# Day 2 Materials

CHRNS Neutron School

## Goals

* Create a lipid bilayer model
* Fit the bilayer model to one- and two-contrast data sets
* Determine structural parameters of the bilayer (completeness, thickness)
* Add a third model and generate full pH curve

## Data sets

### Sample

A TiO2 film was deposited on a silicon wafer by sputter deposition. Nominal thickness is 140 Å. The sample was mounted in the NCNR flow cell; the liquid reservoir was then filled with 3 mg/mL DOPC lipids dissolved in 2-propanol. The 2-propanolic lipid solution was then slowly exchanged with an H2O-based buffer (pH 7 10 mM tris, 150 mM NaCl). The neutron reflectivity was measured; then the solution was exchanged for a D2O based buffer and the measurement repeated. Other pH values were also attempted; the most interesting was pH 11.

To think about:

* What is the difference in SLD between pure H2O and an aqueous 150 mM NaCl solution?

### Data path

ncnrdata/cgd/201806/23396/data/

Intensity scans (high Q): ch061, scans 2282 and 2283

H2O pH 7 data set: ch060 (specular, backgrounds, low Q intensity scan = 2241)

D2O pH 7 data set: ch061 (specular, backgrounds, low Q intensity scan = 2259)

D2O pH 11 data set: ch067 (specular, backgrounds, low Q intensity scan = 2341)

### Useful information

The DOPC lipid has a headgroup attached to two dioleoyl tails. Each tail has molecular formula C17H33 and molecular volume 486 Å3. The PC headgroup has molecular formula C10H18O­8NP and a total molecular volume of 331 Å3.

To think about (calculate the densities and use the neutron SLD calculator below):

* What is the DOPC lipid tail scattering length density?
* What is the DOPC headgroup scattering length density?

## Links

Reductus: <https://reductus.nist.gov>

Refl1D: [Reflectometry Software Installation | NIST](https://www.nist.gov/ncnr/chrns/education-and-outreach/chrns-summer-school-neutron-scattering/course-materials-0)

Neutron activation (and SLD) calculator: <https://www.ncnr.nist.gov/resources/activation/>

or <https://bmaranville.github.io/activation/activation/index_pyodide.html>