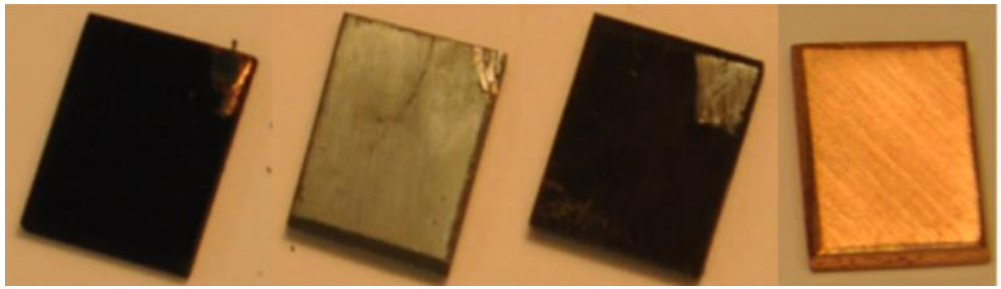
Layer	Thickness	Roughness (Å)
Silicon	–	4 ± 3
Silicon oxide	8 ± 2 Å	5 ± 2
Glue	4 μm	5 ± 2
Mica	6.1 μm	3 ± 1
DDAB	24 ± 2 Å	5.0 ± 0.5

Browning *et al*, JAC, 2014, 47, 1638-1646

Examining Thin Organic Layers on Thick Metal Layers In Buried Systems







Welbourn *et al*, Corrosion Science 115 (2017) 68–77

Thank you for listening