



Introduction to small-angle scattering

**JUDITH HOUSTON
INSTRUMENT SCIENTIST @ THE ESS**

2024-03-11

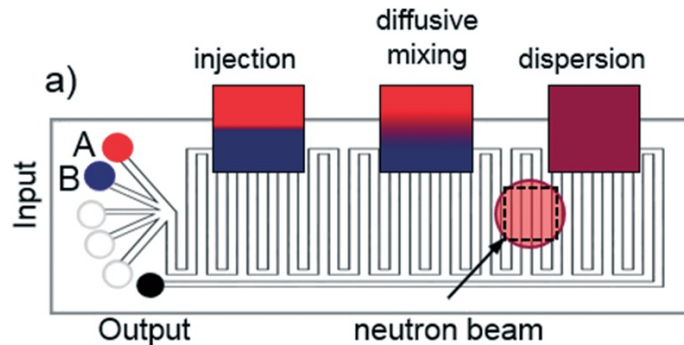


LoKI : SANS for soft matter, materials & bioscience



Microfluidic SANS:

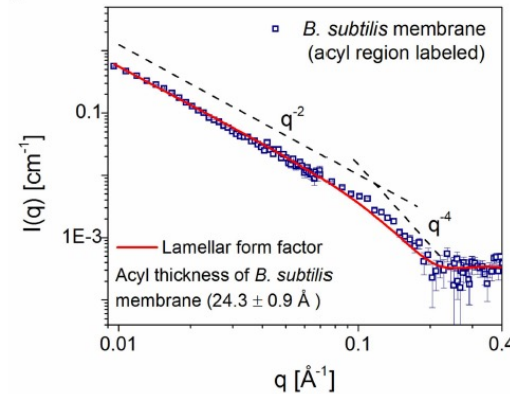
High Throughput Mixing & Tailored Flow Geometry



Lab Chip, 2017, **17**, 1559

Biological Samples:

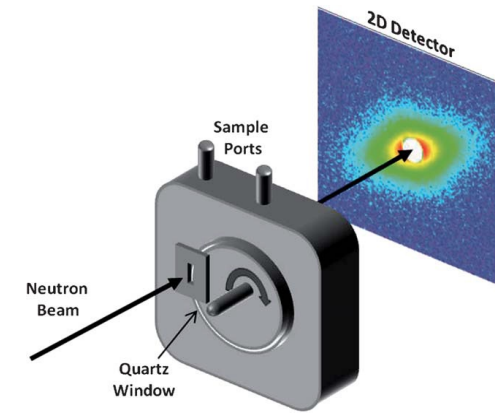
Weak Scatterers & Dilute Solutions



PLoS Bio, 2017, **15**, e2002214

Rheo-SANS:

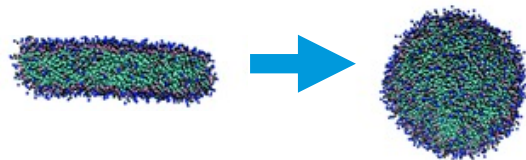
Structures Under Shear



Soft Matter, 2011, **7**, 9992

Non-Equilibrium Studies:

Self-Assembly & Kinetics



Colloid Polym Sci, 2010, **288**, 827

ABILITIES:

- Small beams for **flow-through**, **scanning** & **microfluidic experiments**.
- Perform “**single-shot**” kinetic measurements on **sub-second** timescales.
- Investigate **multiple length scale** systems (simultaneously 0.5-300 nm)
- **High throughput** of regular SANS measurements

→ **high flux & wide simultaneous size range.**

1

Solving life
science problems
with neutron
tools...



Weakly scattering bio-engineered samples



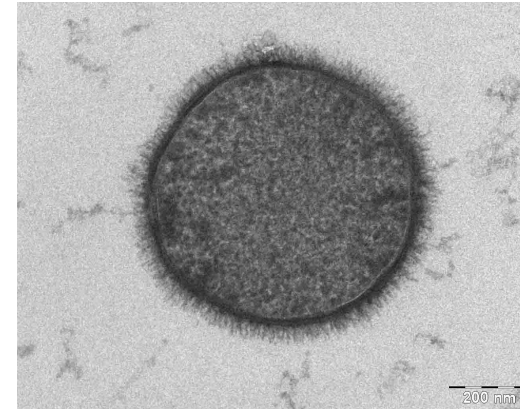
RESEARCH ARTICLE

The in vivo structure of biological membranes and evidence for lipid domains

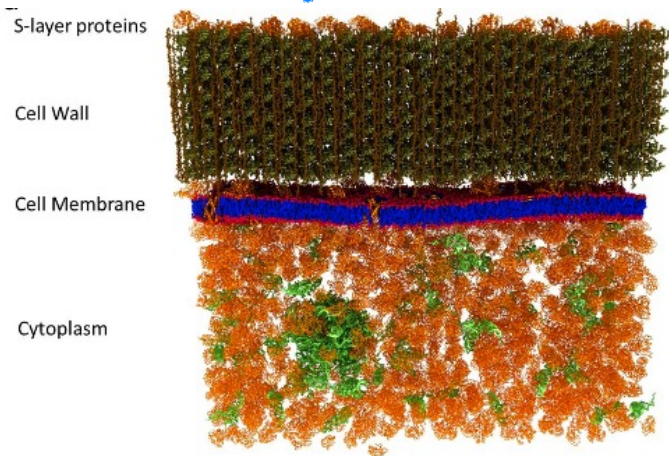
Jonathan D. Nickels^{1,2,3}*, Sneha Chatterjee^{2,4}*, Christopher B. Stanley², Shuo Qian², Xiaolin Cheng^{5,6}, Dean A. A. Myles², Robert F. Standaert^{1,2,4,6}*, James G. Elkins^{4,7}*, John Katsaras^{1,2,3}*

1 Shull Wollan Center—A Joint Institute for Neutron Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, 2 Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, 3 Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, United States of America, 4 Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, 5 Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America, 6 Department of Biochemistry & Cellular and Molecular Biology, University of Tennessee, Knoxville, Tennessee, United States of America, 7 Department of Microbiology, University of Tennessee, Knoxville, Tennessee, United States of America

* These authors contributed equally to this work.
* standaertf@ornl.gov (RFS); elkinsjg@ornl.gov (JGE); katsarasj@ornl.gov (JK)

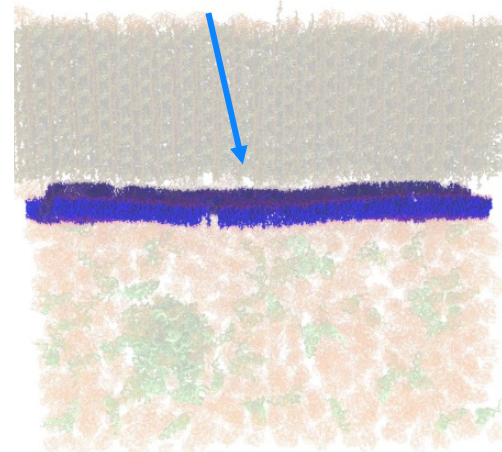


Normal cell components:
everything is visible...

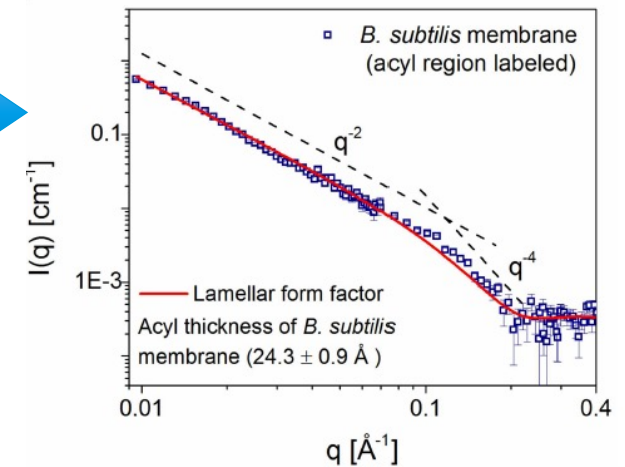


After labelling
with specific
amounts of H
and D

What the neutron
beam sees...



Indirect evidence
of cell membrane
structure!

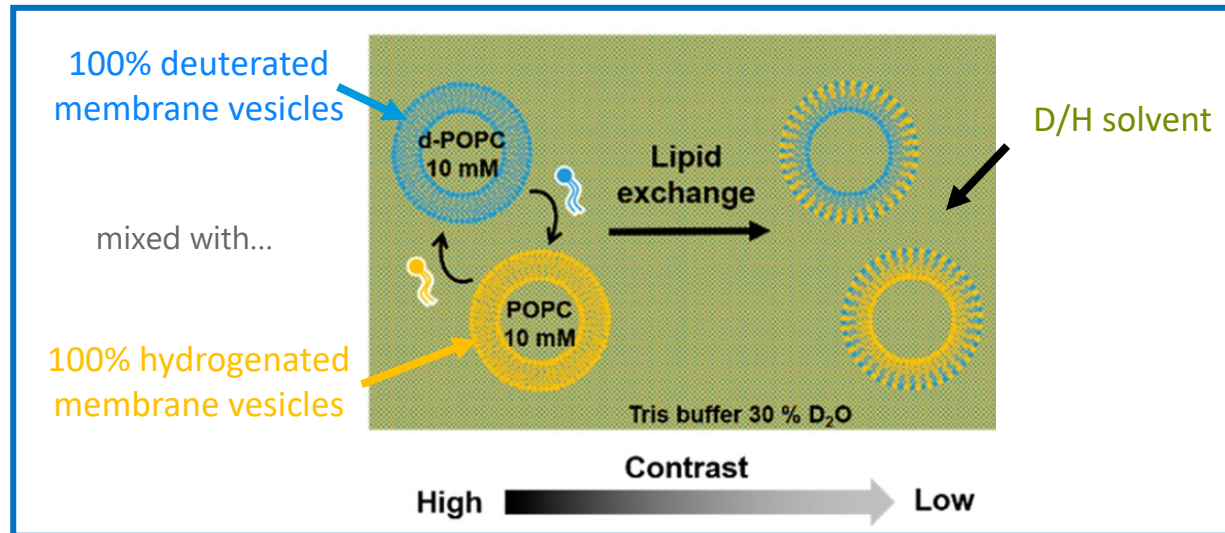


Probing membrane dynamics

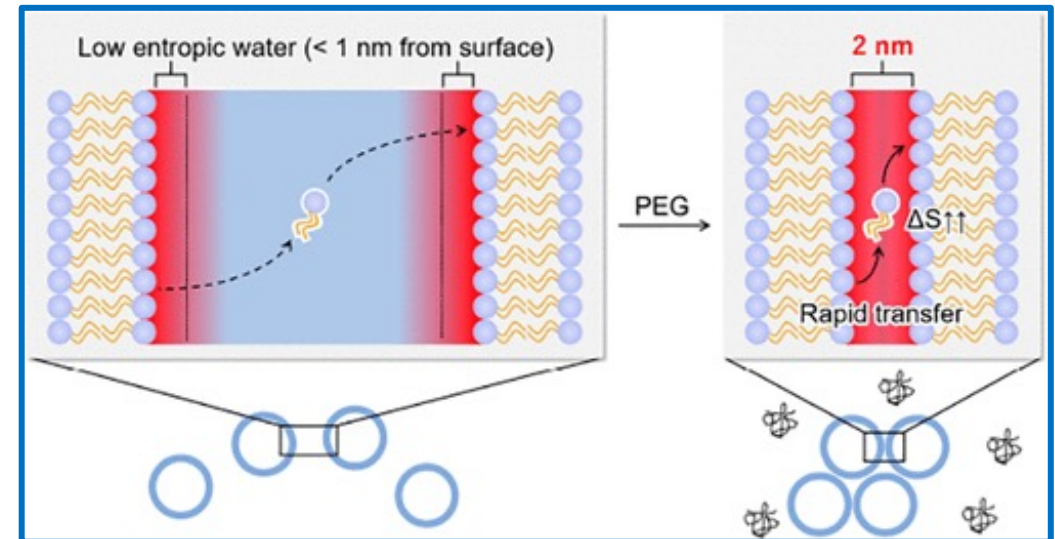
Understanding membrane biofusion



The experiment



The result



- Lipid exchange between the outer leaflets of the vesicles decreases the difference in contrast
- Rate of decrease in contrast directly related to rate of exchange

Gluten vs. gluten-free pasta varieties

The experiment

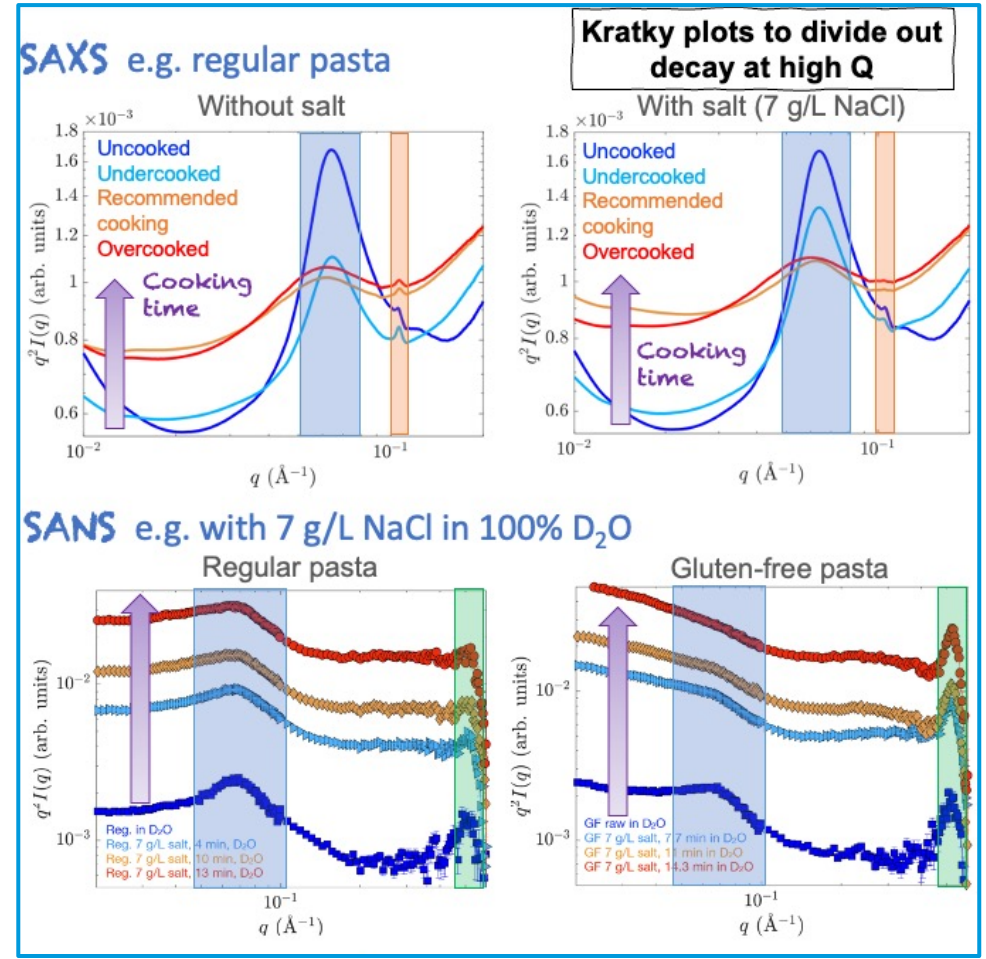
The pasta:

The set-up:

Cooking conditions:

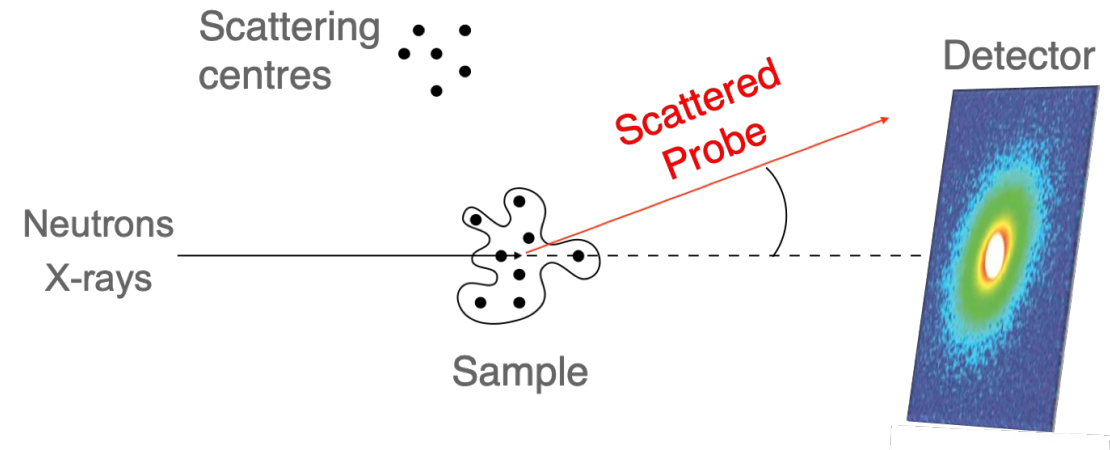
- Salt: 0, 3.5, 7 or 14 g per litre
- Pasta conc.: 100 g per litre
- Cooking time: 70, 100 or 130% of recommended time
- Cooking water: 100, 42 (gluten contrast matched), 0 wt% D₂O

The result



2

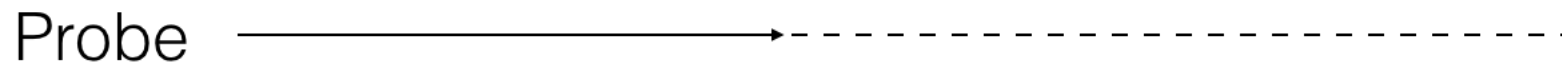
Small-angle scattering and How does it work?





Small-angle scattering

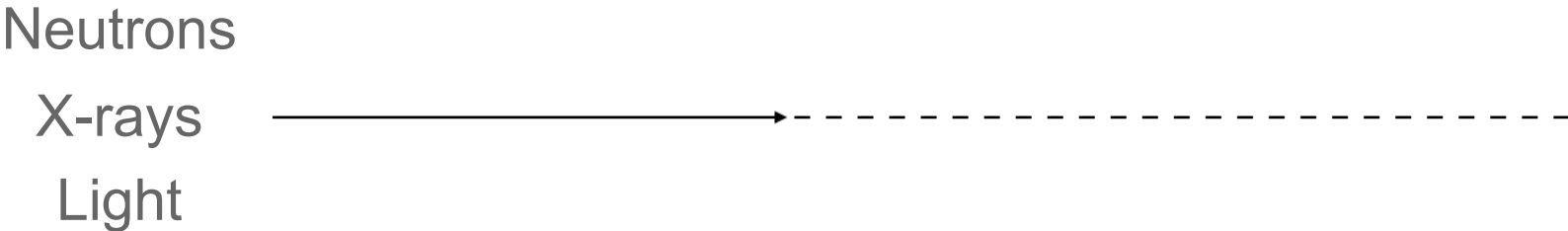
Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of $\sim 1\text{--}200$ nm





Small-angle scattering

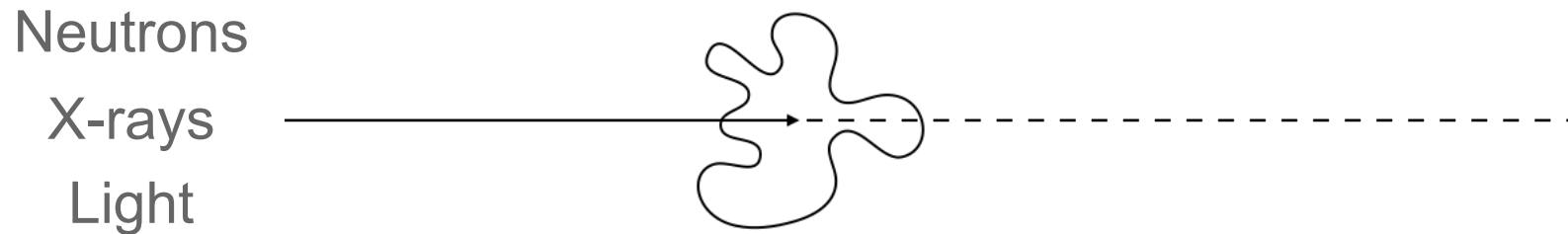
Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of $\sim 1\text{--}200$ nm





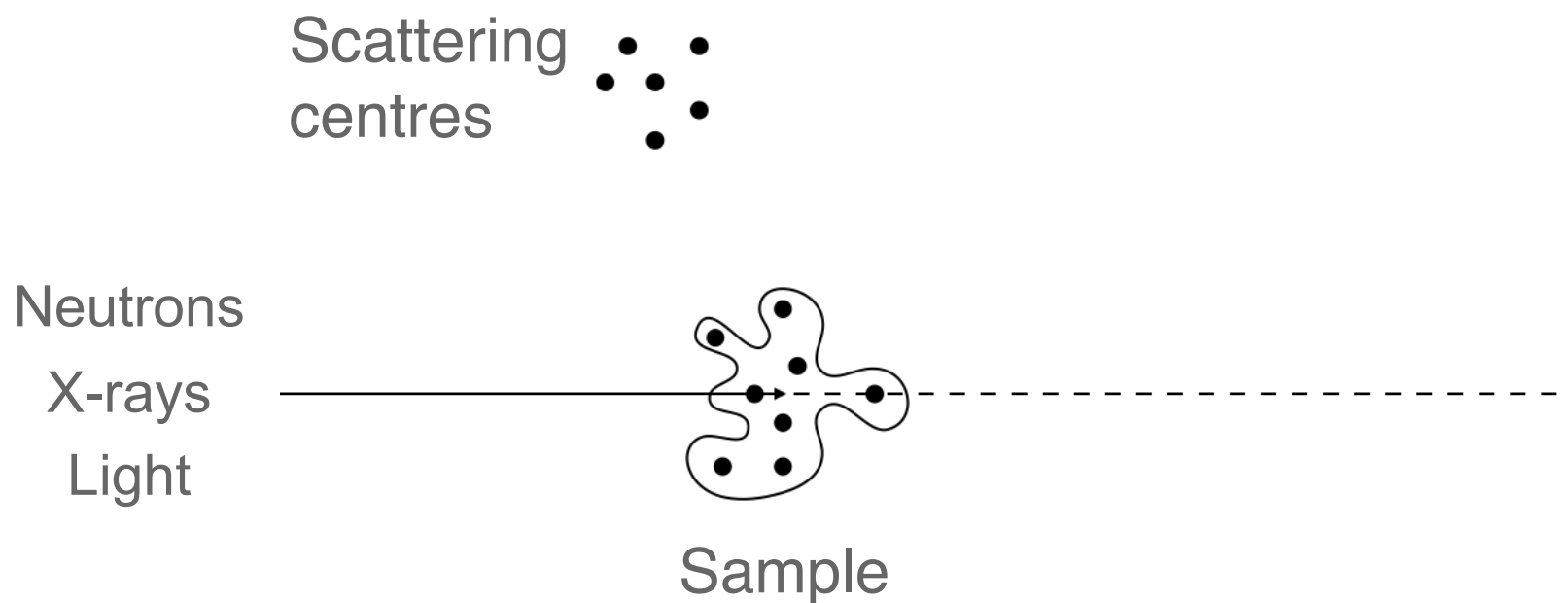
Small-angle scattering

Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of $\sim 1\text{--}200$ nm



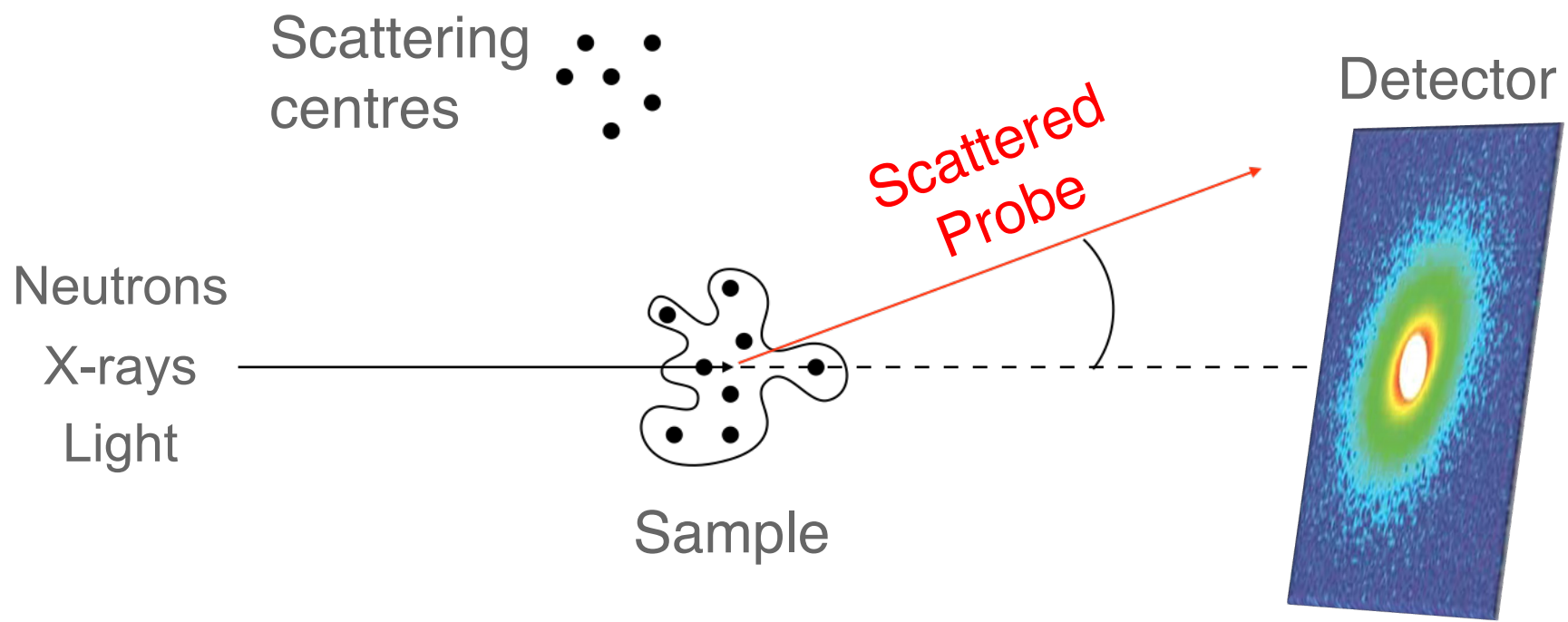
Small-angle scattering

Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of ~1–200 nm

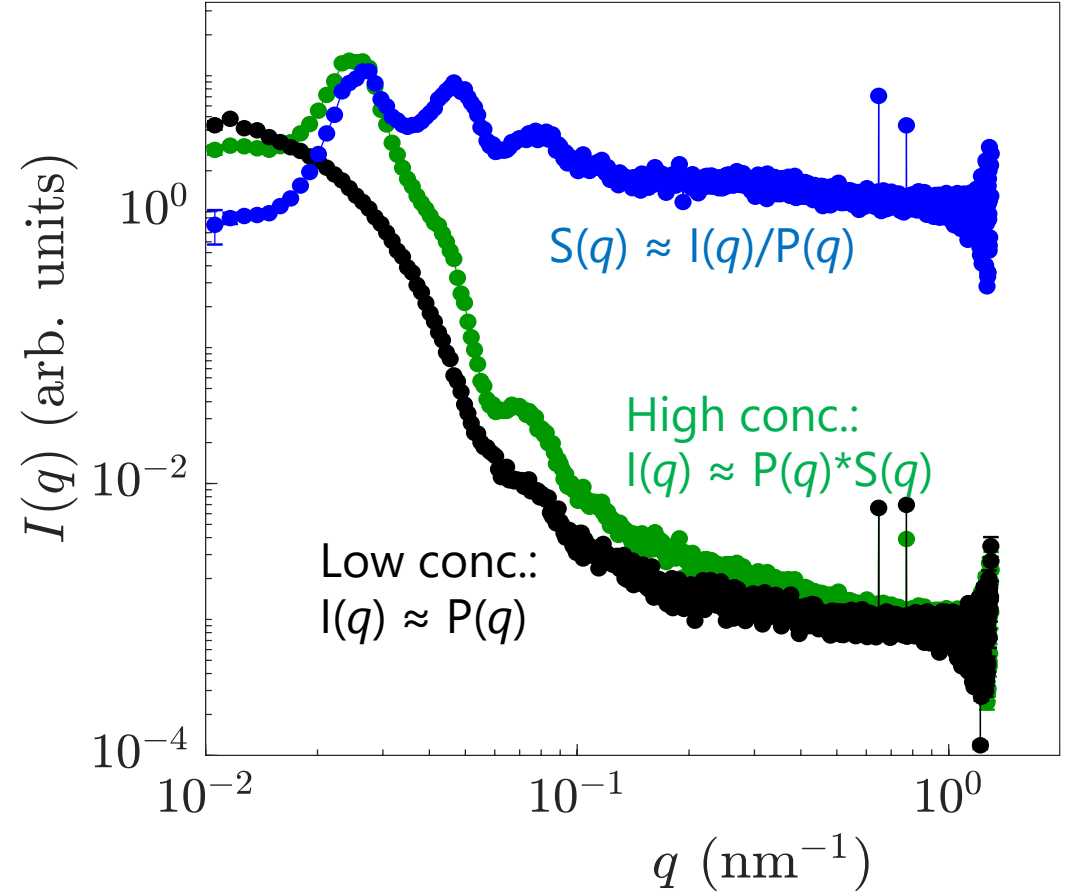
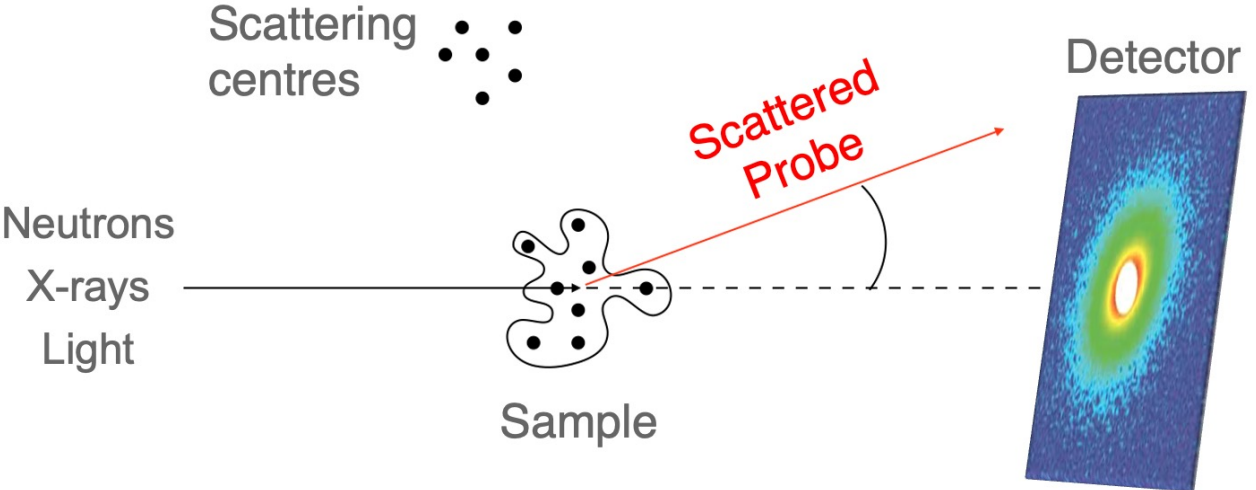


Small-angle scattering

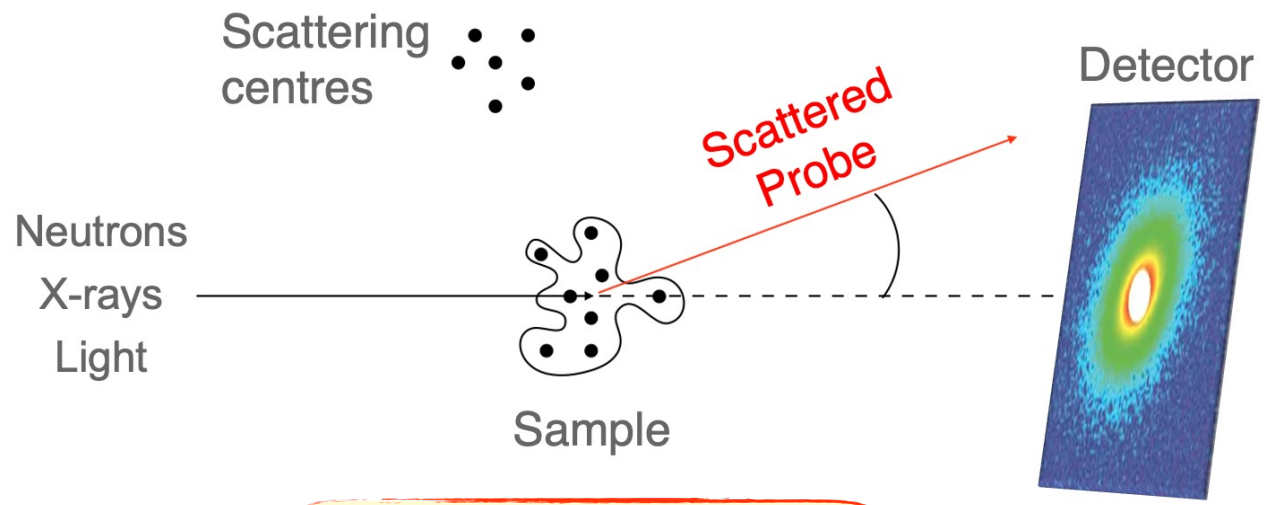
Experimental technique which uses **elastic scattering** at **small angles** to investigate the structure of substances at a mesoscopic scale of $\sim 1\text{--}200\text{ nm}$



Small-angle scattering



Small-angle scattering



n : particle number density
 $\Delta\rho$: scattering contrast
 V : particle volume
 $P(q)$: particle form factor
 $S(q)$: structure factor

$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

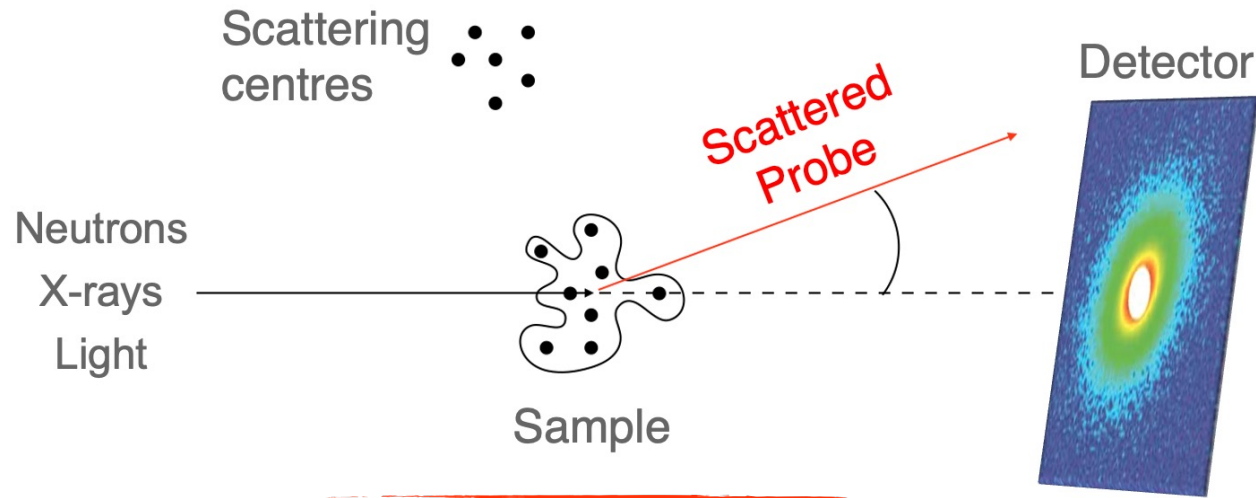
Scattering vector:

$$q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$

Scattering angle

Wavelength of the probe

Small-angle scattering



$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

n : particle number density

$\Delta\rho$: scattering contrast

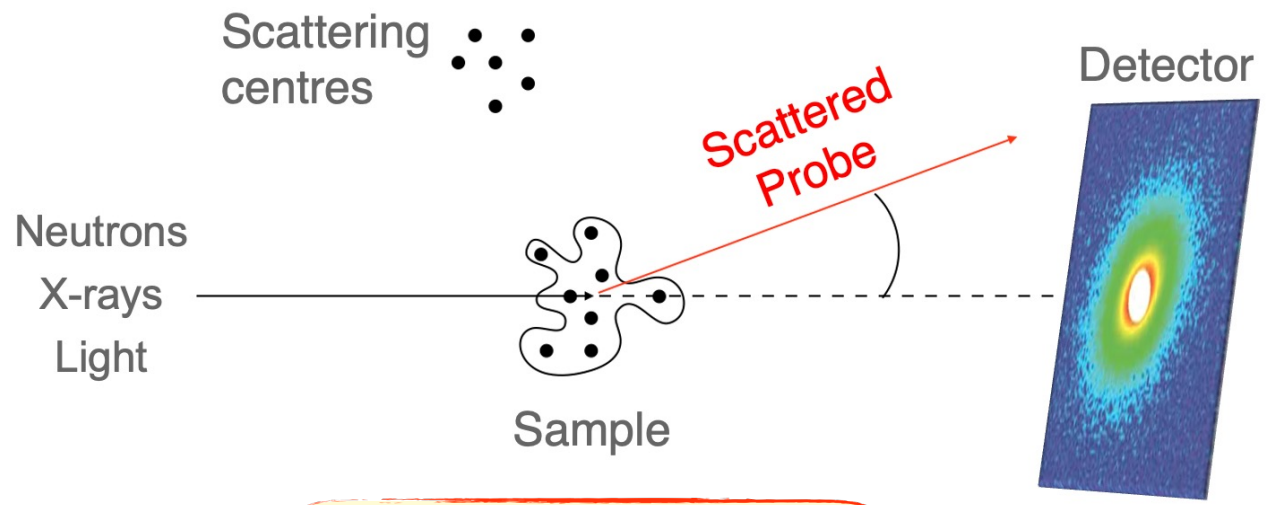
V : particle volume

$P(q)$: particle form factor

$S(q)$: structure factor

Form factor $P(q)$: all information on the single scattering object (shape, architecture, size...)

Small-angle scattering



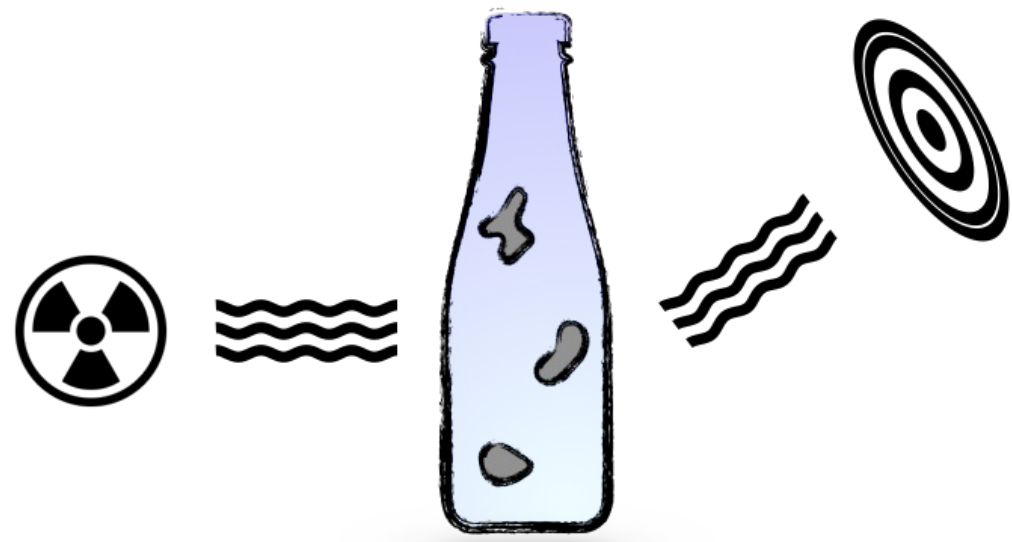
$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

- n : particle number density
- $\Delta\rho$: scattering contrast
- V : particle volume
- $P(q)$: particle form factor
- $S(q)$: structure factor

Form factor $P(q)$: all information on the single scattering object (shape, architecture, size...)

Structure factor $S(q)$: all information on the arrangement in the sample (nearest neighbour distance, phase, crystalline lattice)

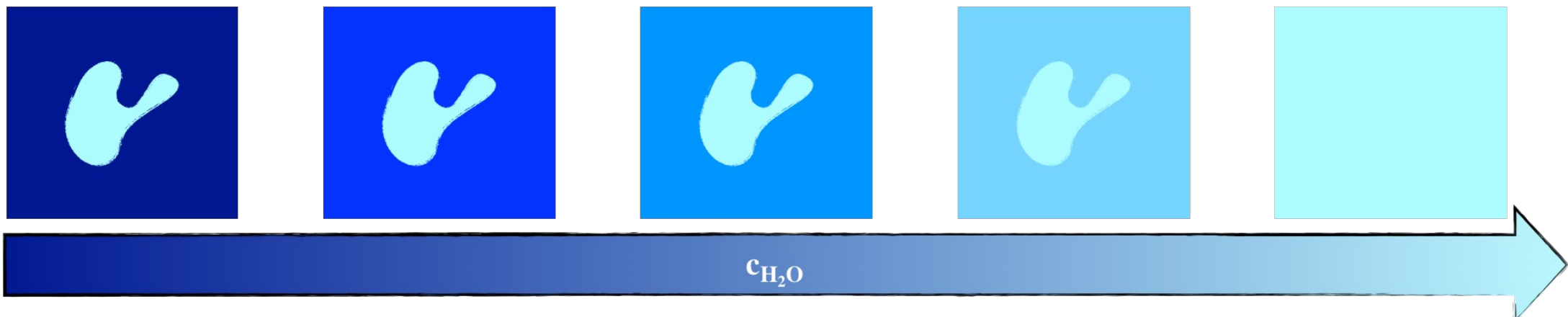
Scattering contrast, $\Delta\rho$



$$I_{exp}(q) = n \Delta\rho^2 V^2 P(q) S(q)$$

$\Delta\rho$: difference in scattering length density between solvent and sample.

$$\Delta\rho = |\rho_{H_2O} - \rho_{SiO_2}|$$



Contrast matching



*When the monster came,
Lola remained undetected.*

*Harold, of course, was
immediately devoured.*

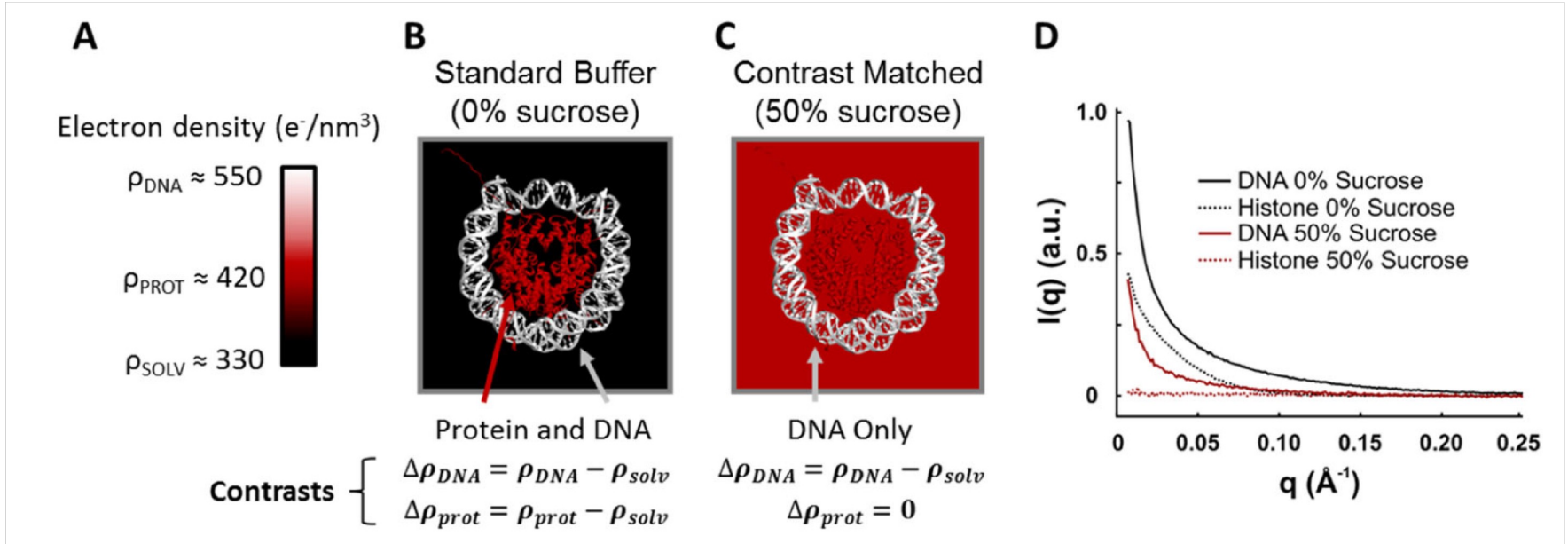
Contrast matching using light



Laura Waller on youtube.com

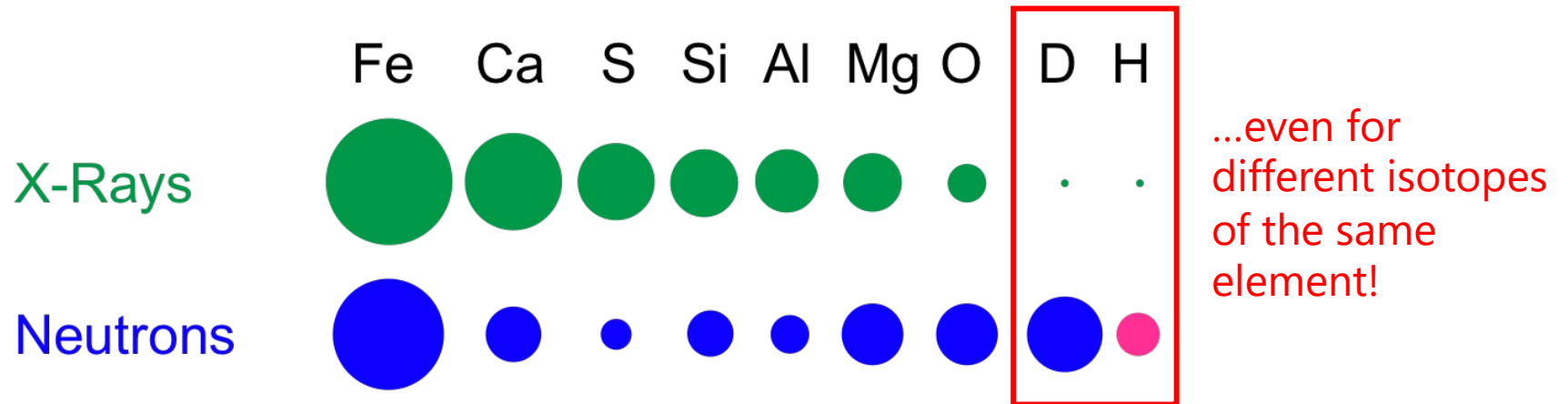
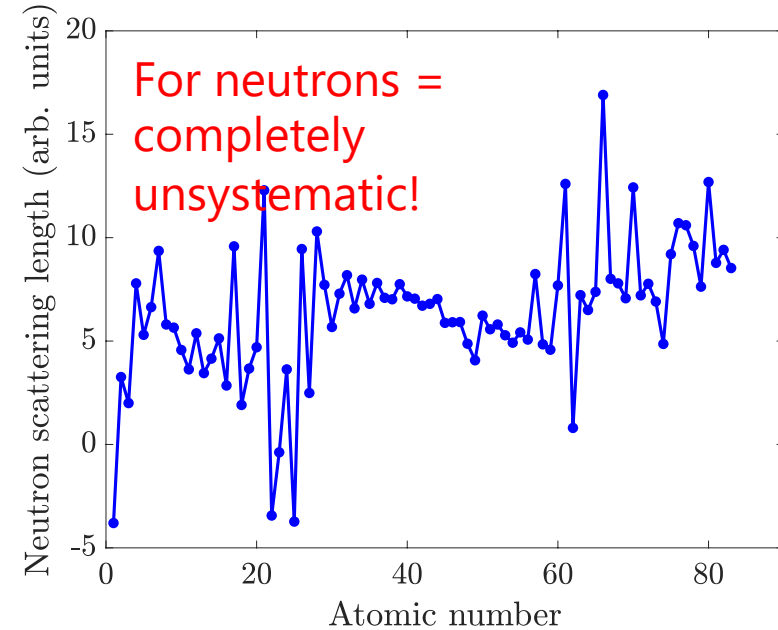
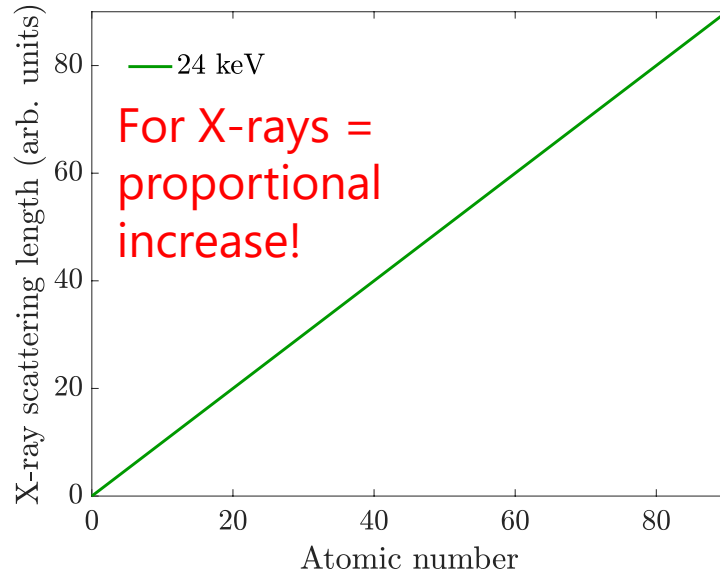
Contrast matching using light and X-rays

- Contrast matching is possible for all the scattering methods.
- Light: match the between the **refractive index** of the sample and the solvent.
- X-ray: match the **electron density** between the sample and the solvent.



This same idea works for neutrons by playing with H/D substitution!

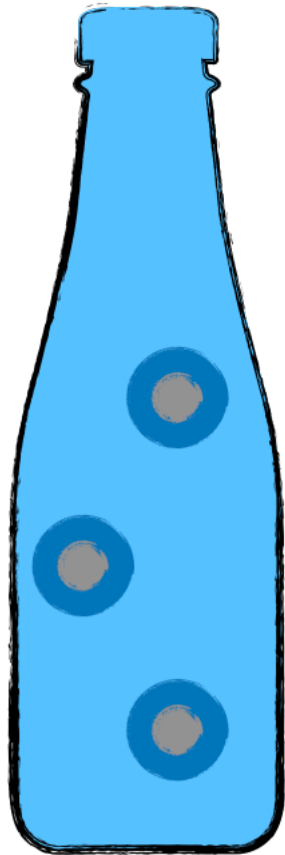
Recap: X-rays and neutrons see things differently!



Neutrons and contrast matching

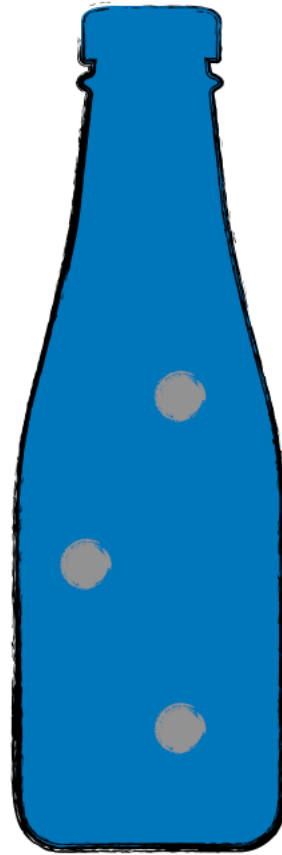


Solvent 1



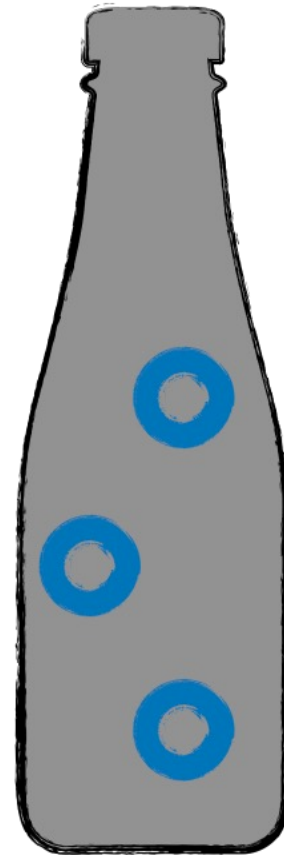
Core-shell particle

Solvent 2



Core-only

Solvent 3



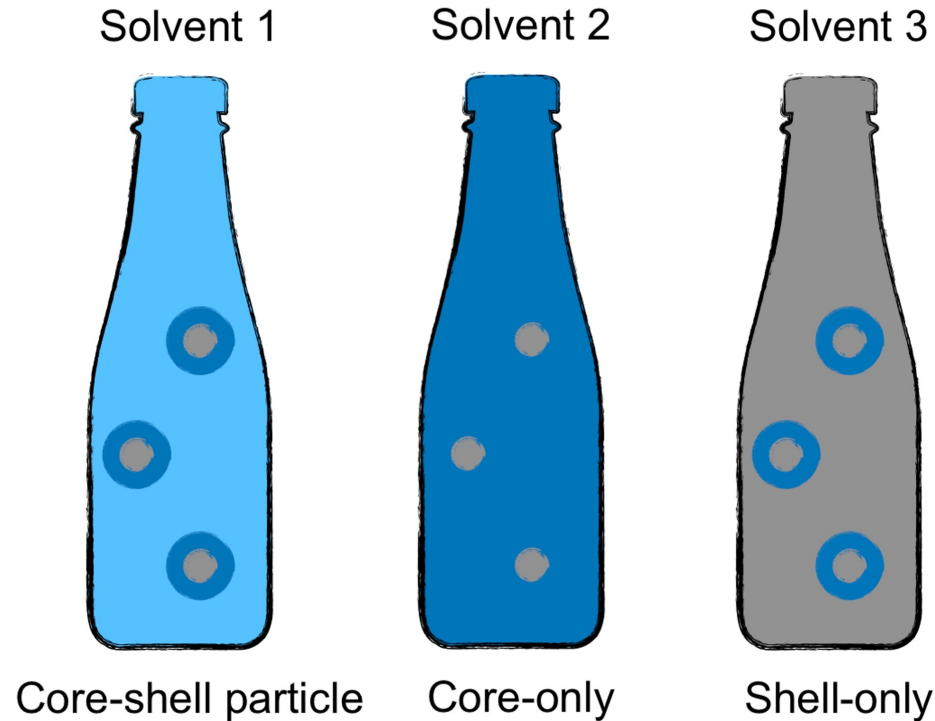
Shell-only

$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

Selective deuteration in combination with neutrons lets us investigate selected parts of complex assemblies.

Combining X-Ray and Neutron measurements provides more information

Neutrons and contrast matching



$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

Selective deuteration in combination with neutrons lets us investigate selected parts of complex assemblies.

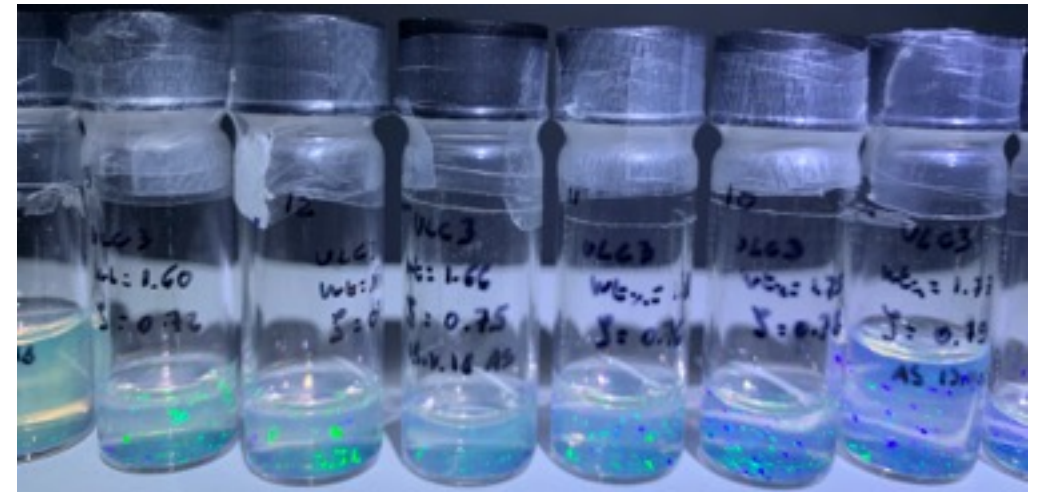
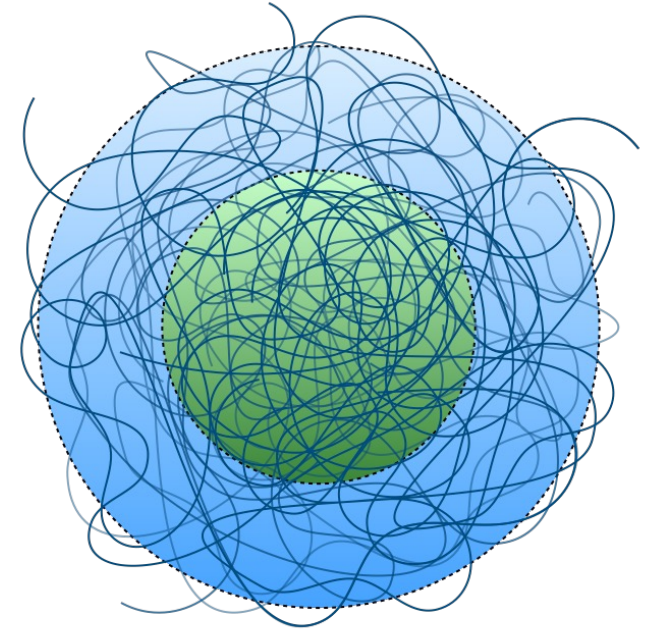
Combining X-Ray and Neutron measurements provides more information

Why is it so important for Life Science?

- one of the easiest way to change the contrast is switching from H → D
- one of the main elements of biological matter is H, thus neutron scattering and CV is natural tool

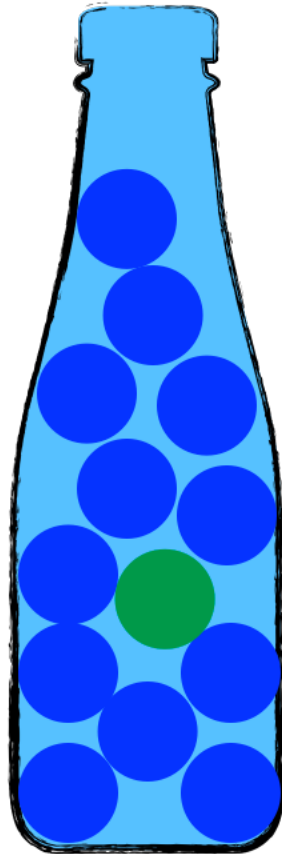
3

Colloidal particles in a crowded environment



Example: Colloidal particles in crowded environment

Solvent 1



All particles visible

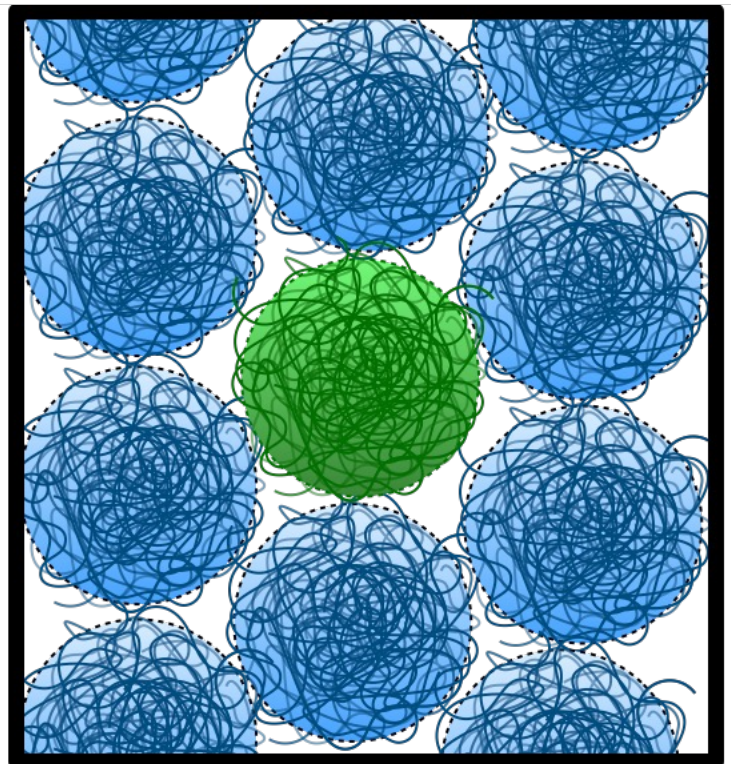
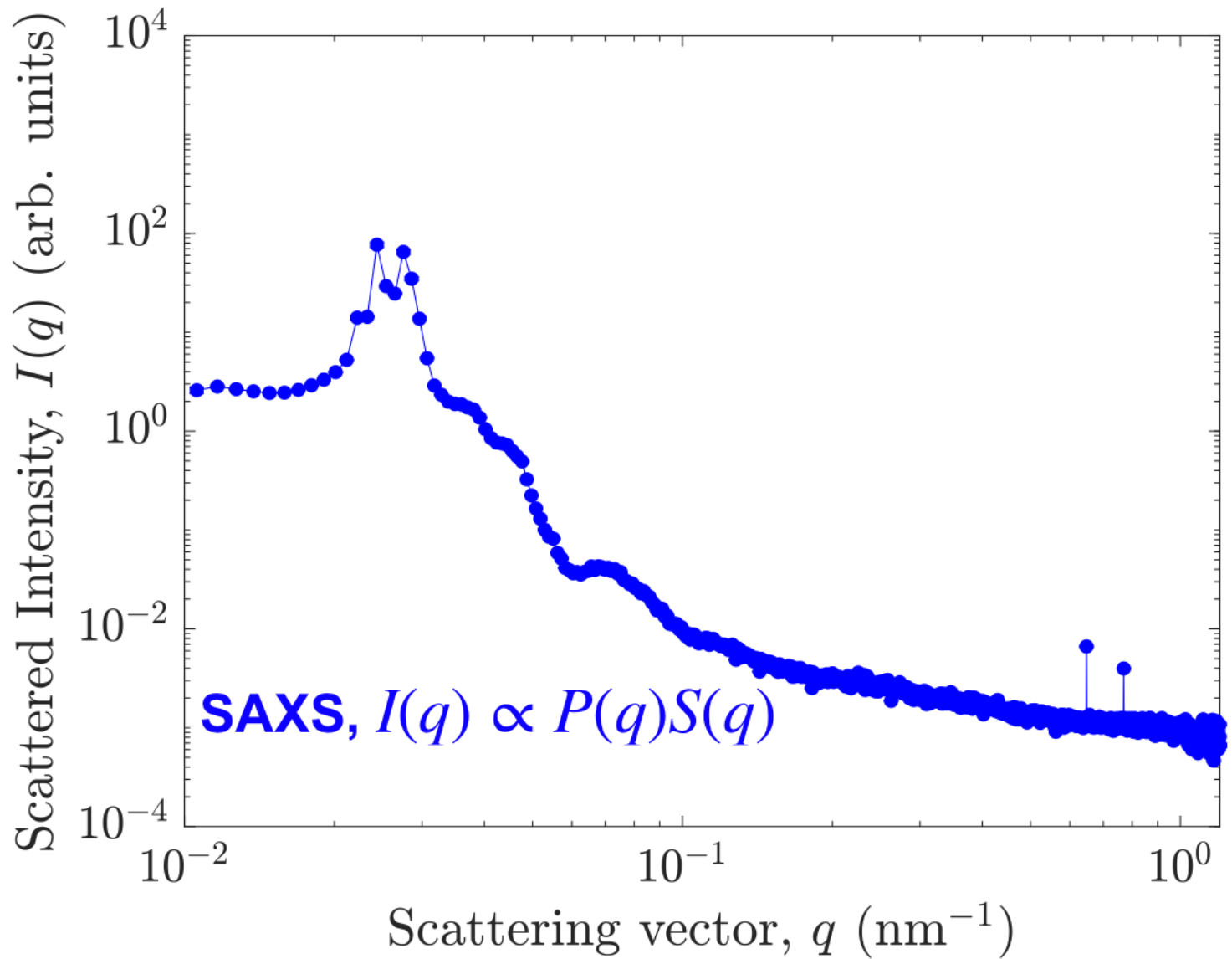
Question:
how does a
soft colloid
respond to crowding?

Problem:
in concentrated solutions
 $I(q) \propto P(q)S(q)$

 Hydrogenated particle

 Deuterated particle

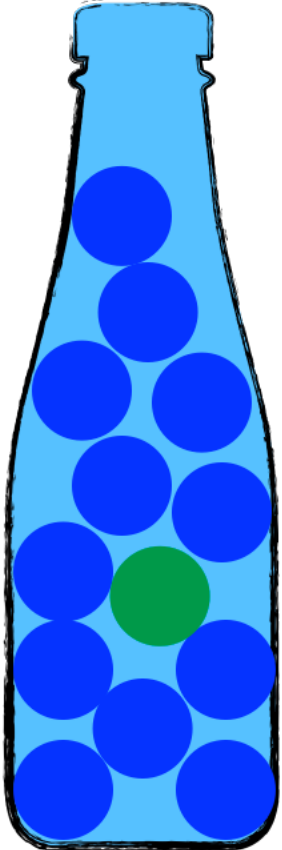
Example: Colloidal particles in crowded environment



Courtesy of Andrea Scotti (RWTH)

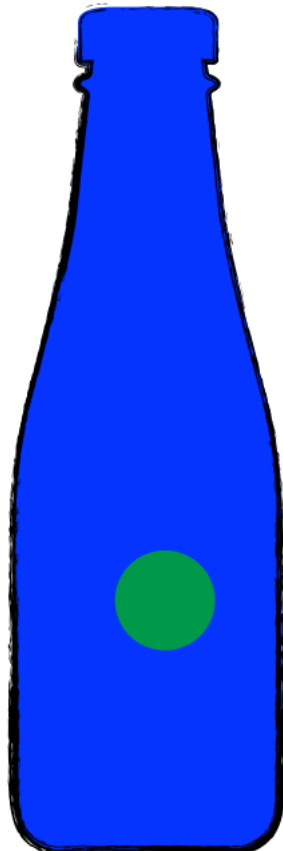
Example: Colloidal particles in crowded environment

Solvent 1





All particles visible

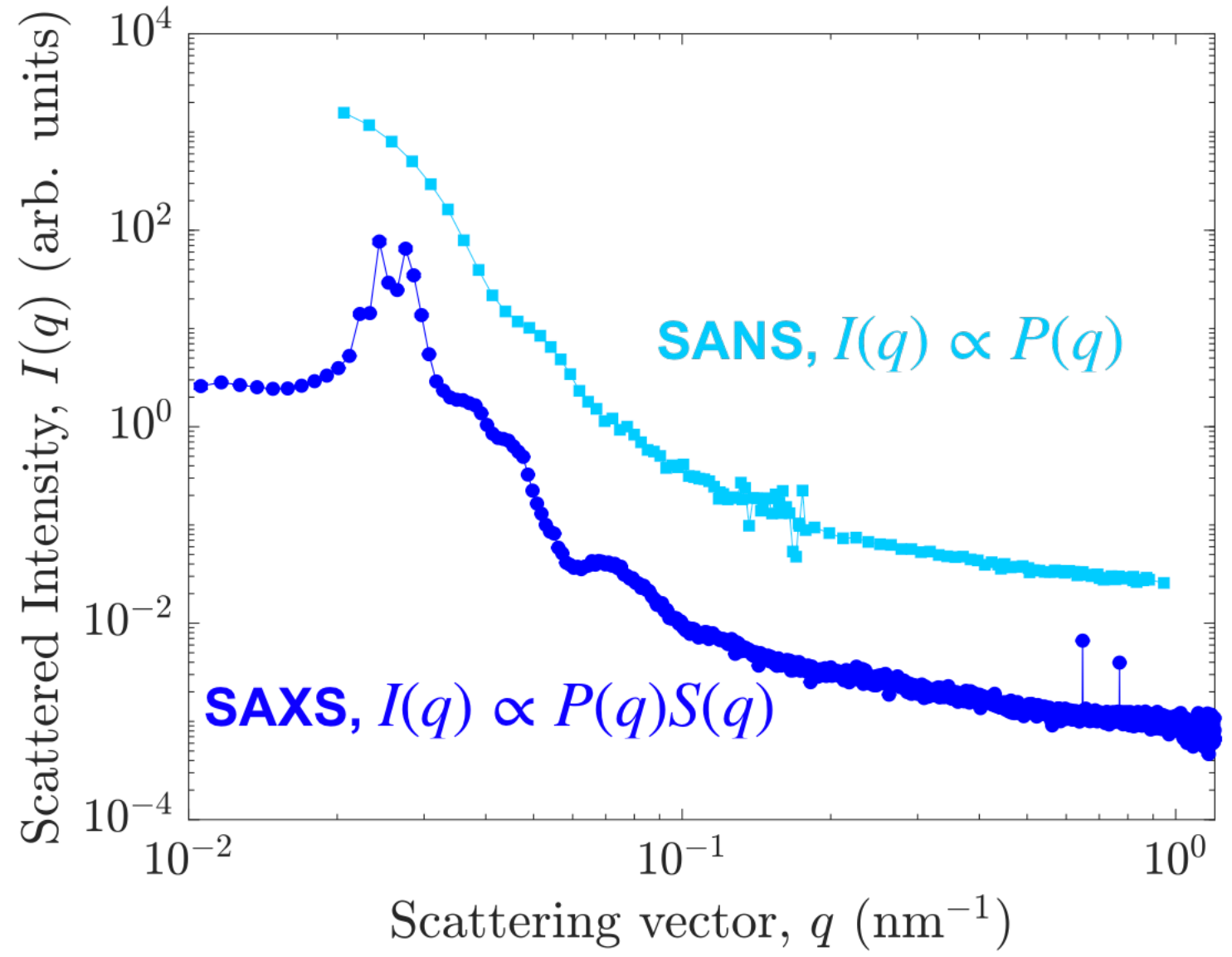
Solvent 2



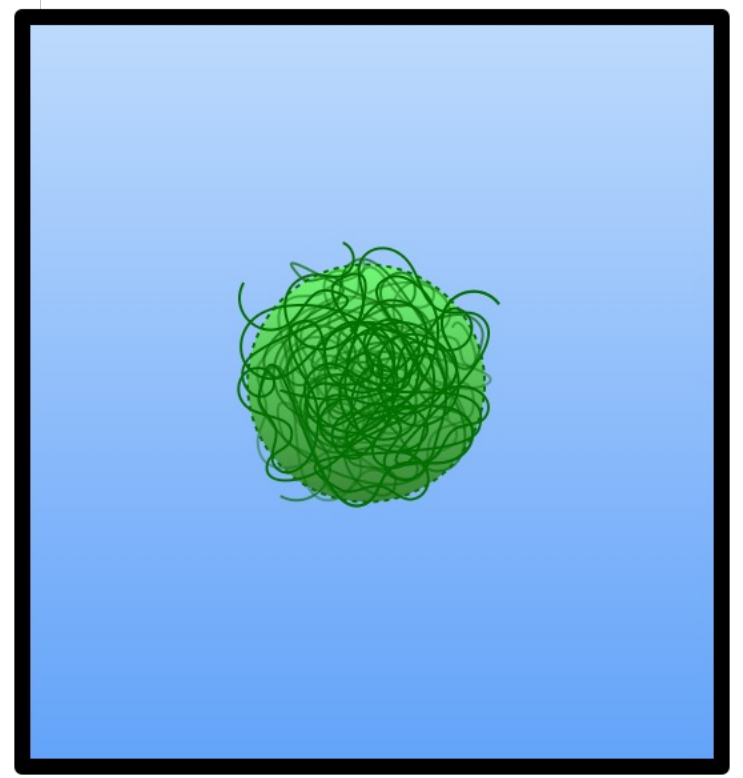
Only the labelled particle is visible

-  Hydrogenated particle
-  Deuterated particle

Example: Colloidal particles in crowded environment



SANS, $I(q) \propto P(q)$



Courtesy of Andrea Scotti (RWTH)

How do we experimentally determine the contrast matching point? Method 1

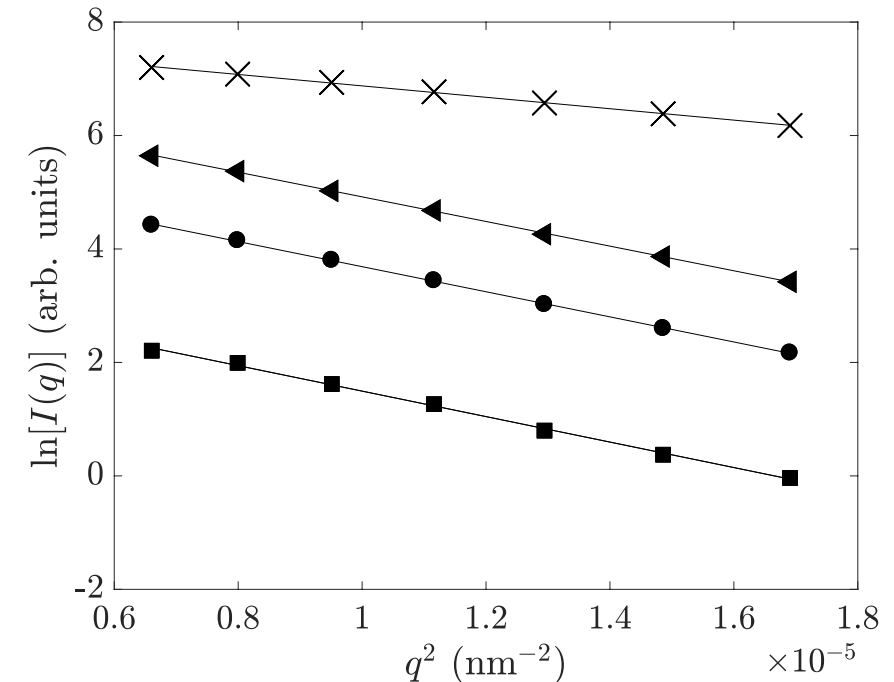
Step 1: prepare a series of the same sample (highly diluted) in different solvents (e.g. water/heavy water mixtures).

Step 2: perform small-angle neutron scattering measurements at low-Q (Guinier regime).

Step 3: fit the data at low-Q with the Guinier approximation for all the different solvents

$$\lim_{q \rightarrow 0} P(q) = I(0) \exp \left[-\frac{q^2 \langle S^2 \rangle}{3} \right]$$

Step 4: plot the values of $I(0)$ obtained from the fits versus the solvent composition and look for the intercept with the x-axes



- × 0 wt% D₂O/ 100 wt% H₂O
- ◄ 28 wt% D₂O/ 62 wt% H₂O
- 58 wt% D₂O/ 42 wt% H₂O
- 100 wt% D₂O/ 0 wt% H₂O

How do we experimentally determine the contrast matching point? Method 1

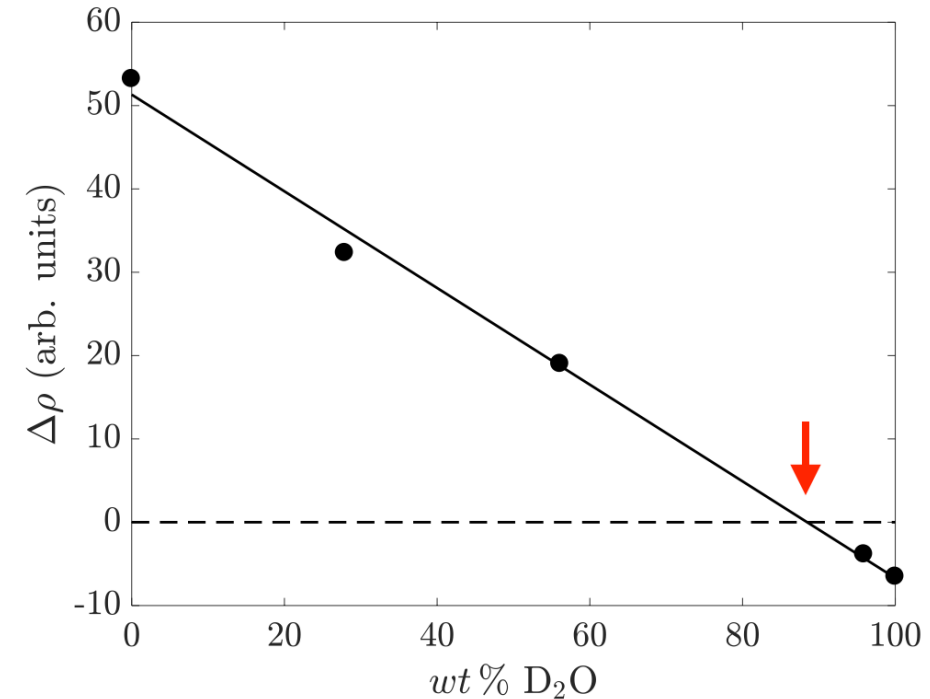
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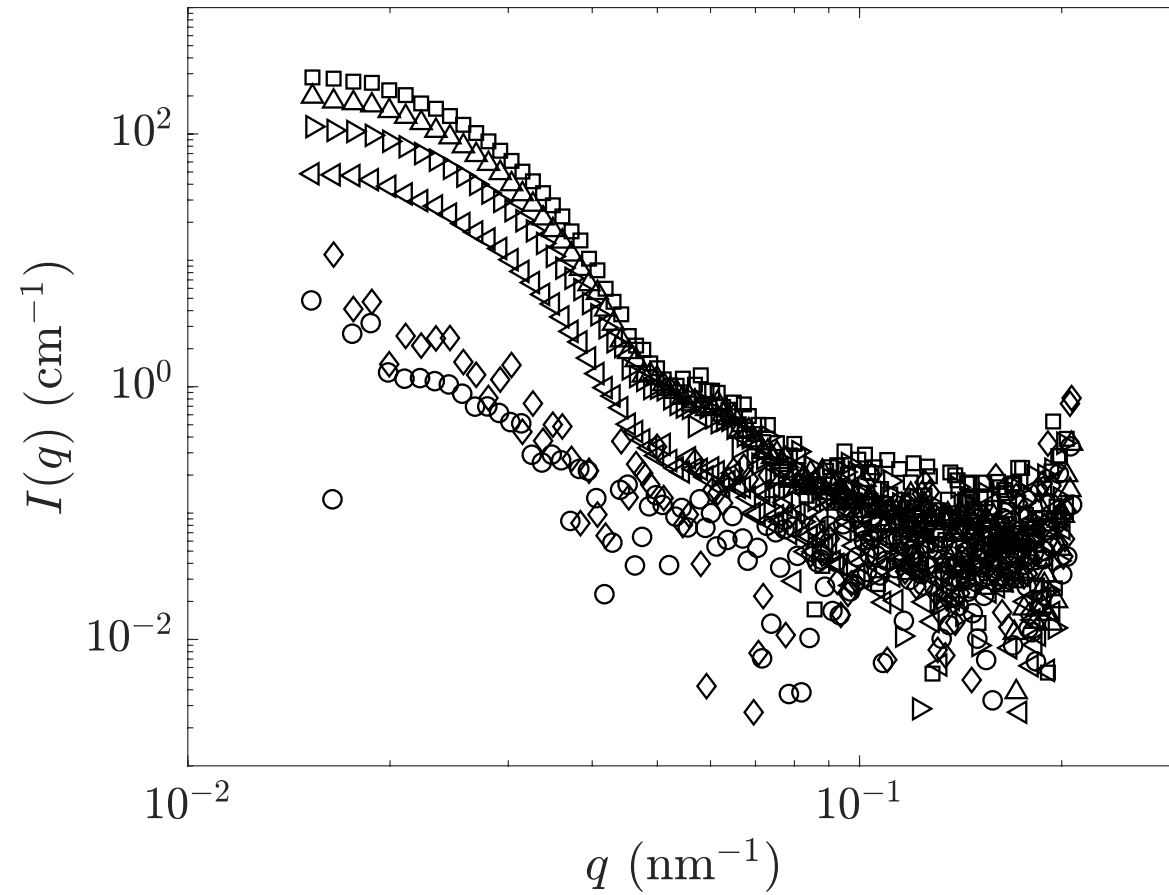
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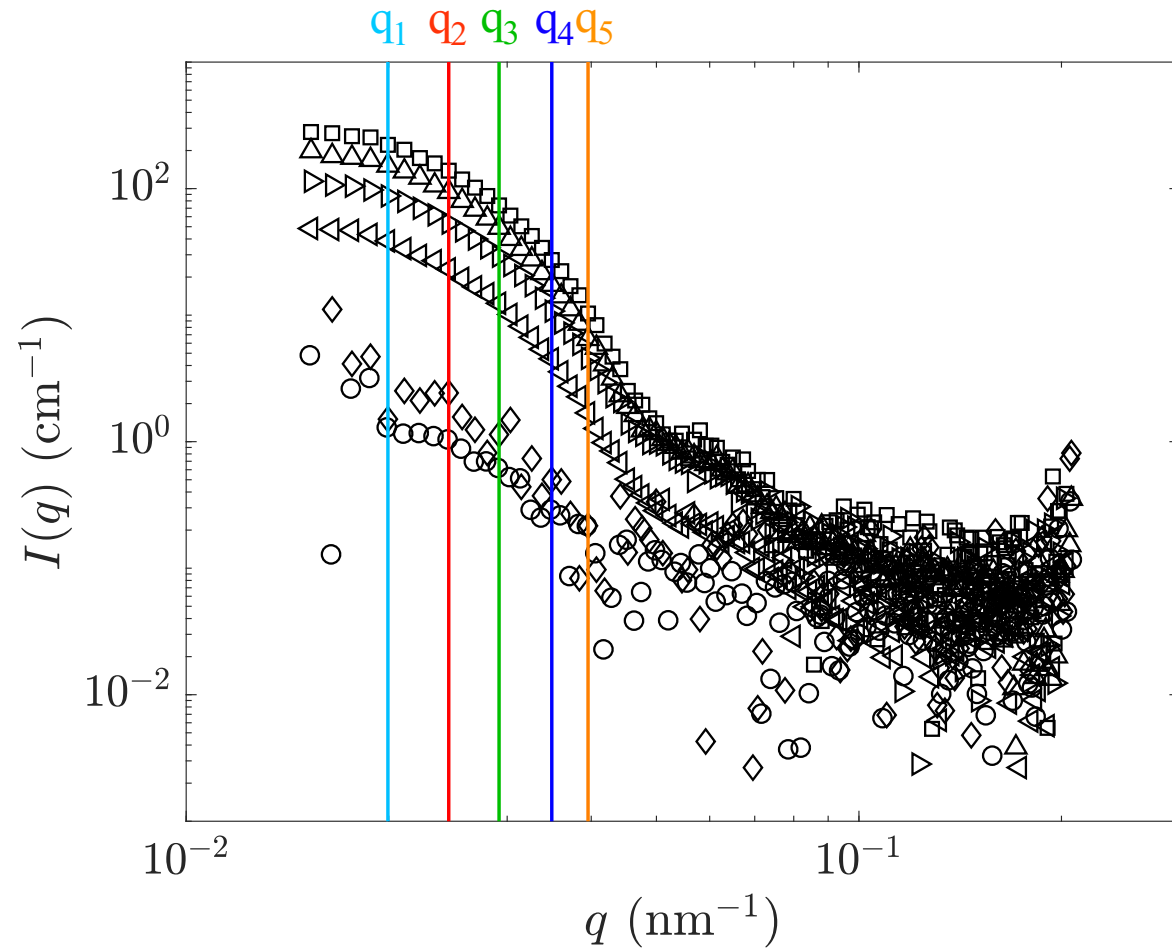


How do we experimentally determine the contrast matching point? Method 2



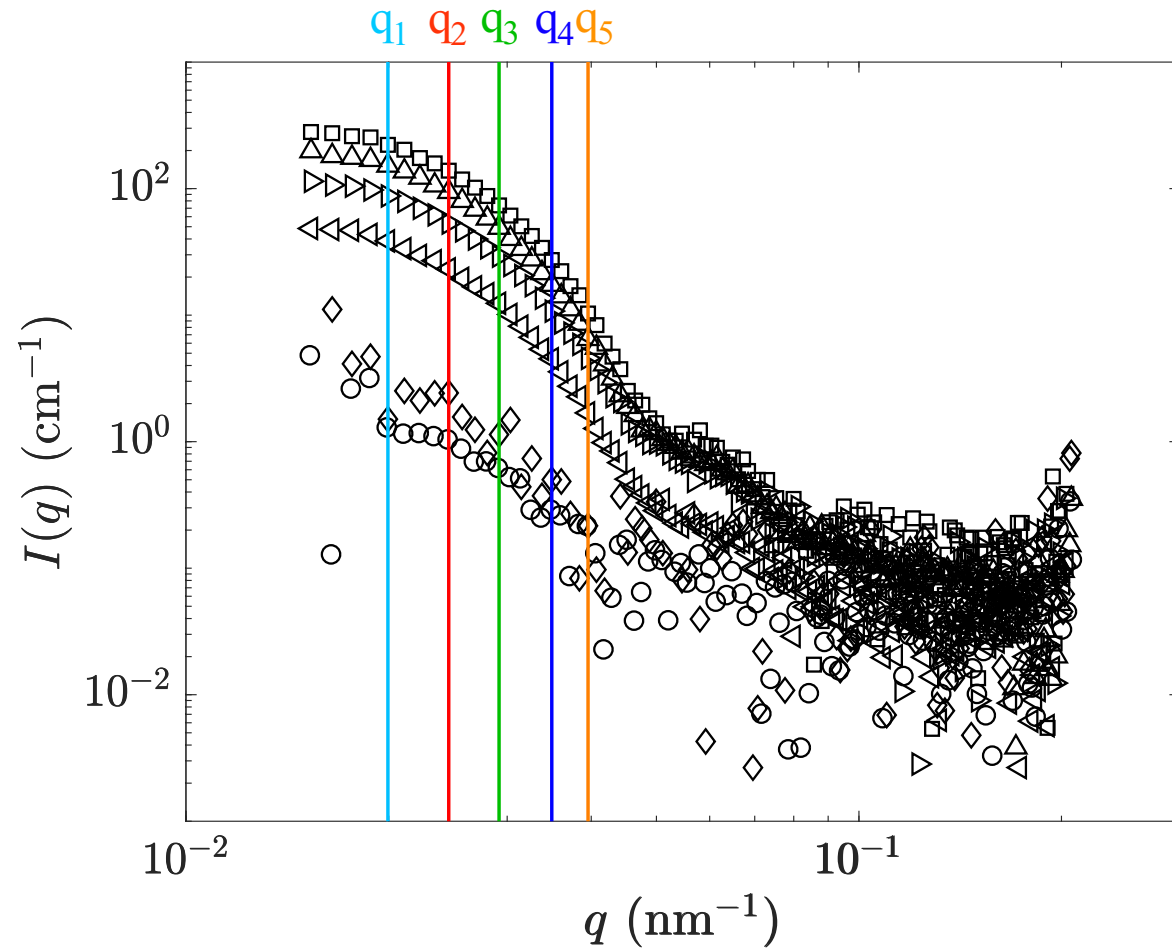
- 0 wt% D_2O / 100 wt% H_2O
- ▷ 20 wt% D_2O / 80 wt% H_2O
- ◇ 50 wt% D_2O / 50 wt% H_2O
- 60 wt% D_2O / 40 wt% H_2O
- ◁ 80 wt% D_2O / 20 wt% H_2O
- △ 100 wt% D_2O / 0 wt% H_2O

How do we experimentally determine the contrast matching point? Method 2



- 0 wt% D_2O / 100 wt% H_2O
- ▷ 20 wt% D_2O / 80 wt% H_2O
- ◇ 50 wt% D_2O / 50 wt% H_2O
- 60 wt% D_2O / 40 wt% H_2O
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- △ 100 wt% D_2O / 0 wt% H_2O

How do we experimentally determine the contrast matching point? Method 2

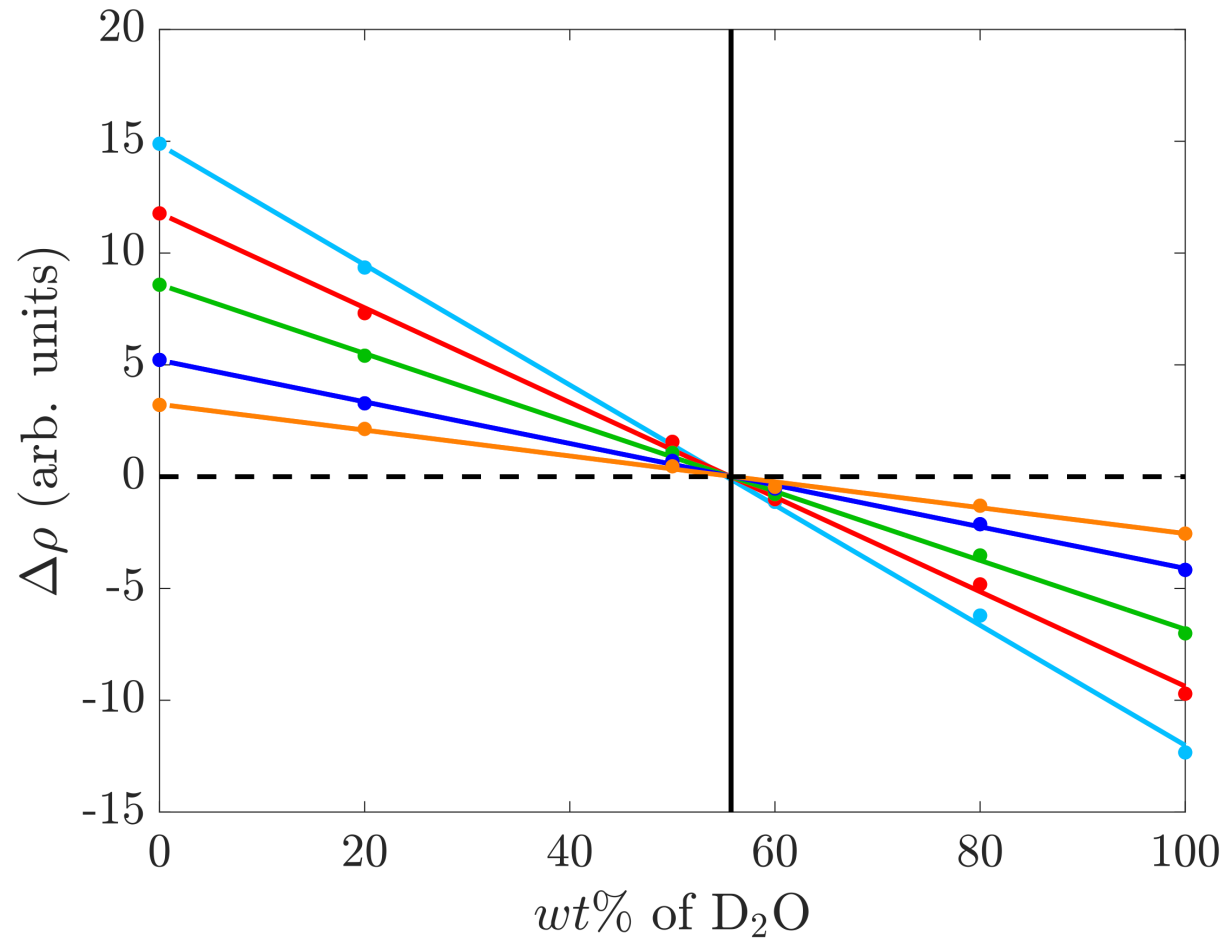


- 0 wt% D₂O / 100 wt% H₂O
- ▷ 20 wt% D₂O / 80 wt% H₂O
- ◇ 50 wt% D₂O / 50 wt% H₂O
- 60 wt% D₂O / 40 wt% H₂O
- ◁ 80 wt% D₂O / 20 wt% H₂O
- △ 100 wt% D₂O / 0 wt% H₂O

$$I_{exp}(q) = n\Delta\rho^2 V^2 P(q) S(q)$$

All the samples have the same concentration of the same particles.

How do we experimentally determine the contrast matching point? Method 2



$$I(q_1) \propto \Delta\rho$$

$$I(q_2) \propto \Delta\rho$$

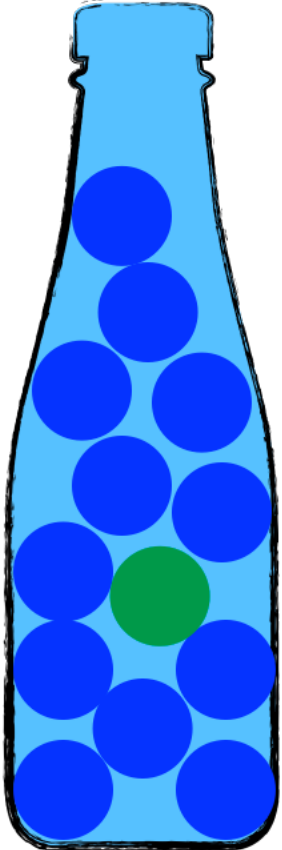
$$I(q_3) \propto \Delta\rho$$

$$I(q_4) \propto \Delta\rho$$

$$I(q_5) \propto \Delta\rho$$

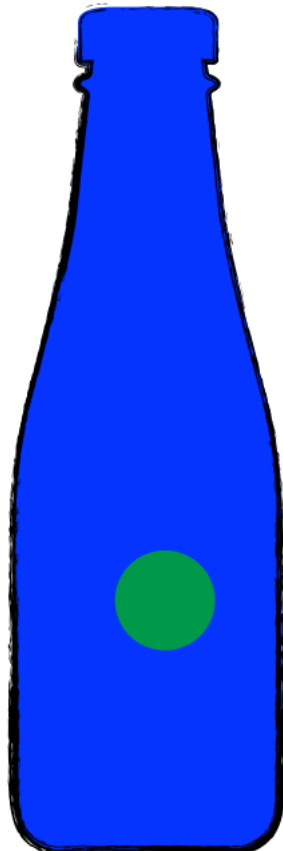
Example: Colloidal particles in crowded environment

Solvent 1





All particles visible

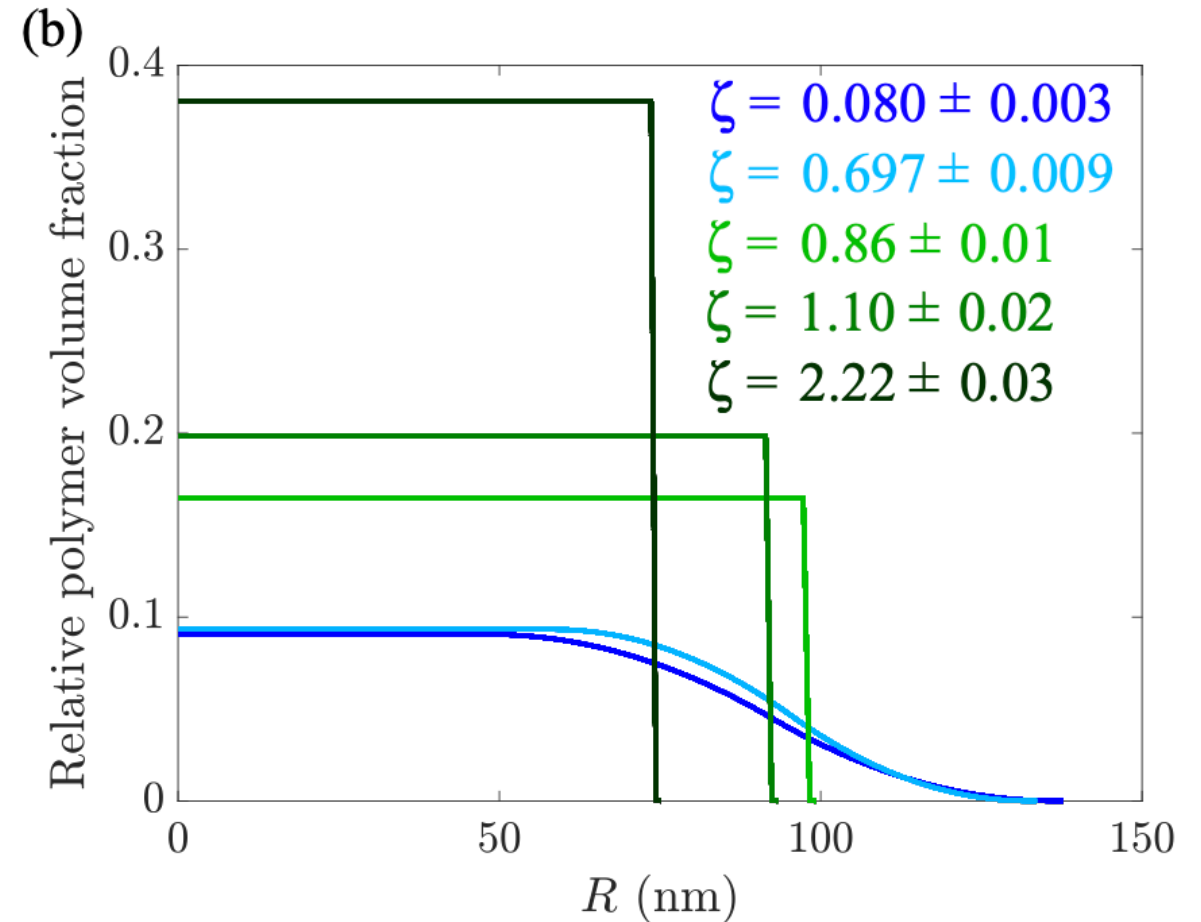
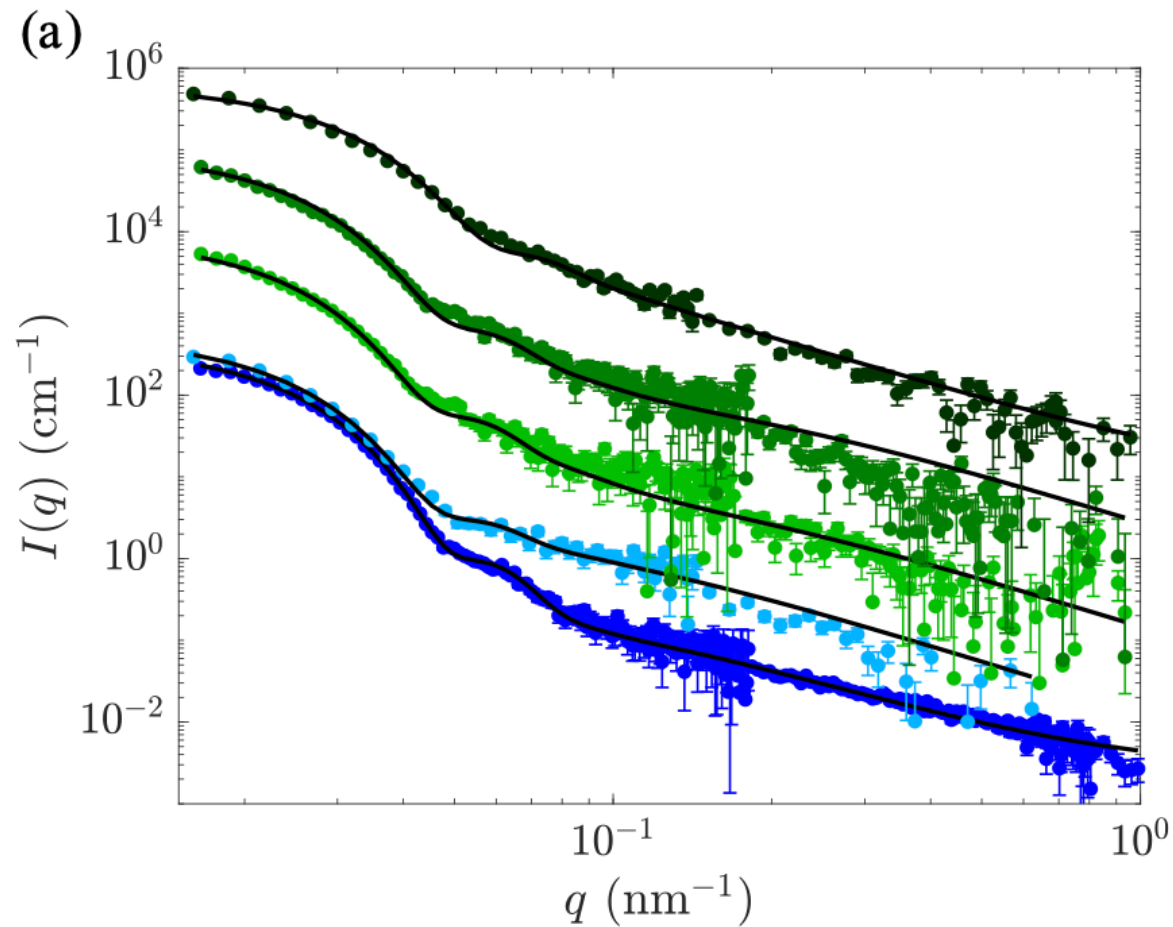
Solvent 2



Only the labelled particle is visible

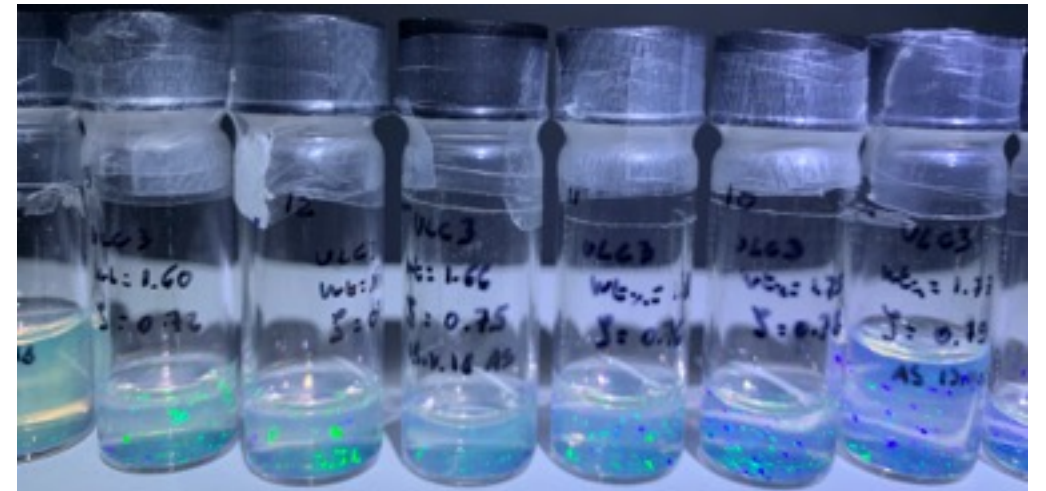
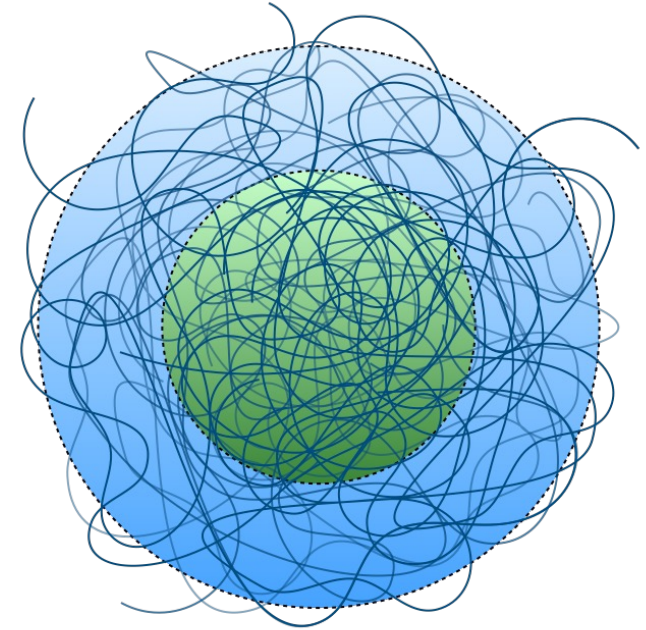
-  Hydrogenated particle
-  Deuterated particle

Small-angle neutron scattering with contrast variation



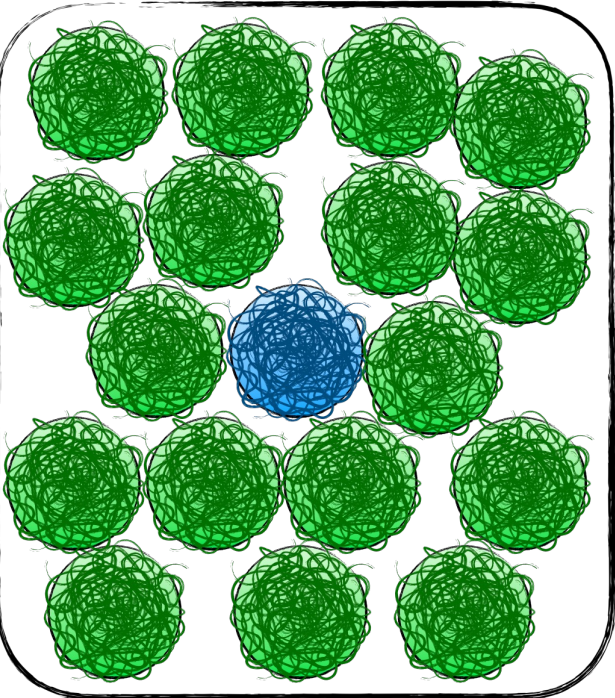
4

Using SAS to quantify the softness of small colloids

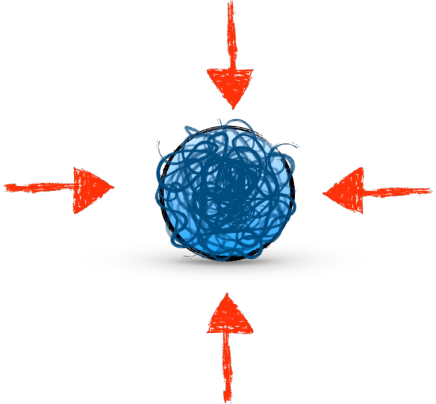


Colloids in crowded suspensions

Deswelling



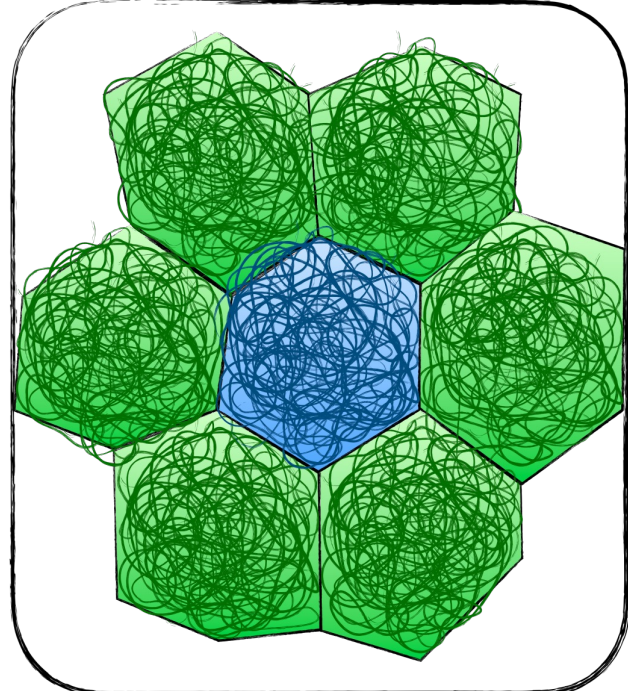
We need the **bulk modulus!**



Bulk modulus

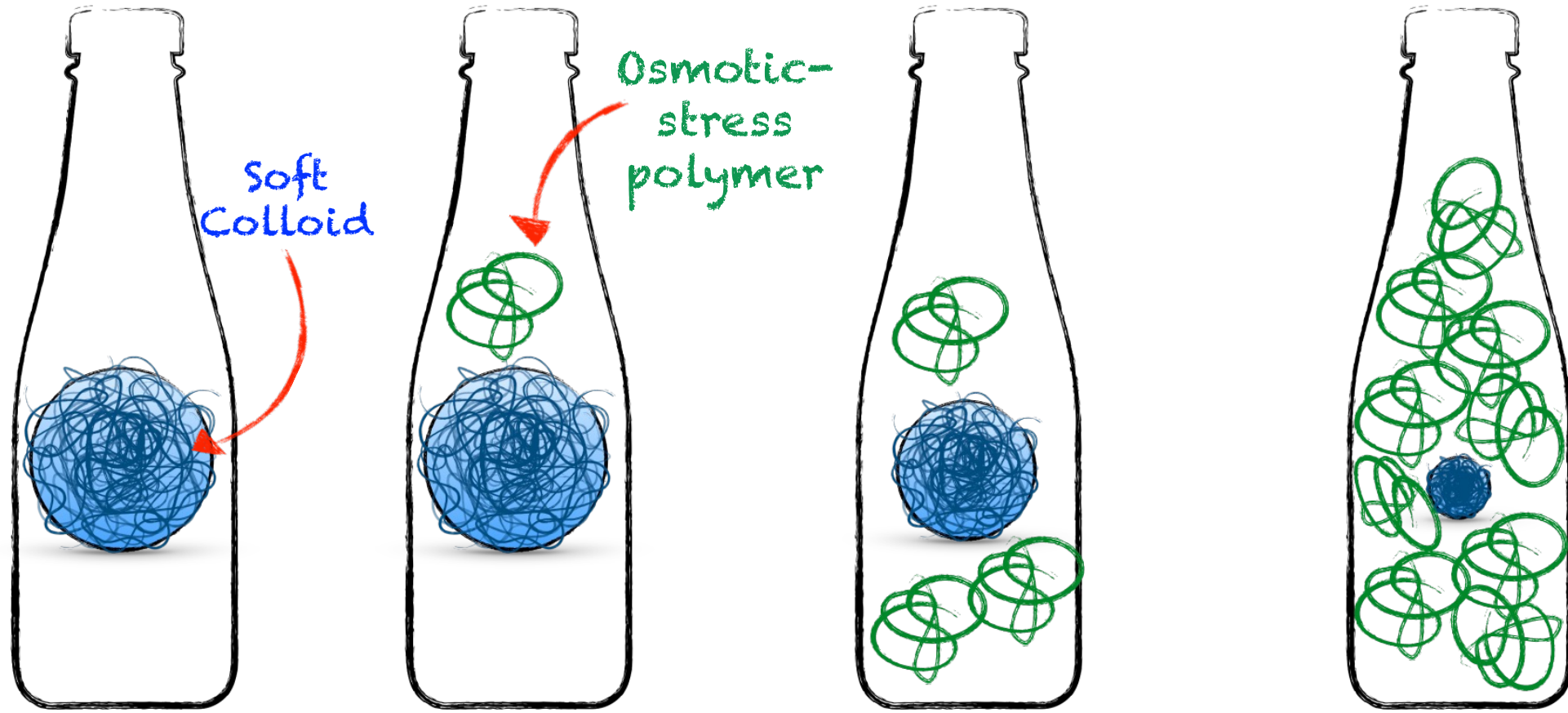
$$K = -v \frac{d\pi}{dv}$$

Faceting



We cannot use microscopy, particles too small!

How do we measure K ? Osmotic stress solutions

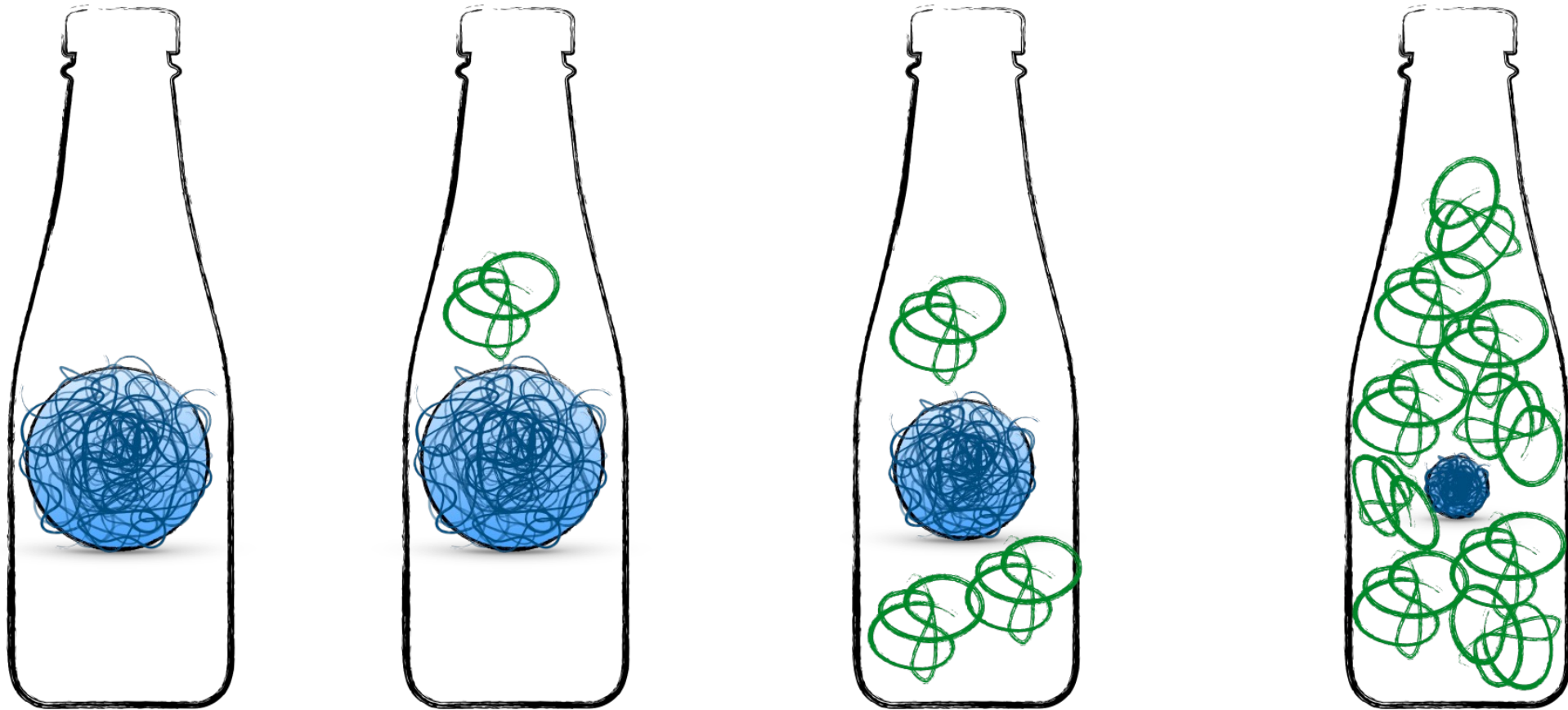


Soft Colloid

Osmotic-stress polymer

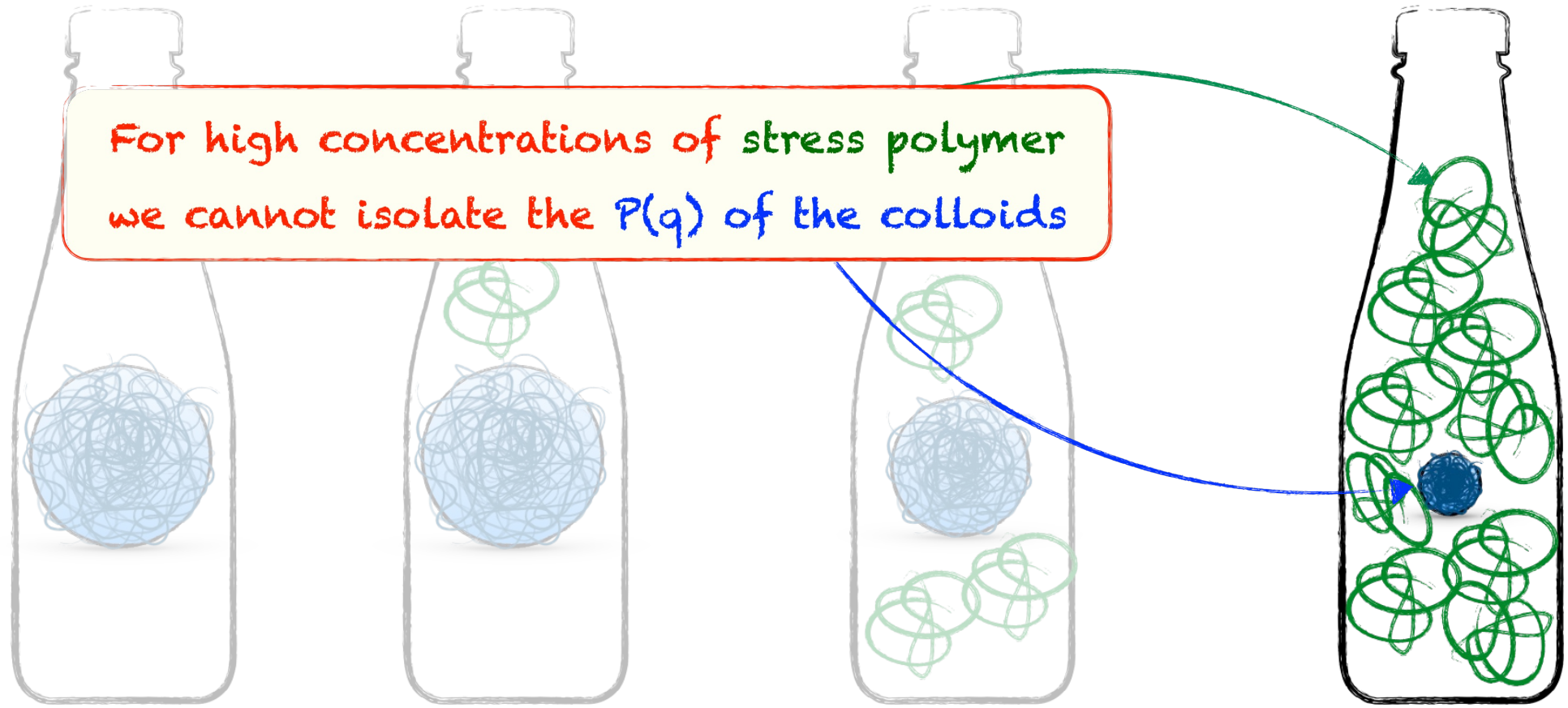
Concentration osmotic stress polymer

Information not accessible at high pressures



Information not accessible at high pressures

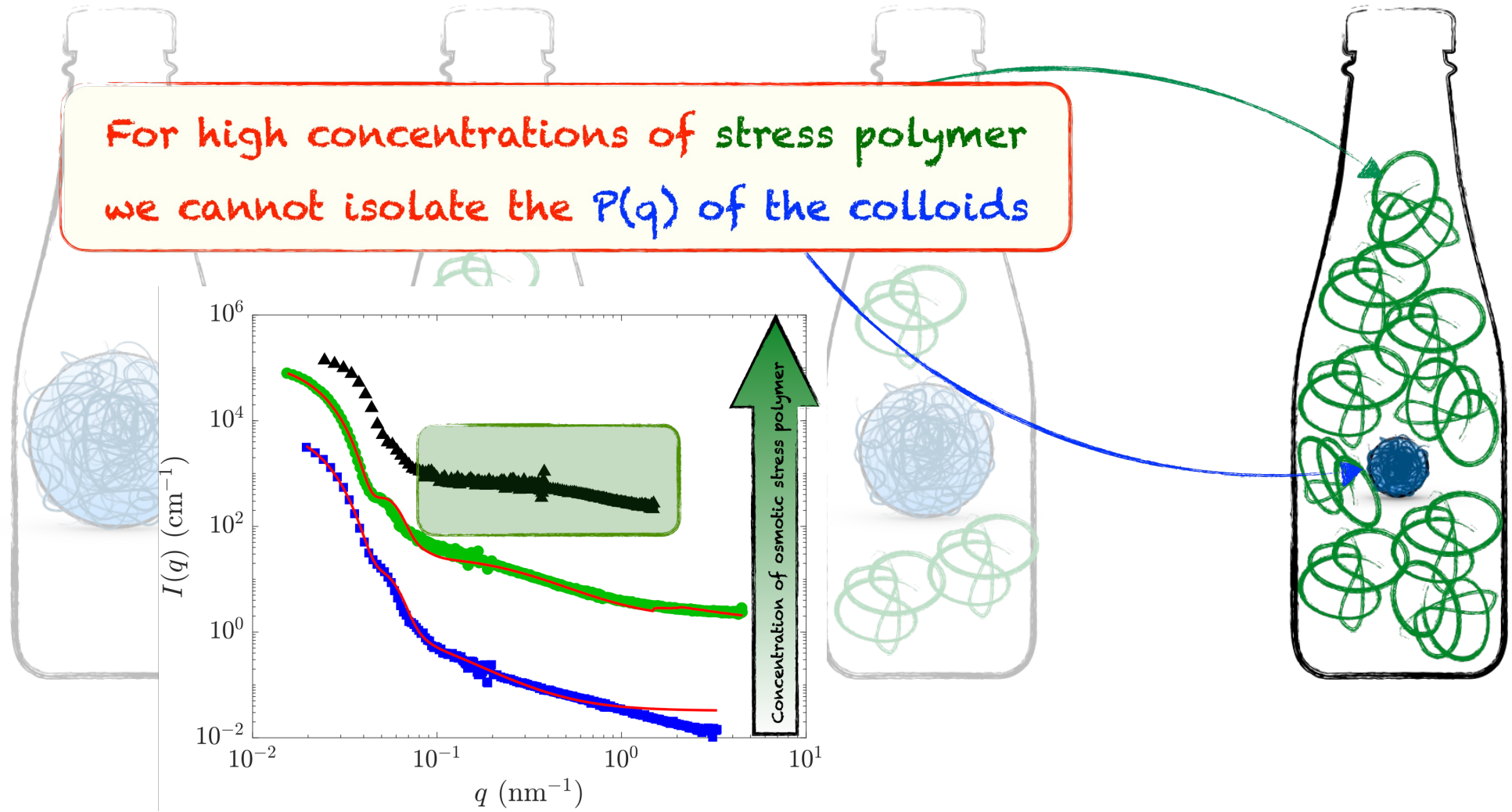
For high concentrations of stress polymer we cannot isolate the $P(q)$ of the colloids



Information not accessible at high pressures



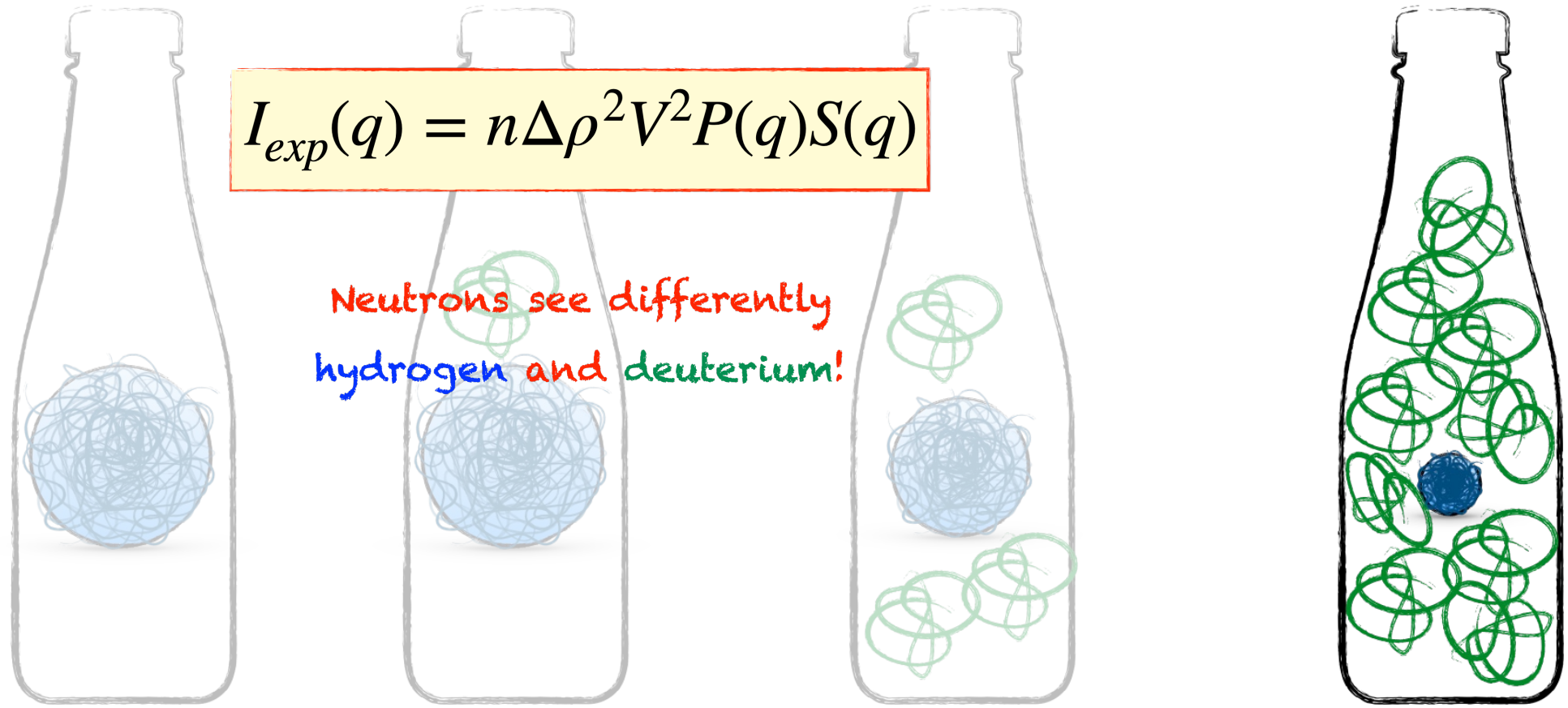
For high concentrations of stress polymer we cannot isolate the $P(q)$ of the colloids



Neutrons and contrast variation

$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

Neutrons see differently
hydrogen and deuterium!

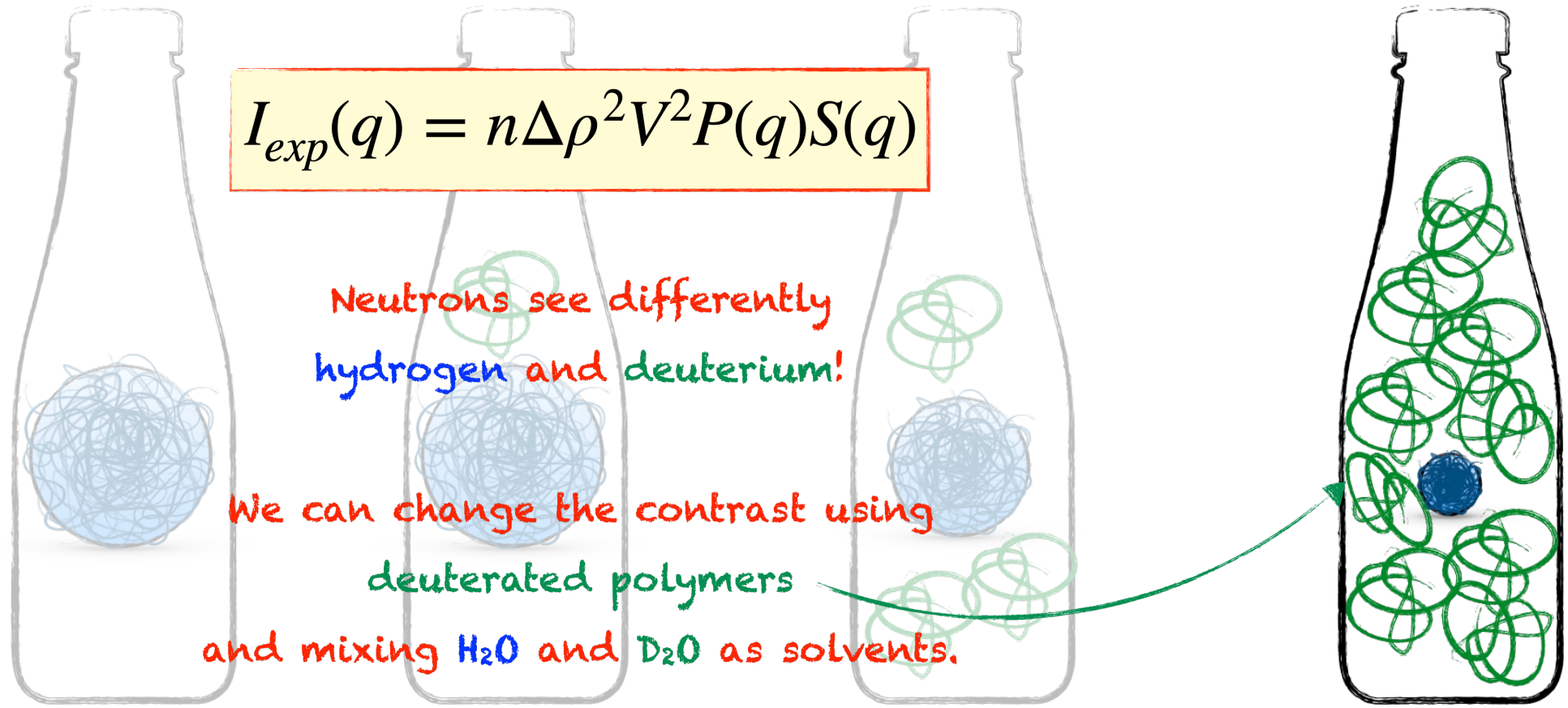


Neutrons and contrast variation

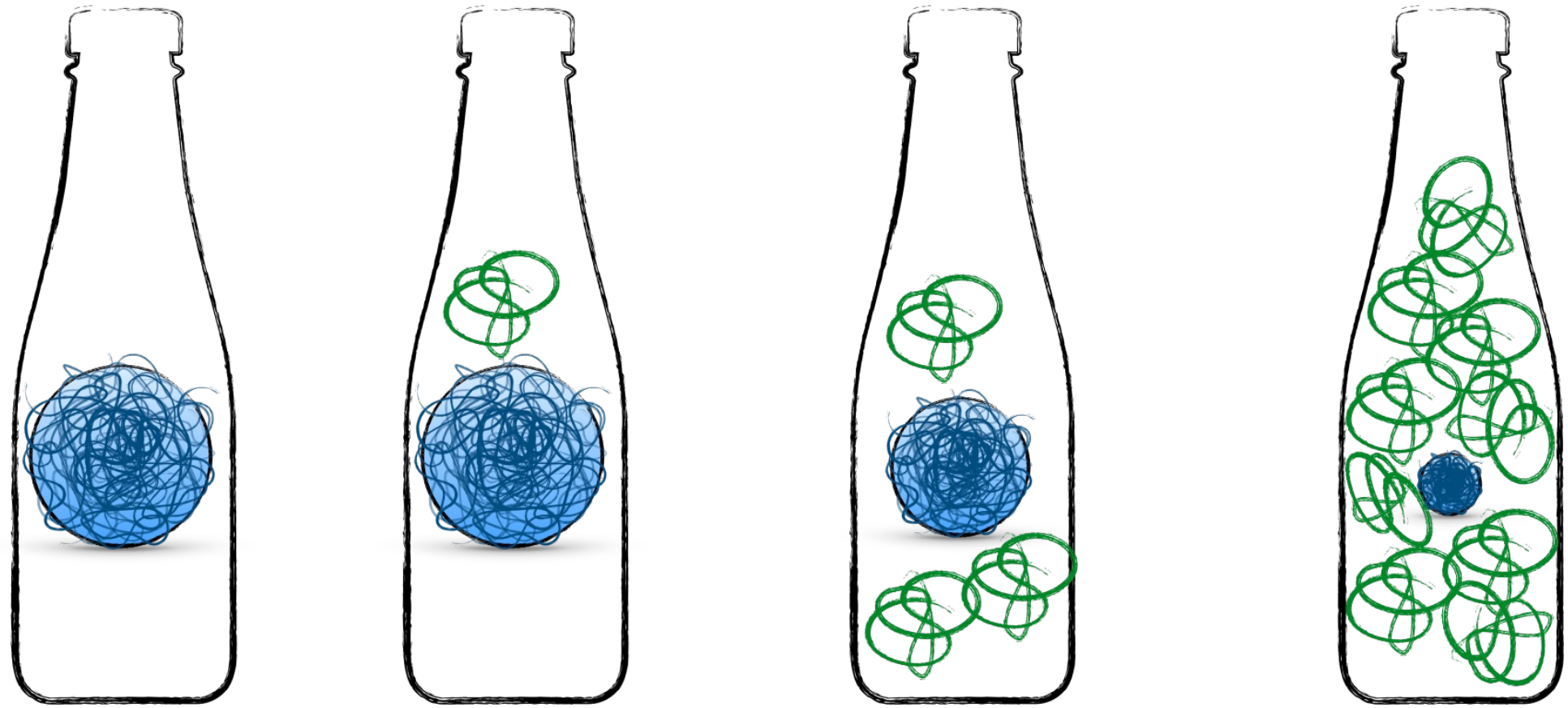
$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$

Neutrons see differently
hydrogen and deuterium!

We can change the contrast using
deuterated polymers
and mixing H₂O and D₂O as solvents.



Osmotic stress solutions for small colloids



Concentration osmotic stress polymer

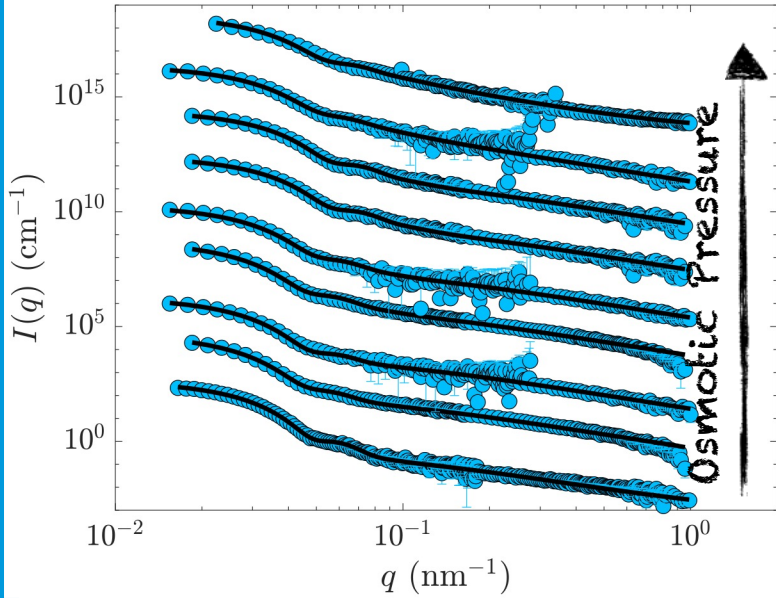
Now we see only the colloids!



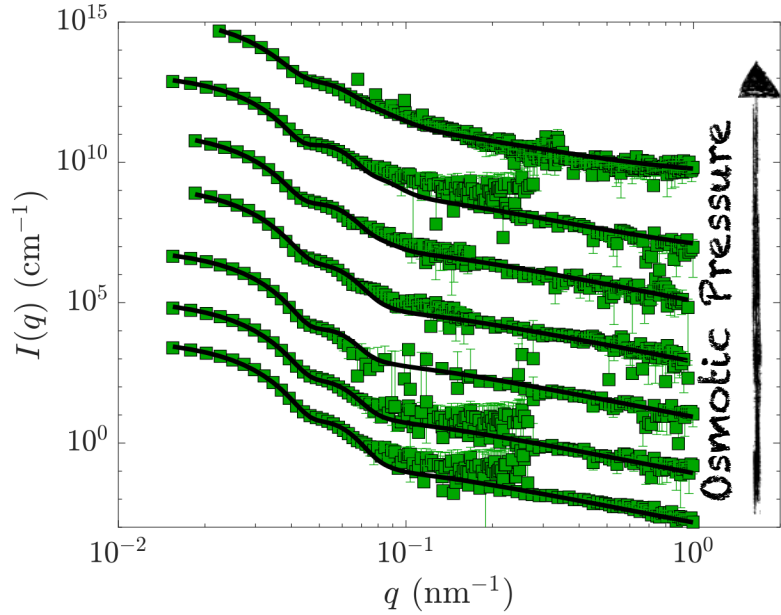
Concentration osmotic stress polymer

How do we measure the elastic moduli?

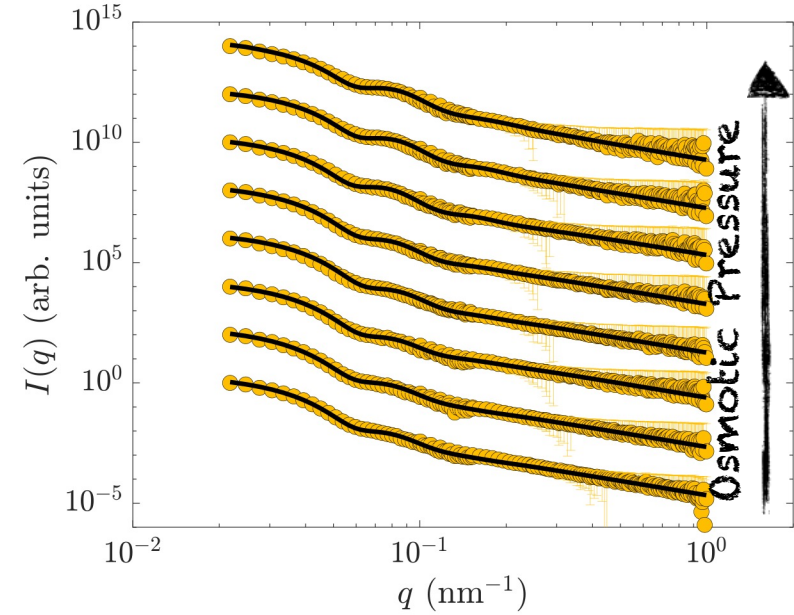
Ultra-soft



Hard

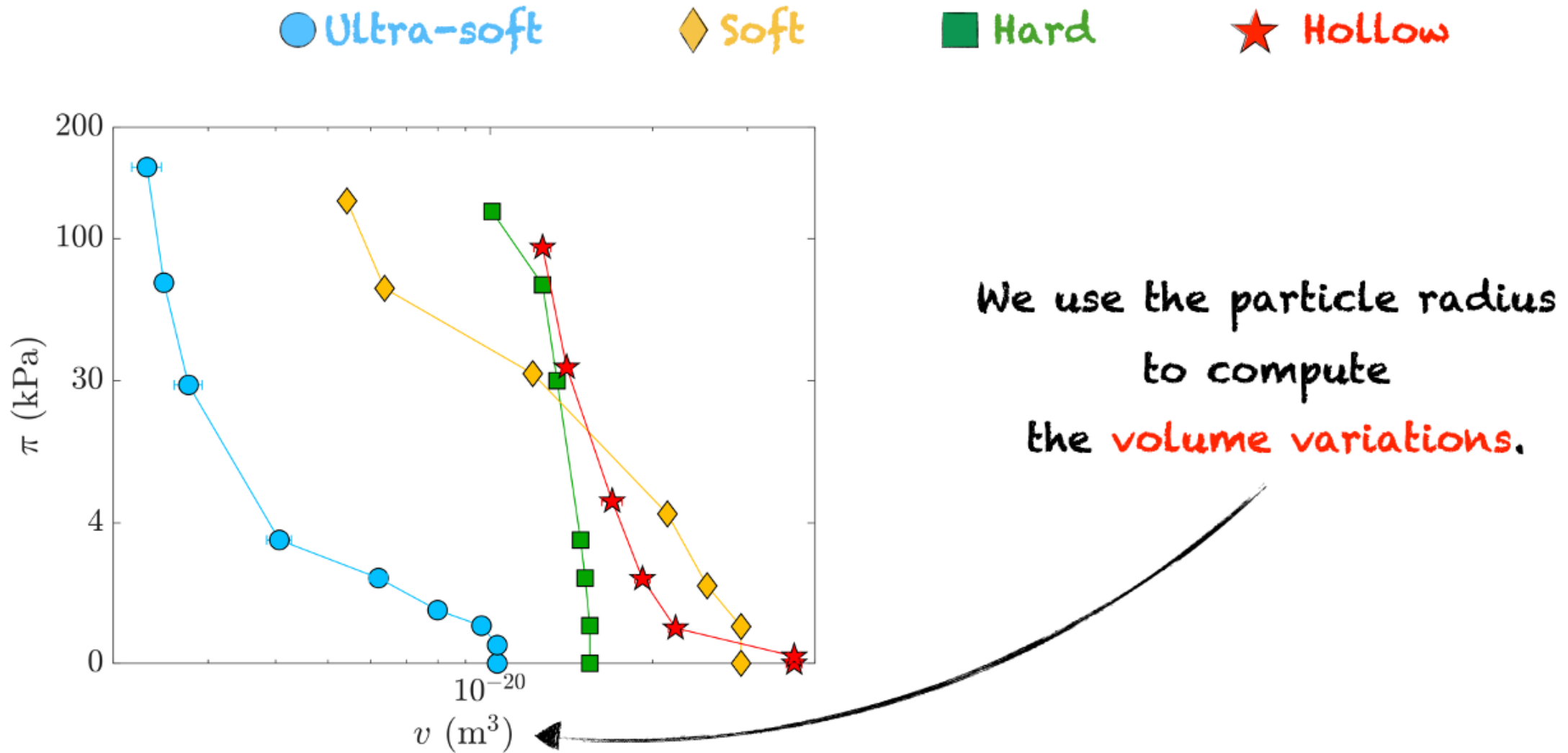


Hollow



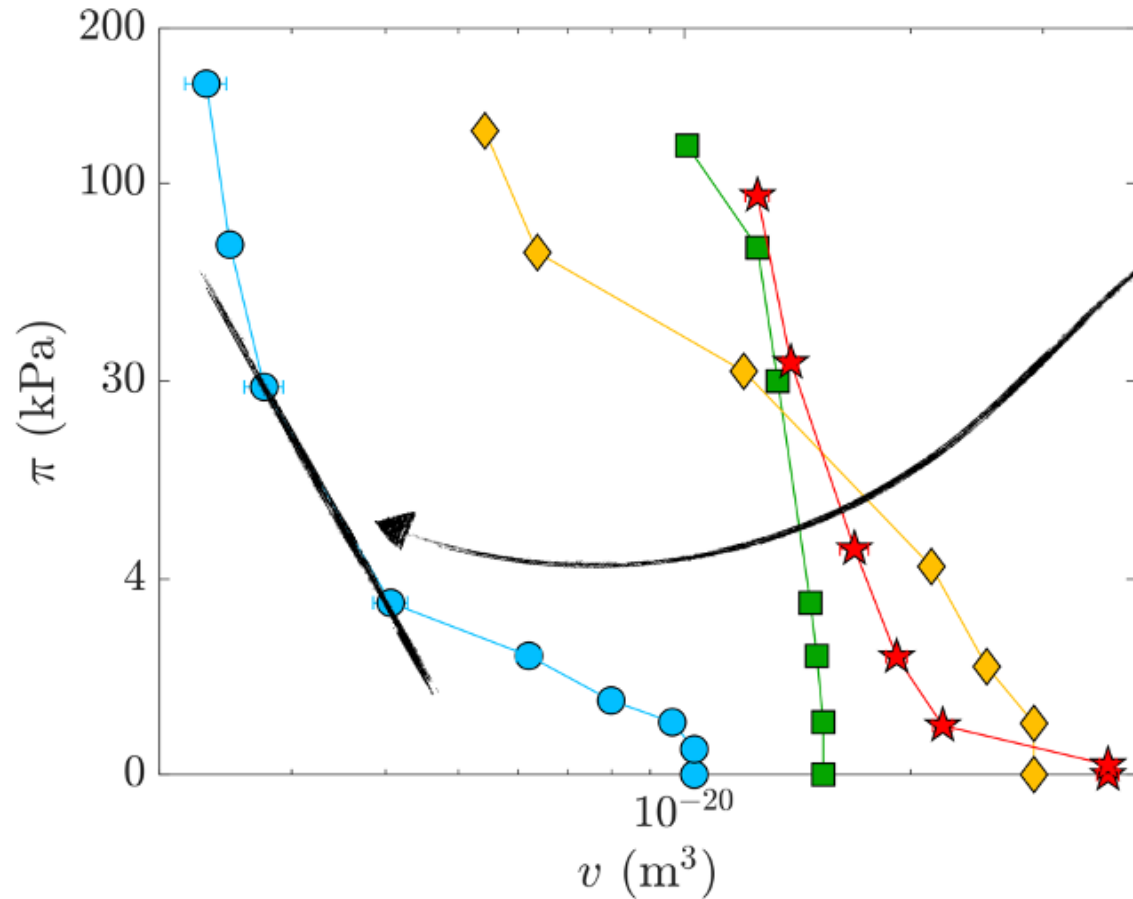
We probe a **larger range of pressures** (contrast-variation)
and we can obtain the **characteristic lengths**.

An unusual representation of the results



An unusual representation of the results

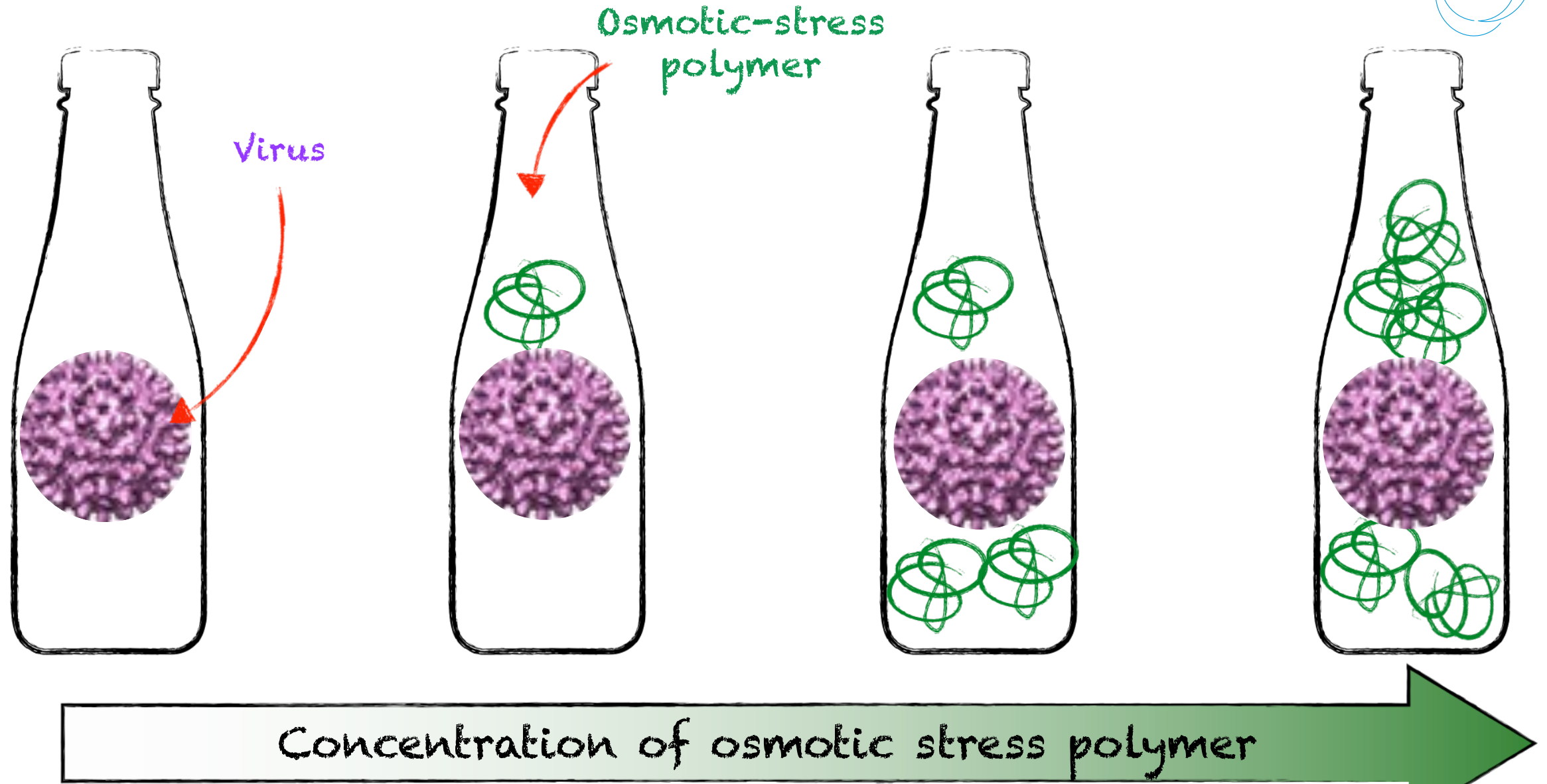
● Ultra-soft
 ◆ Soft
 ■ Hard
 ★ Hollow



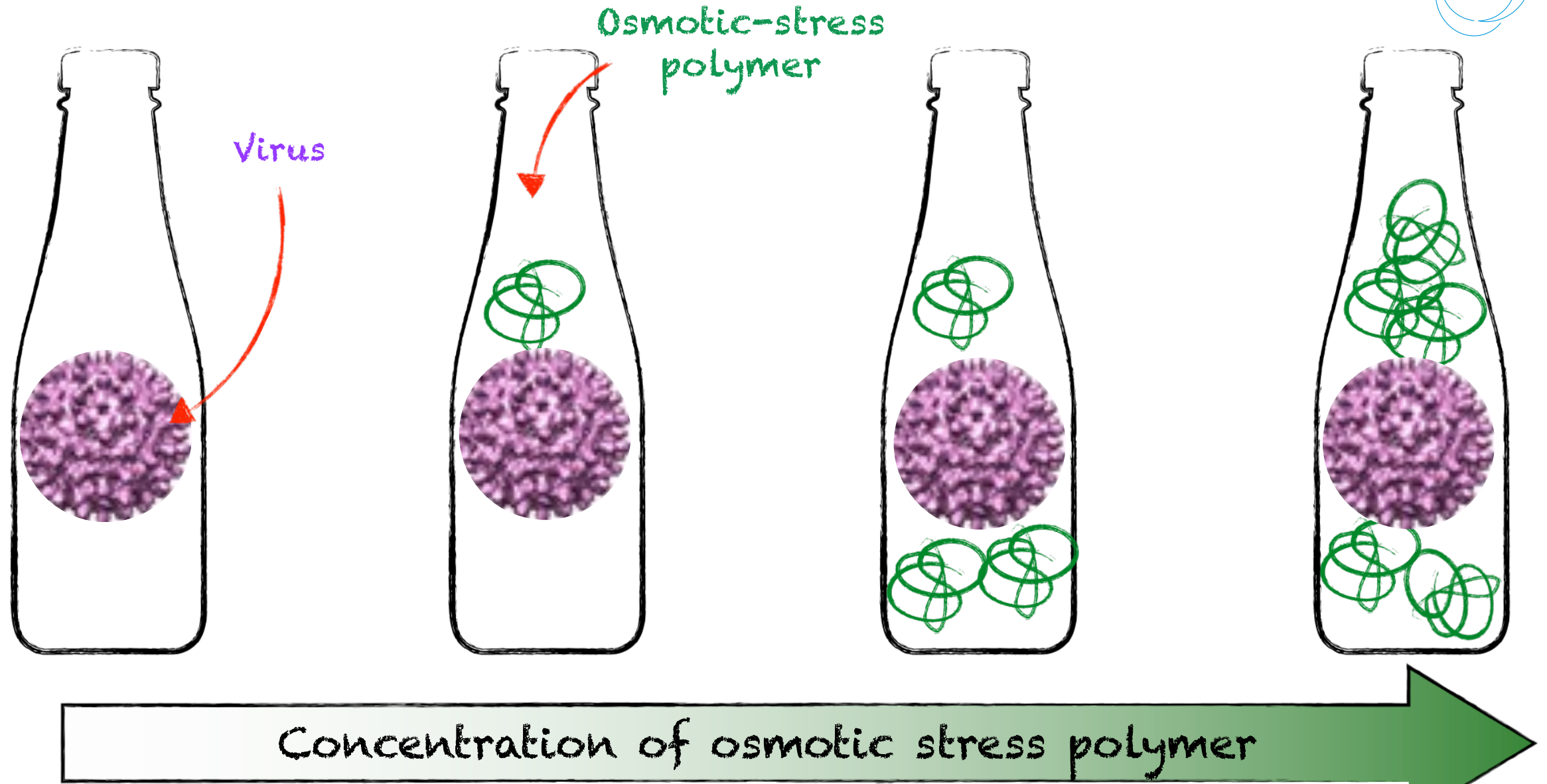
The (local) slope gives the bulk modulus:

$$K = -v \frac{d\pi}{dv}$$

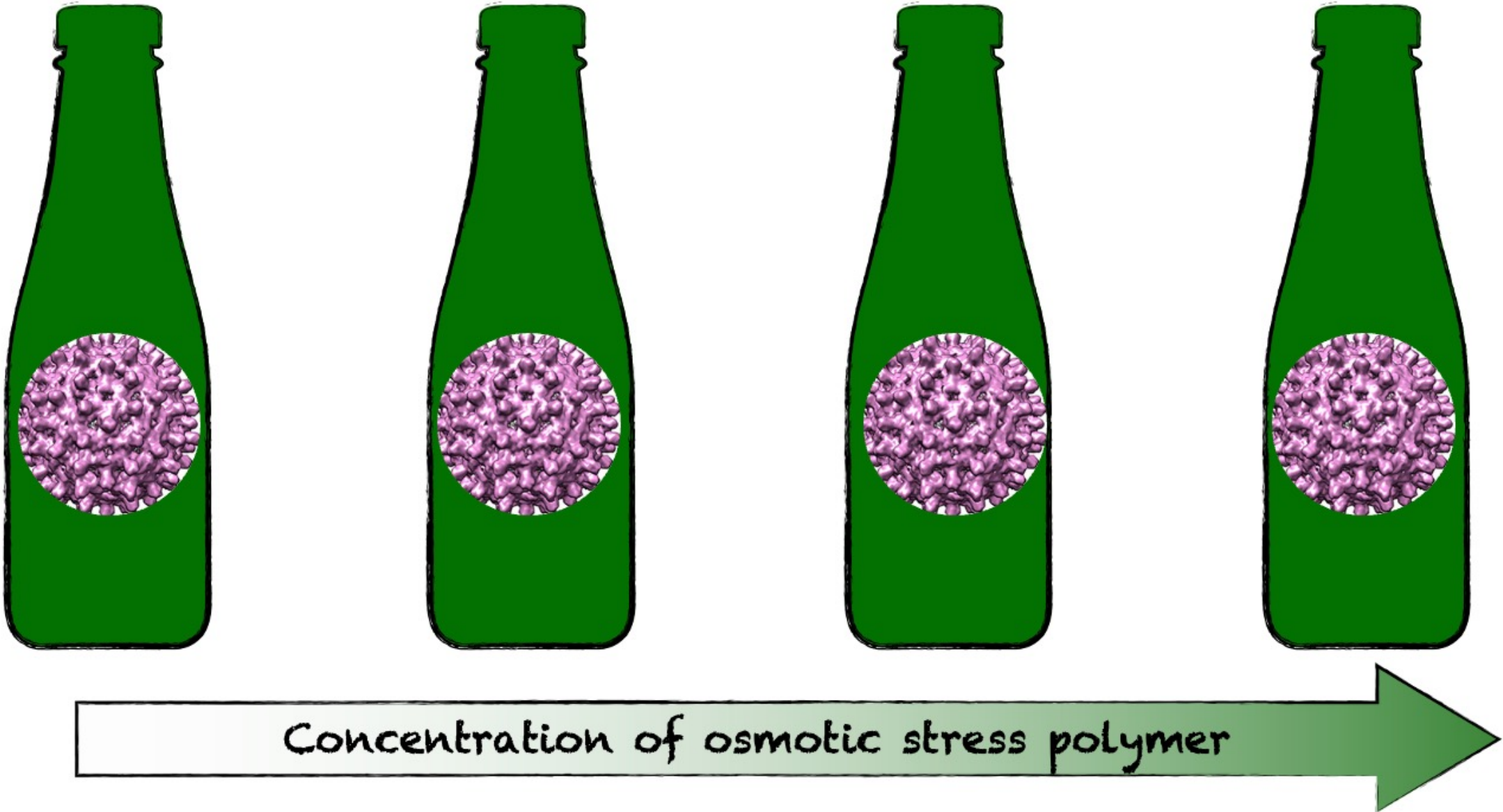
Bio-colloids and osmotic stress



Bio-colloids and osmotic stress



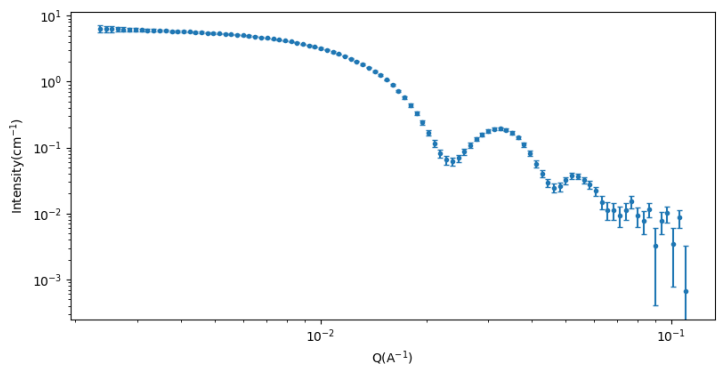
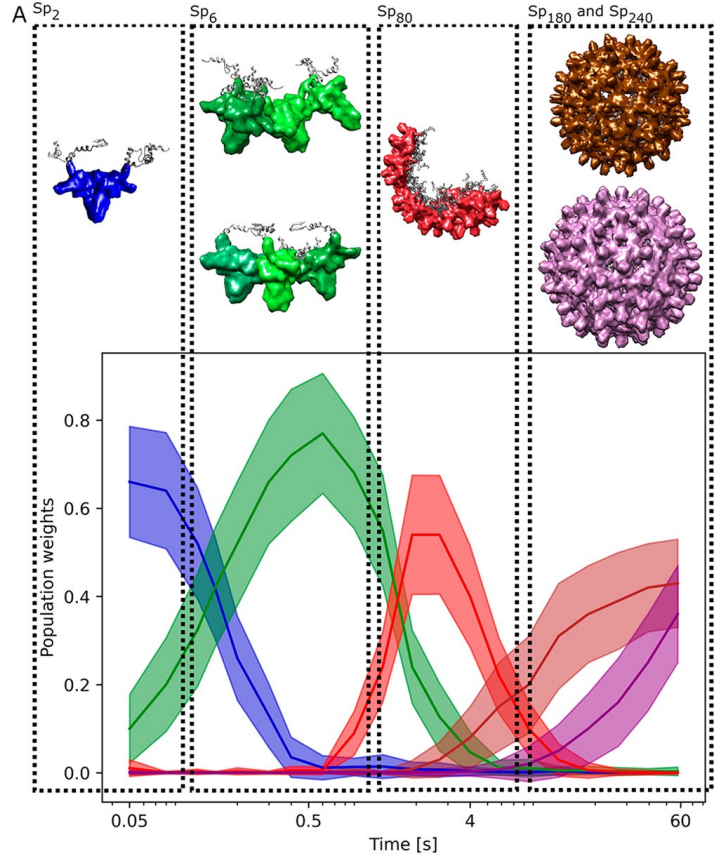
Bio-colloids and osmotic stress, contrast





Interesting also for bio-relevant colloids

Explore the effects of different osmotic stress on the final architecture of the viral capsid and the self-assembly.



I. André (LU, Sweden)

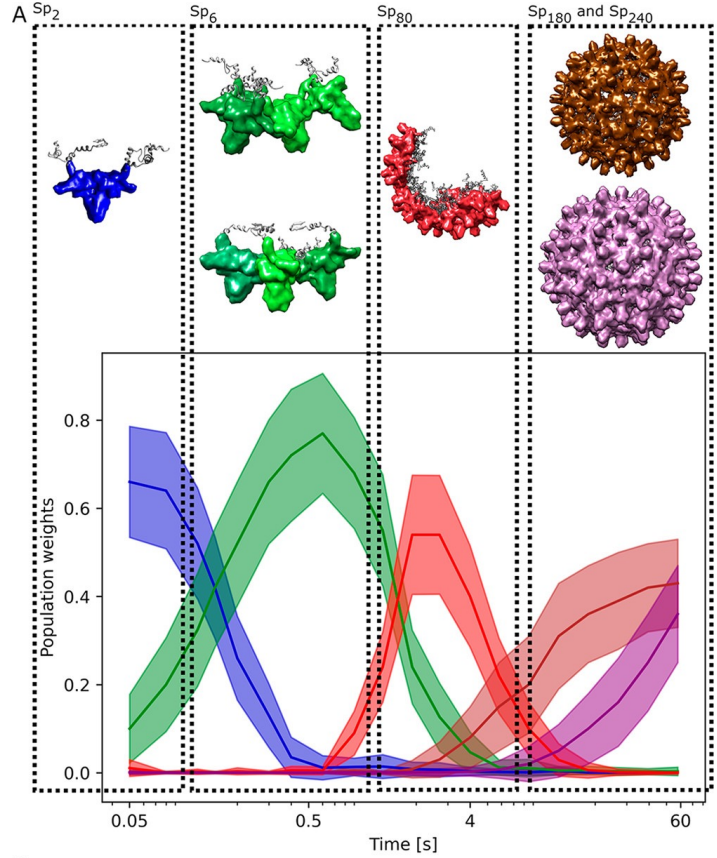


W. Potrzebowski (ESS, Sweden)



A. Scotti (Lund/Malmö, Sweden)

Interesting also for bio-relevant colloids



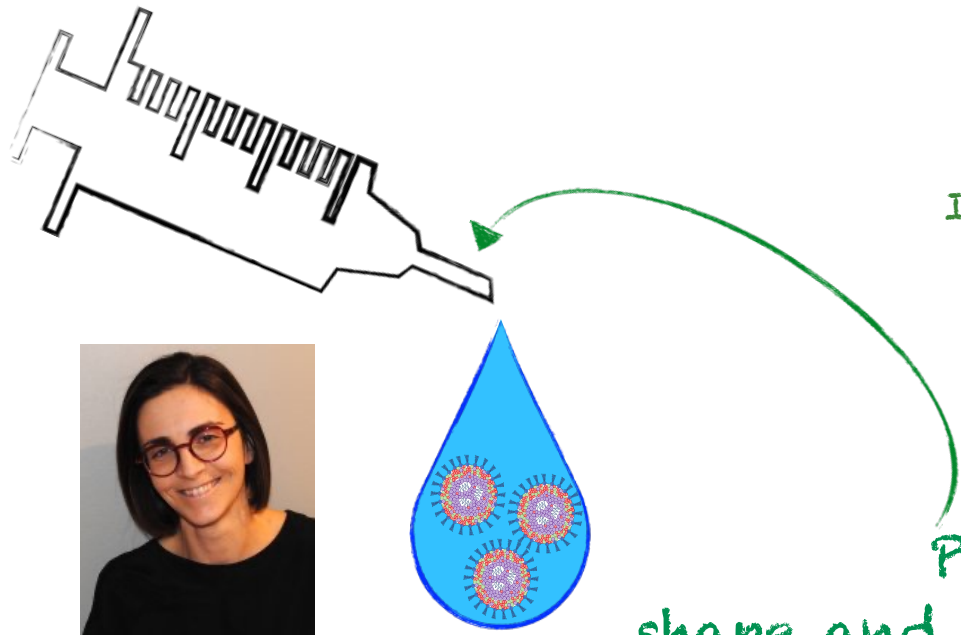
← Explore the effects of different osmotic stress on the final architecture of the viral capsid and the self-assembly.



I. André (LU, Sweden)

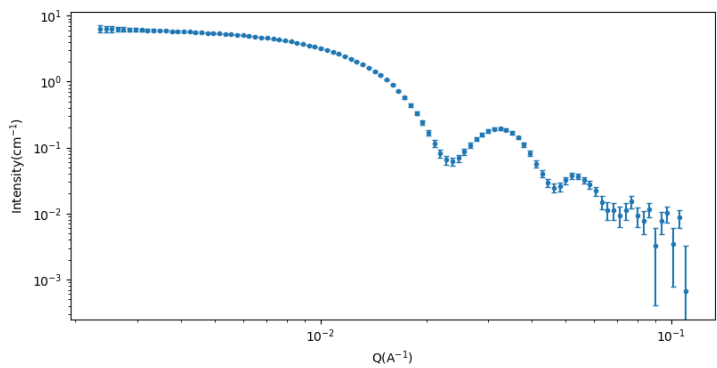


W. Potrzebowski (ESS, Sweden)



F. Sebastiani (Copenhagen Uni, Denmark)

Probe the shape and internal structure of lipid nanoparticles under different osmotic stress.



CATTERING



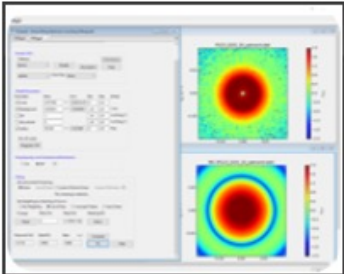
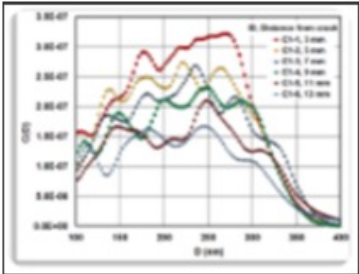
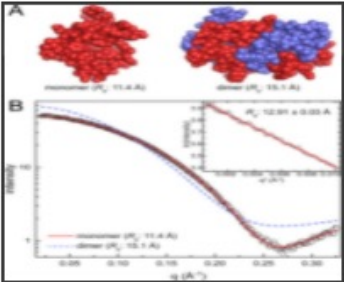
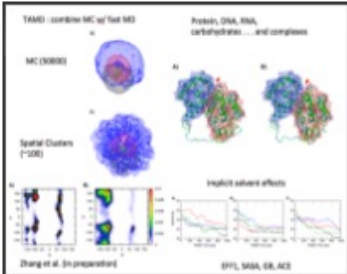
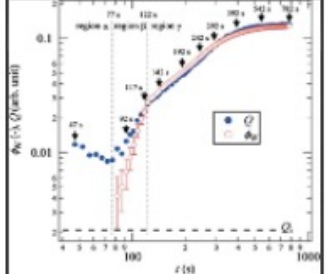
5

Small-Angle Scattering Data Analysis

Data analysis

Few different options for SAS data

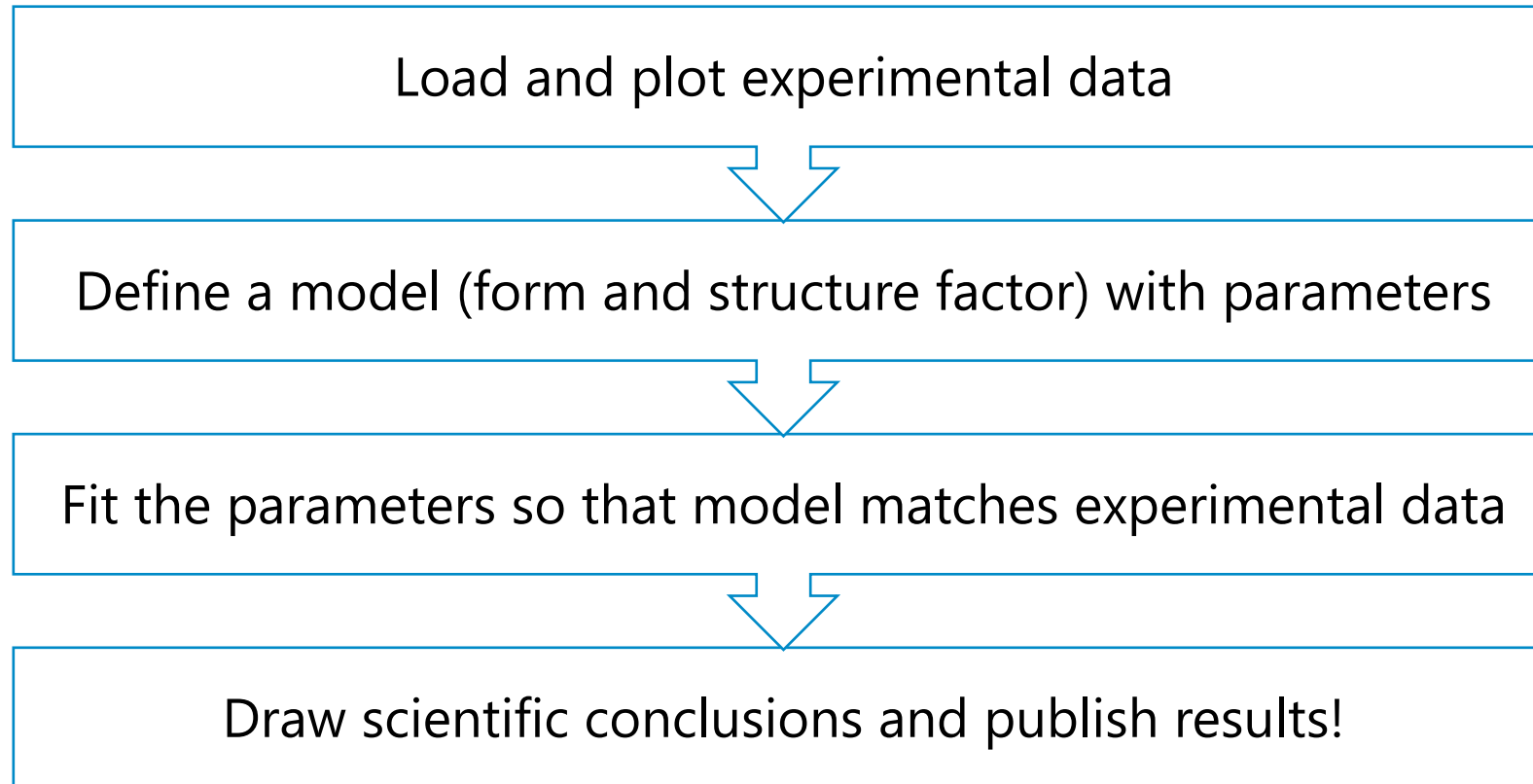


Model-Fitting Methods	Real-Space Methods	<i>Ab-Initio</i> Methods	MC/MD Methods	Other Methods
 <p>Example of 2D model-fitting using the SasView application</p>	 <p>Cavity size distributions in a steel weldment as derived from SANS 10.1179/1743284714Y.0000000577</p>	 <p><i>Ab-initio</i> modelling of polcalcin constrained by SAXS 10.1002/pro.3376</p>	 <p>MC & TAMD modelling of proteins constrained by SANS 10.1016/j.jmgs.2017.02.010</p>	 <p>Time evolution of the invariant during crystallisation of P4MP1 10.1038/pj.2012.204</p>

<https://www.isis.stfc.ac.uk/Pages/SANSdataanalysisOverview.aspx>

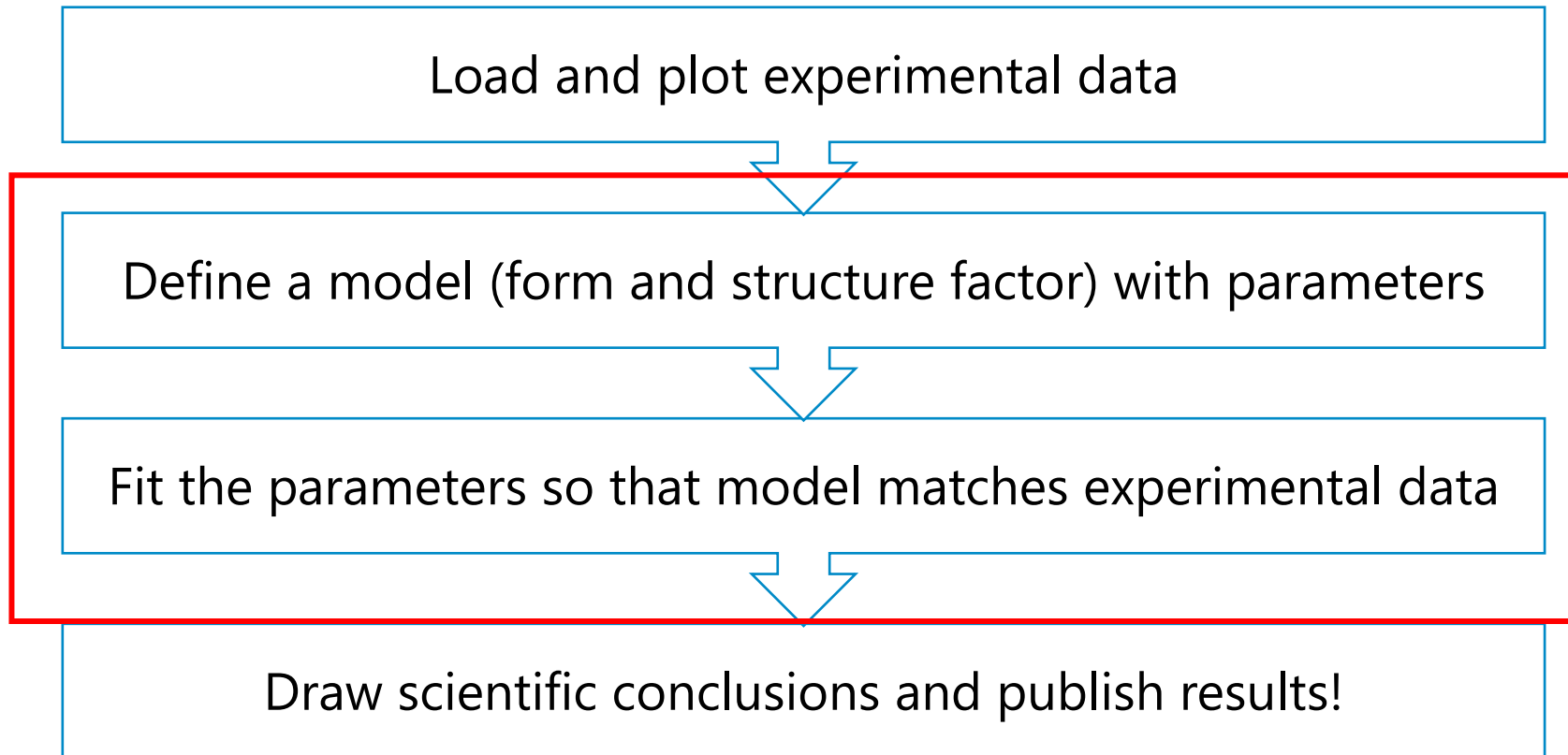
Typical data fitting workflow

For reduced data:



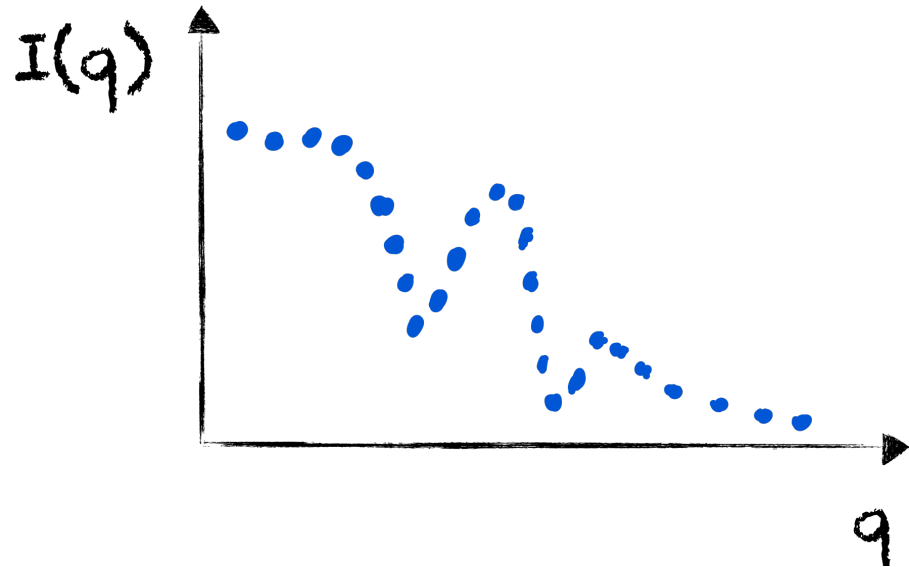
Typical data fitting workflow

For reduced data:



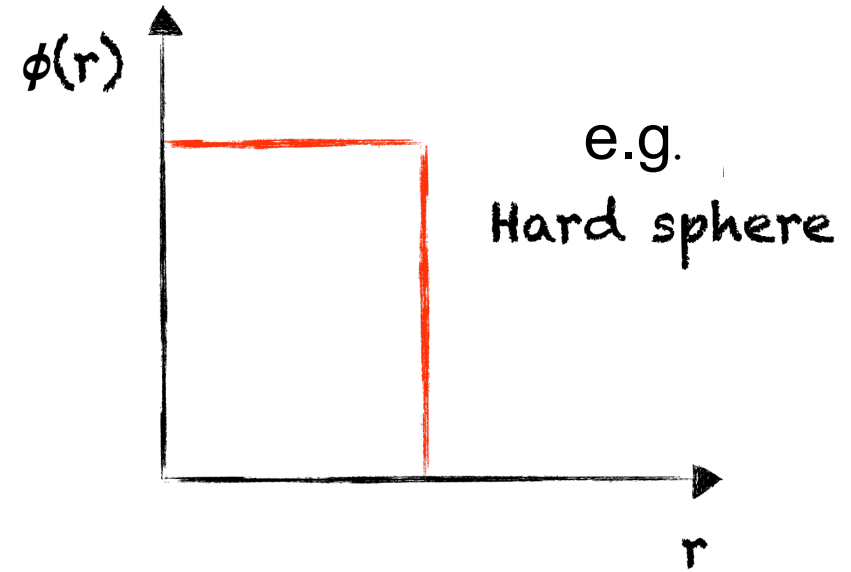
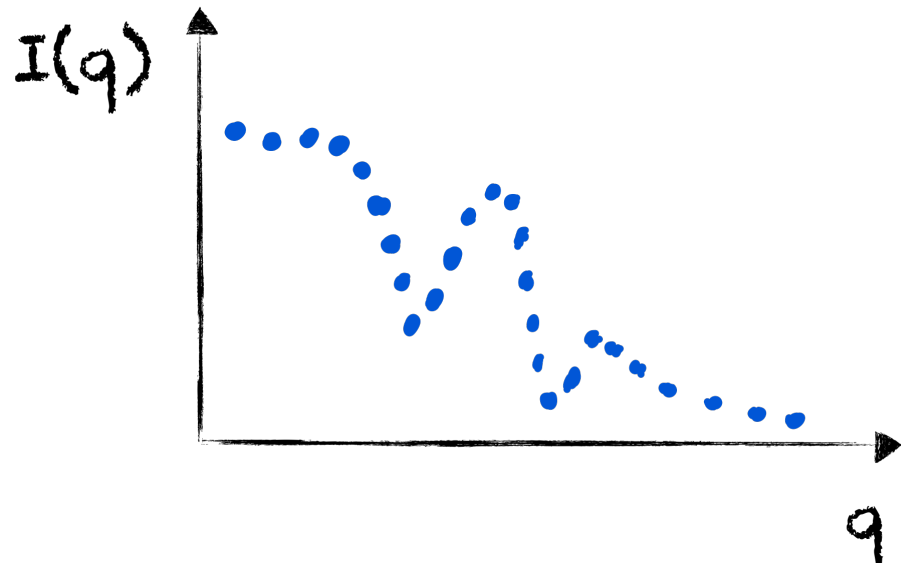
What is data fitting for SAS?

Experiment
(dilute suspension)



What is data fitting for SAS?

Experiment
(dilute suspension)

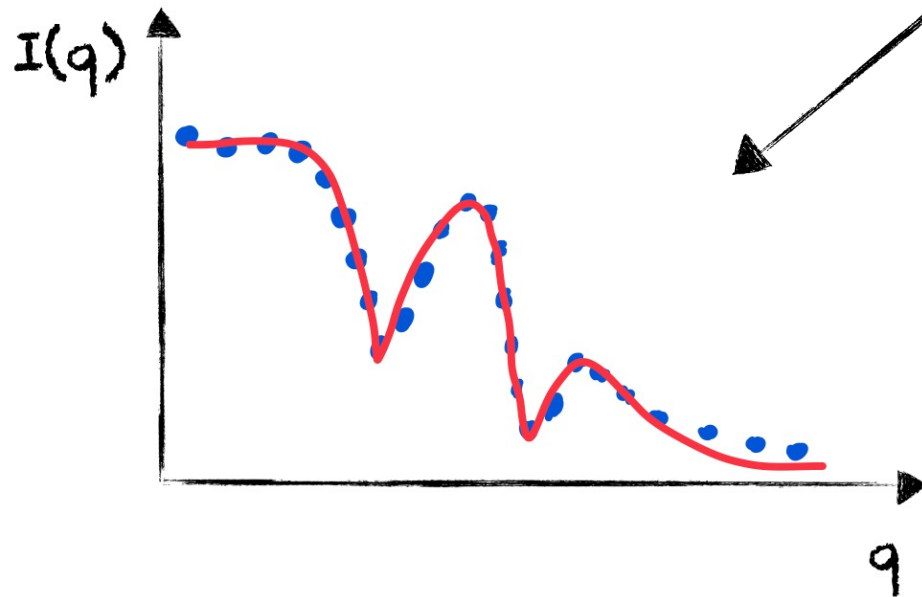


Idea of a model

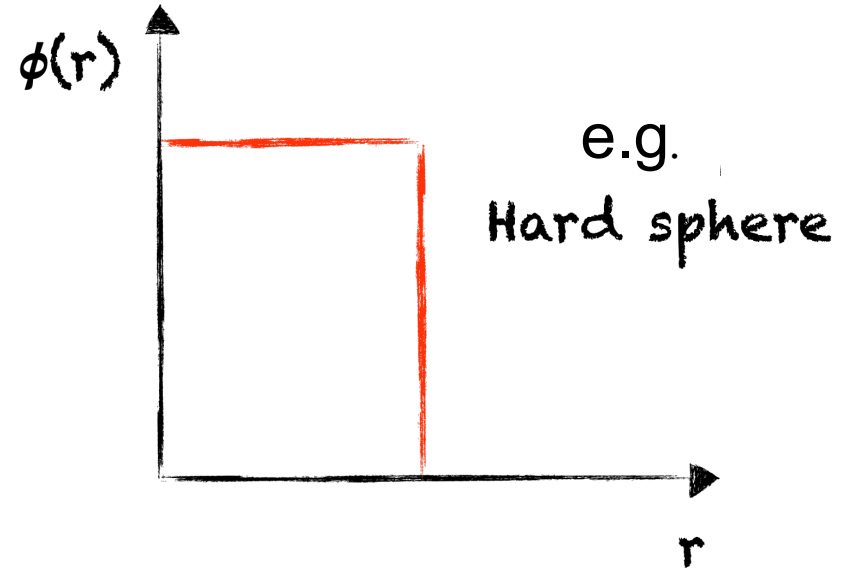
What is data fitting for SAS?

Model 1

Experiment
(dilute suspension)



Fit the data and obtain
characteristic lengths

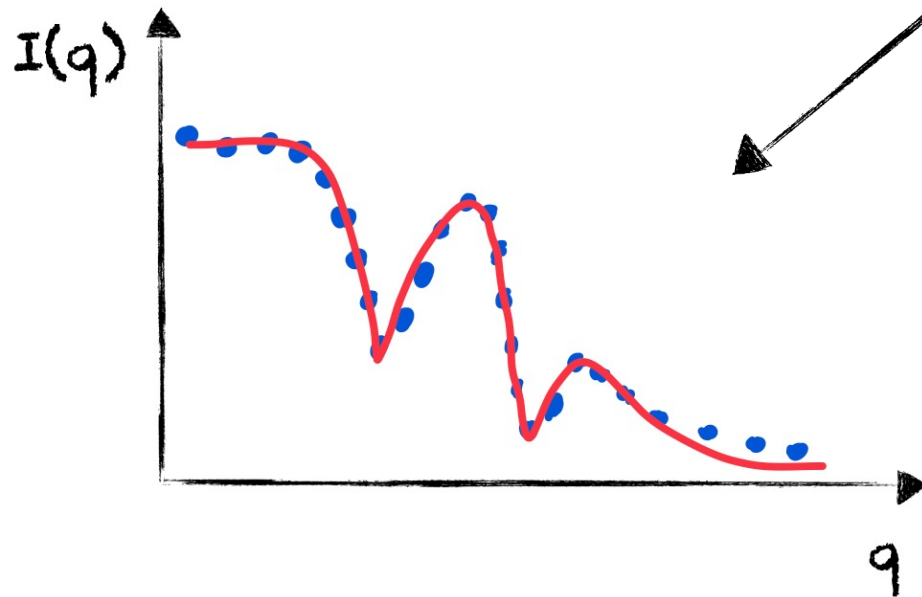


Idea of a model

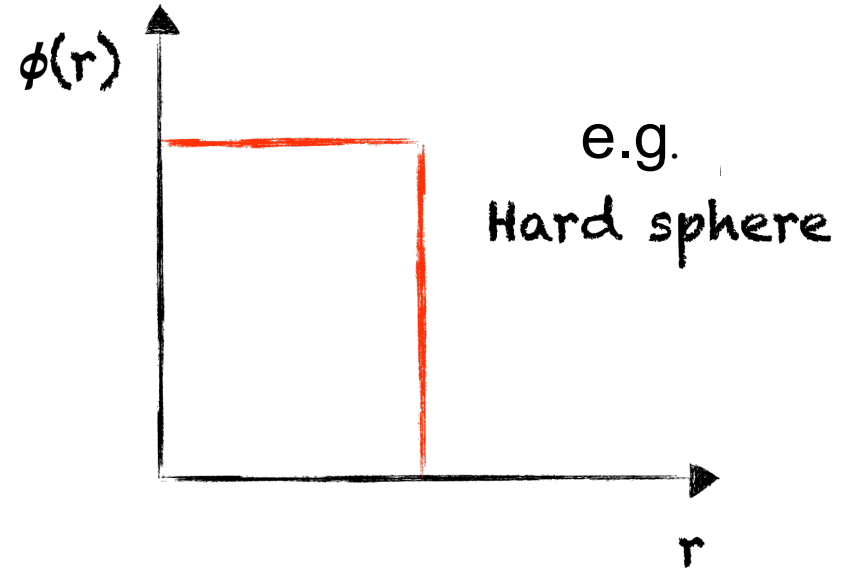
What is data fitting for SAS?

Model 1

Experiment
(dilute suspension)



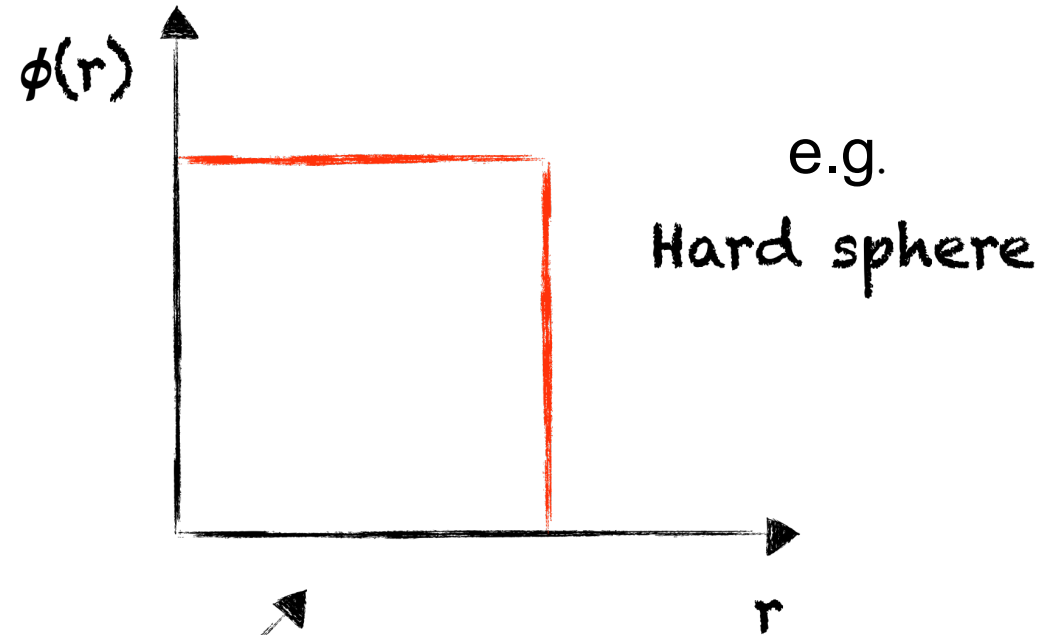
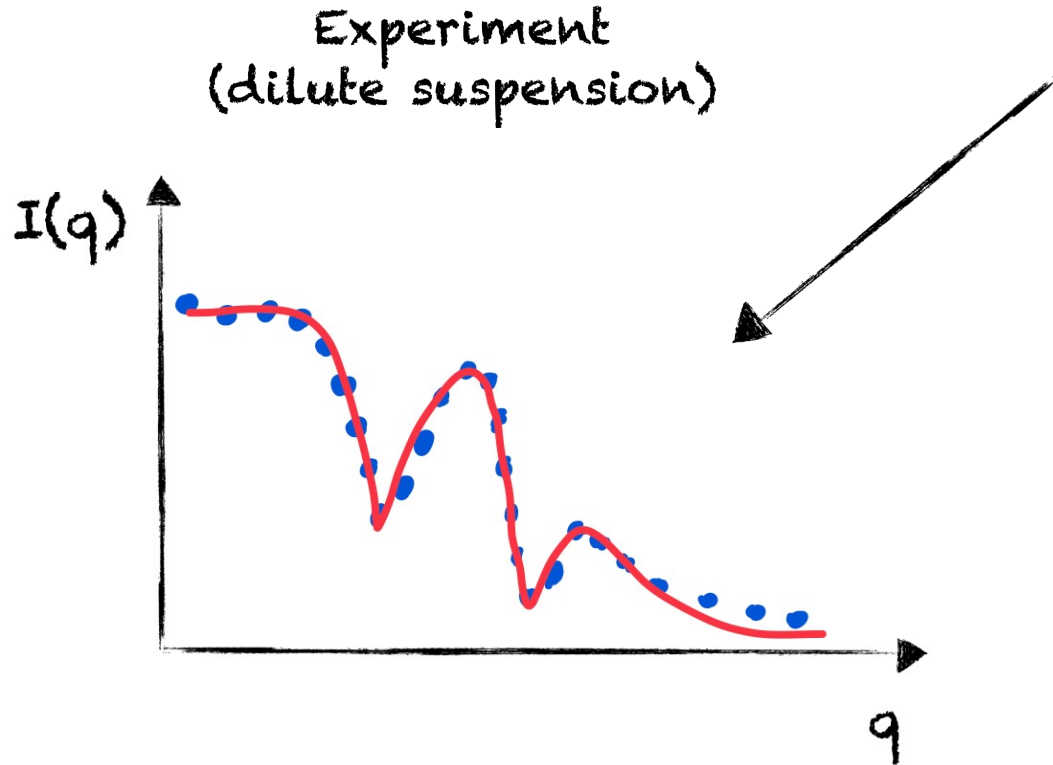
Fit the data and obtain
characteristic lengths



Idea of a model

What is data fitting for SAS?

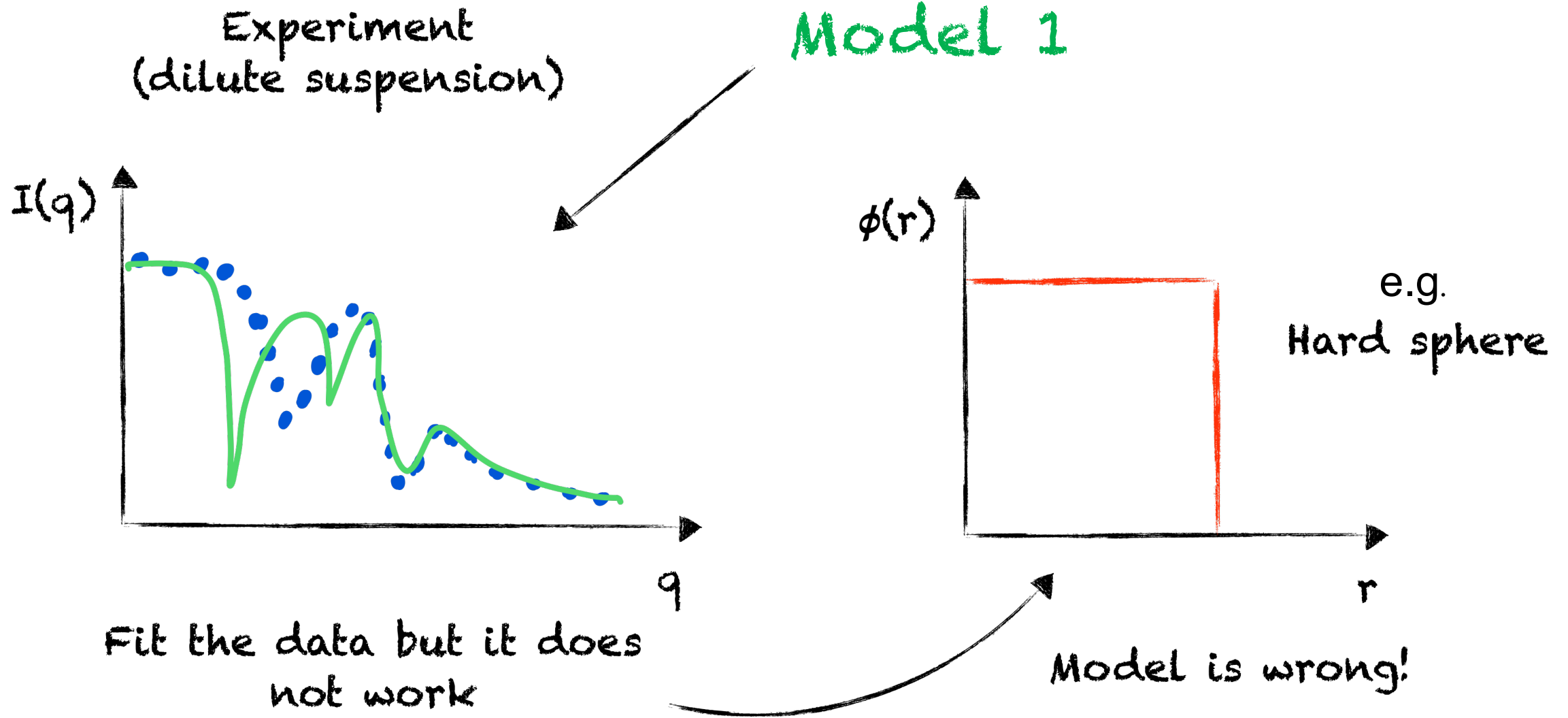
Model 1



Fit the data and obtain
characteristic lengths

Model is OK!

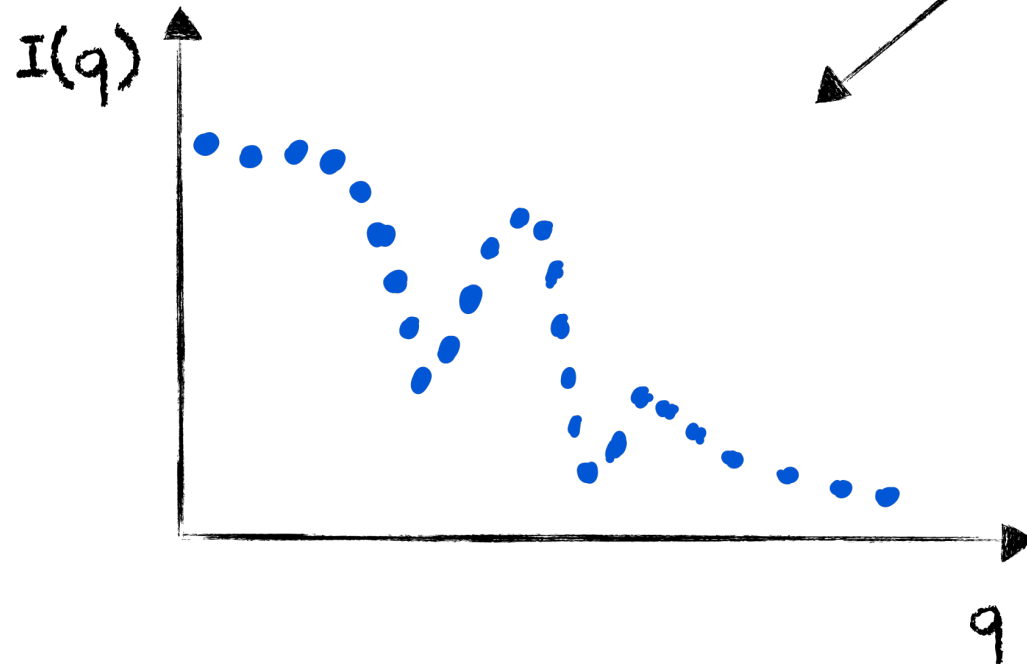
What is data fitting for SAS?



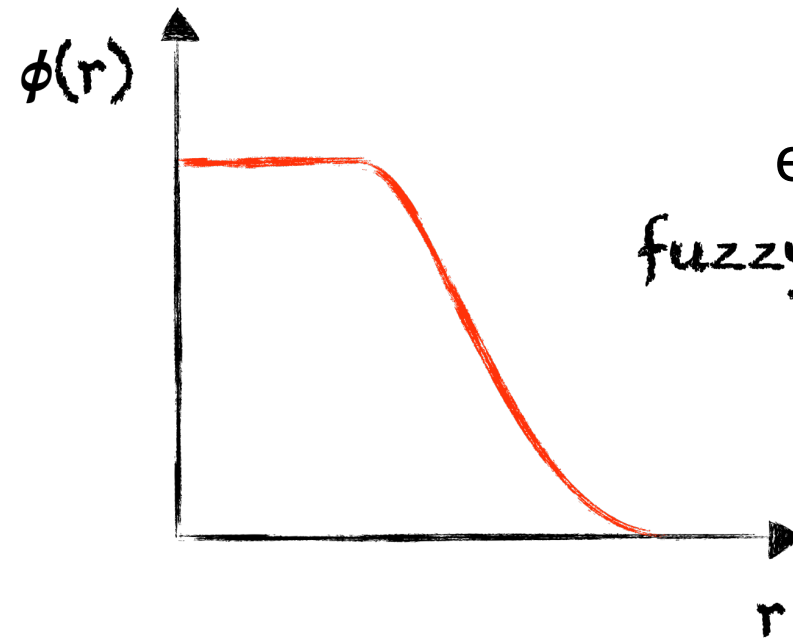
What is data fitting for SAS?

Experiment
(dilute suspension)

Model 2



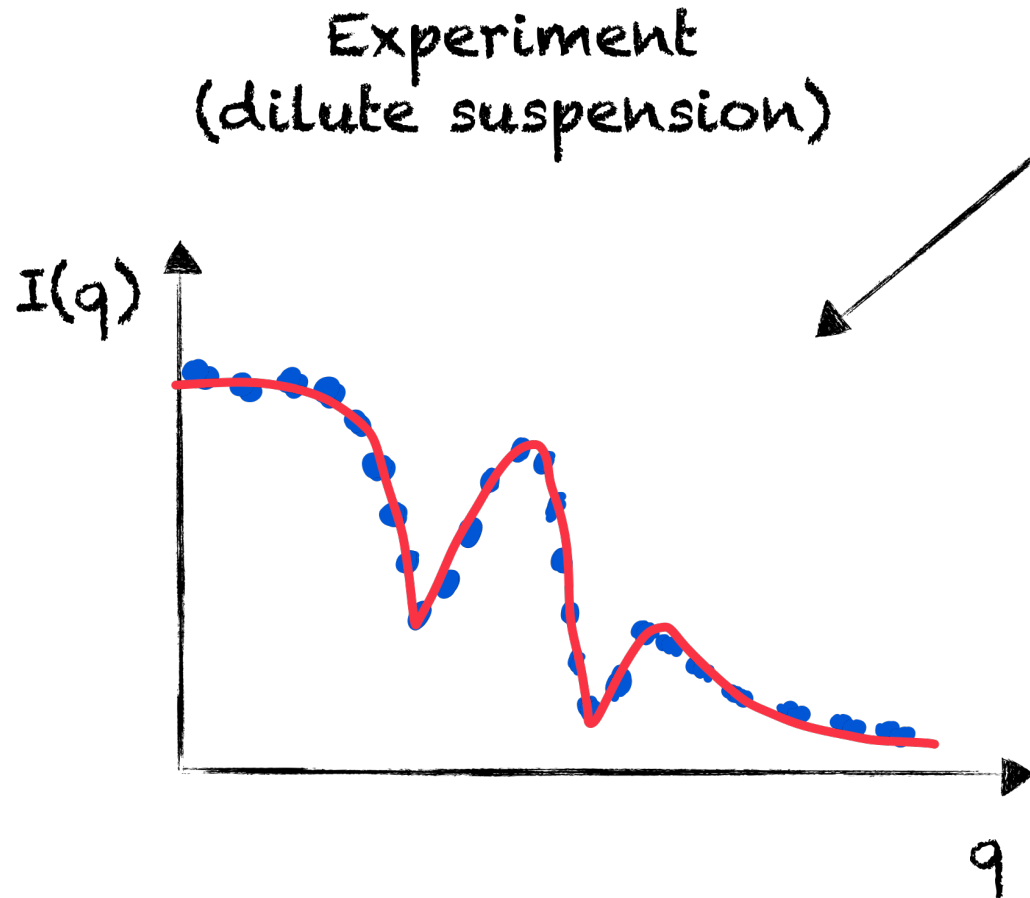
Fit the data and obtain
characteristic lengths



e.g.
fuzzy sphere

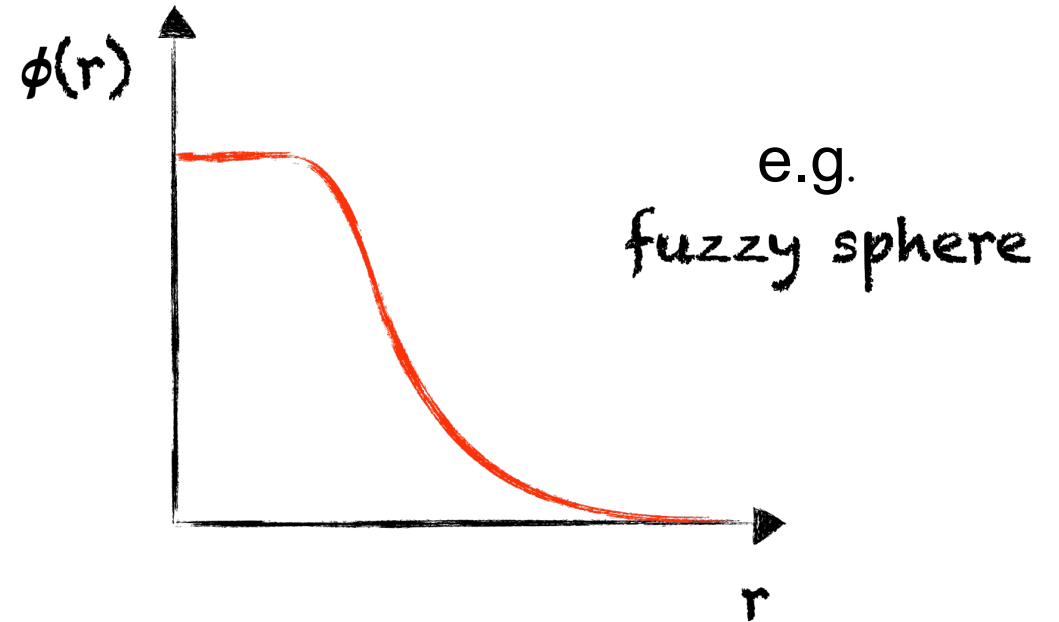
New model!

What is data fitting for SAS?



Fit the data and obtain characteristic lengths

Model 2



Model is OK!

Fitting in SasView

70+ models to explain data



Wide choice of built-in models (> 70)
F(Q), S(Q) & F(Q)*S(Q)

Single, batch and simultaneous
1D and 2D fitting

The screenshot shows the SasView 5.0.6 interface. On the left, the 'Data Explorer' panel shows a list of data files, with '2% SDS in D2O_SANS' selected. The main panel displays the 'FitPage3' window for the 'ellipsoid' model. The 'Model' section shows a table of parameters:

Parameter	Value	Error	Min	Max
ellipsoid				
<input type="checkbox"/> sld	2.2256		-∞	∞
<input type="checkbox"/> sld...	6.39		-∞	∞
<input checked="" type="checkbox"/> radi...	17.22	1.0248	0.0	∞
<input checked="" type="checkbox"/> radi...	21.14	0.58958	0.0	∞
hayter_...				
<input type="checkbox"/> radi...	19.817		0.0	∞
<input checked="" type="checkbox"/> volfr...	0.016792	0.00018291	0.0	0.74
<input checked="" type="checkbox"/> char...	20.607	0.40757	1e-06	200.0
<input type="checkbox"/> tem...	298		0.0	450.0
<input type="checkbox"/> con...	0.0		0.0	∞
<input checked="" type="checkbox"/> diel...	78.06		-∞	∞

The 'Options' section shows 'Polydispersity' and 'Magne' checkboxes. The 'Fitting details' section shows 'Min range 0.009 Å⁻¹' and 'Max range 0.281 Å⁻¹'. The 'Fitting error' section shows 'χ² 0.85246'. On the right, the 'Graph4' window shows two plots: 'Intensity(cm⁻¹)' vs 'Q(Å⁻¹)' and 'Residuals(normaliz)' vs 'Q(Å⁻¹)'. The top plot shows a log-log plot of intensity with data points and a fit line. The bottom plot shows a linear plot of residuals.

Data management
Common data formats
supported, including
NXCansas & cansas1D

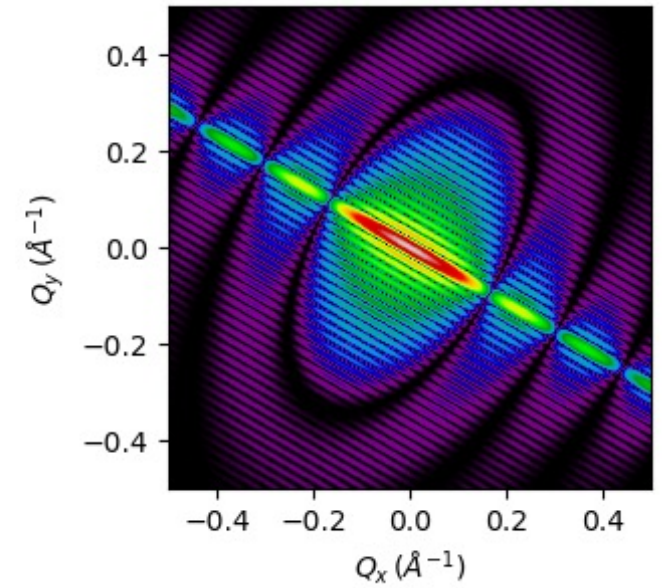
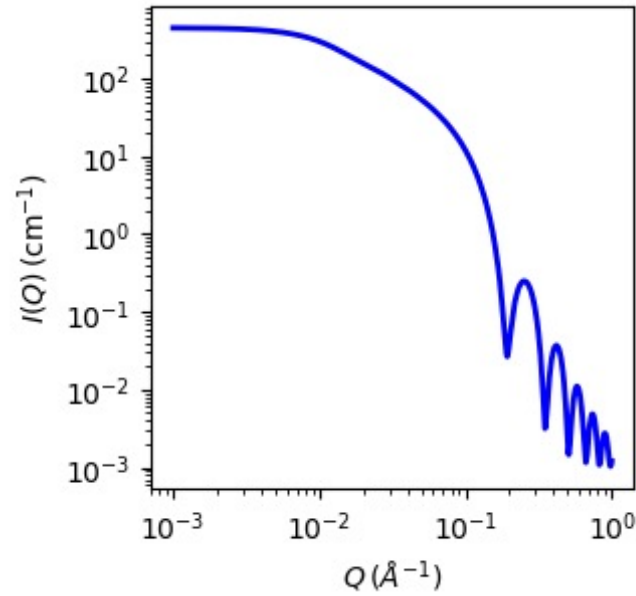
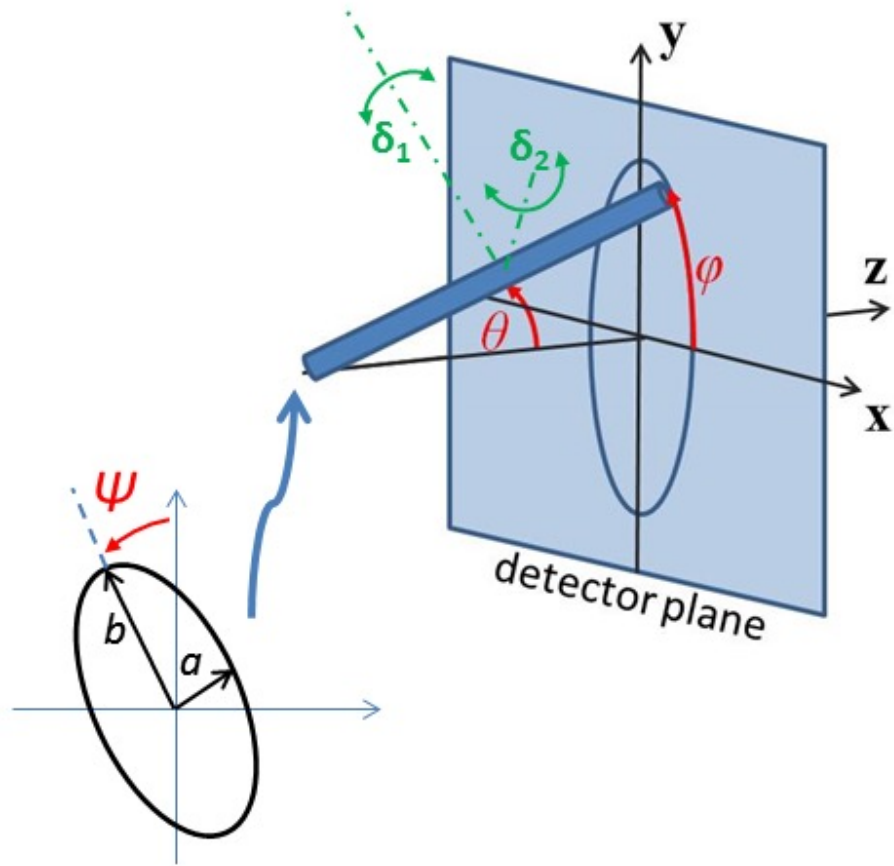
Analysis Tool Choice
&
Plotting

Polydispersity (choice of distribution and
distribution parameters)

Resolution smearing (pinhole and slit)
Automatically from data or provide parameters

2D fitting

For oriented or magnetic particles

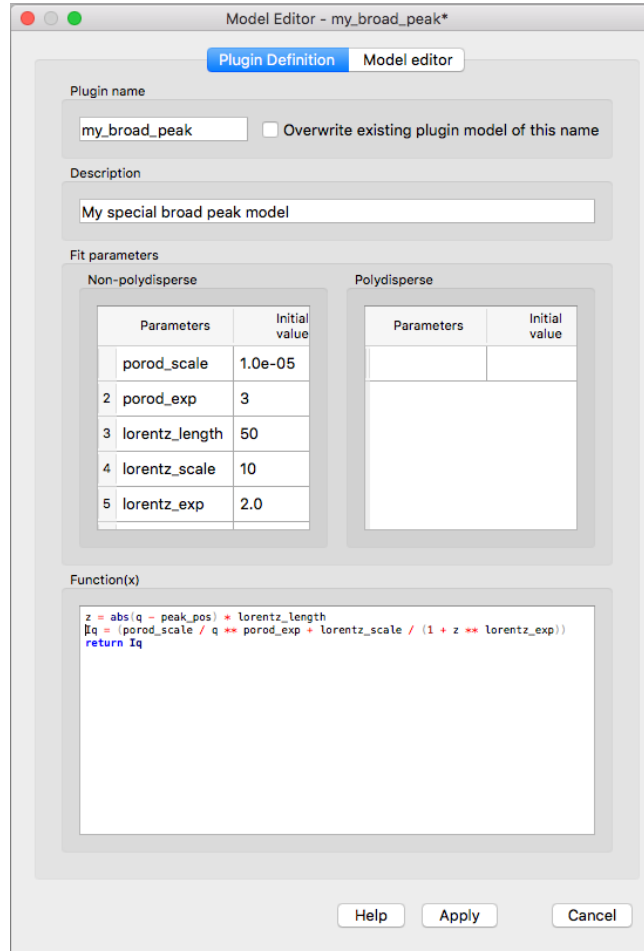


1D and 2D cylinder model

Plugin models

SasView provides tools and infrastructure for custom/plugin models

- Dedicated editor
- Syntax and performance testing
- Directly available in SasView ecosystem
- Community developed models can be deposited to marketplace: <https://marketplace.sasview.org/>



Model Editor - my_broad_peak*

Plugin Definition | Model editor

Plugin name: my_broad_peak Overwrite existing plugin model of this name

Description: My special broad peak model

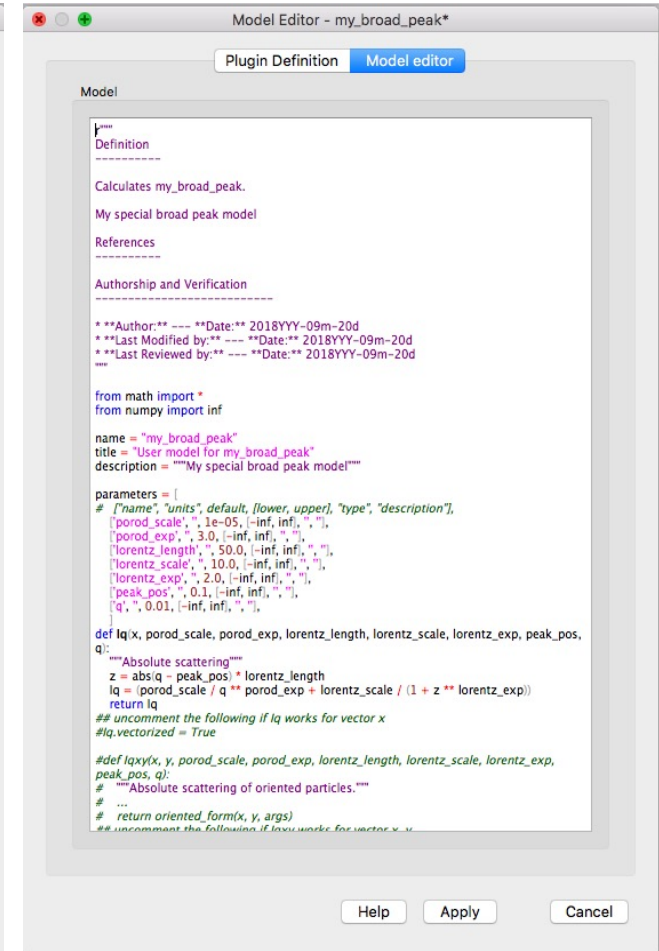
Fit parameters

Non-polydisperse		Polydisperse	
Parameters	Initial value	Parameters	Initial value
porod_scale	1.0e-05		
2 porod_exp	3		
3 lorentz_length	50		
4 lorentz_scale	10		
5 lorentz_exp	2.0		

Function(x)

```
z = abs(q - peak_pos) * lorentz_length
Iq = (porod_scale / q ** porod_exp + lorentz_scale / (1 + z ** lorentz_exp))
return Iq
```

Buttons: Help, Apply, Cancel



Model Editor - my_broad_peak*

Plugin Definition | Model editor

Model

```
"""
Definition
-----
Calculates my_broad_peak.
My special broad peak model
References
-----
Authorship and Verification
-----
**Author:** --- **Date:** 2018YYY-09m-20d
**Last Modified by:** --- **Date:** 2018YYY-09m-20d
**Last Reviewed by:** --- **Date:** 2018YYY-09m-20d
"""

from math import *
from numpy import inf

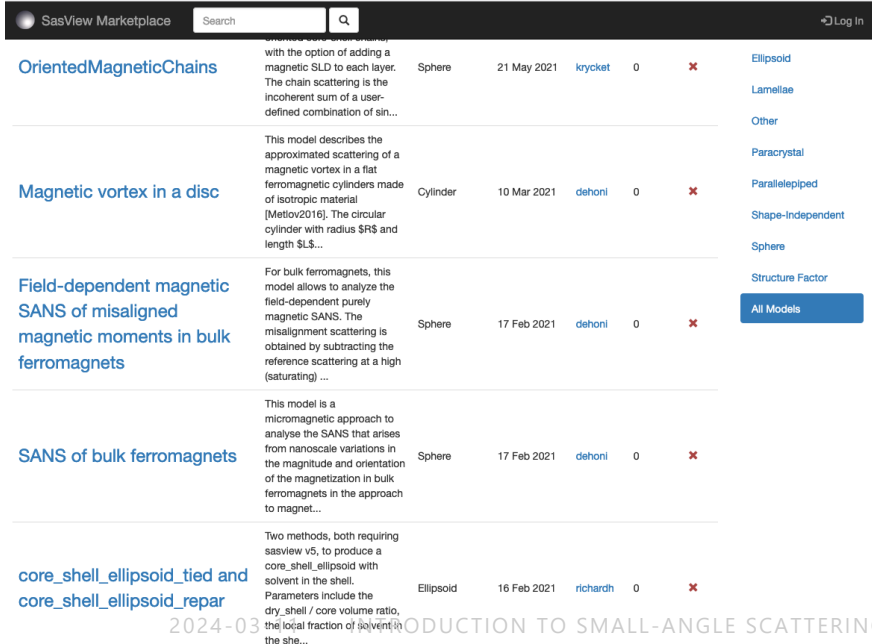
name = "my_broad_peak"
title = "User model for my_broad_peak"
description = ""My special broad peak model""

parameters = [
    # ["name", "units", "default", "lower", "upper", "type", "description"],
    ["porod_scale", "1", 1e-05, [-inf, inf], "r", ""],
    ["porod_exp", "3", 3.0, [-inf, inf], "r", ""],
    ["lorentz_length", "50", 50.0, [-inf, inf], "r", ""],
    ["lorentz_scale", "10", 10.0, [-inf, inf], "r", ""],
    ["lorentz_exp", "2", 2.0, [-inf, inf], "r", ""],
    ["peak_pos", "0.1", 0.1, [-inf, inf], "r", ""],
    ["q", "0.01", [-inf, inf], "r", ""],
]

def Iq(x, porod_scale, porod_exp, lorentz_length, lorentz_scale, lorentz_exp, peak_pos, q):
    """Absolute scattering"""
    z = abs(q - peak_pos) * lorentz_length
    Iq = (porod_scale / q ** porod_exp + lorentz_scale / (1 + z ** lorentz_exp))
    return Iq
    ## uncomment the following if Iq works for vector x
    ##Iq.vectorized = True

def Iqyx(x, y, porod_scale, porod_exp, lorentz_length, lorentz_scale, lorentz_exp, peak_pos, q):
    """Absolute scattering of oriented particles"""
    # ...
    # return oriented_form(x, y, args)
    ## uncomment the following if Iqyx works for vector x, y
```

Buttons: Help, Apply, Cancel



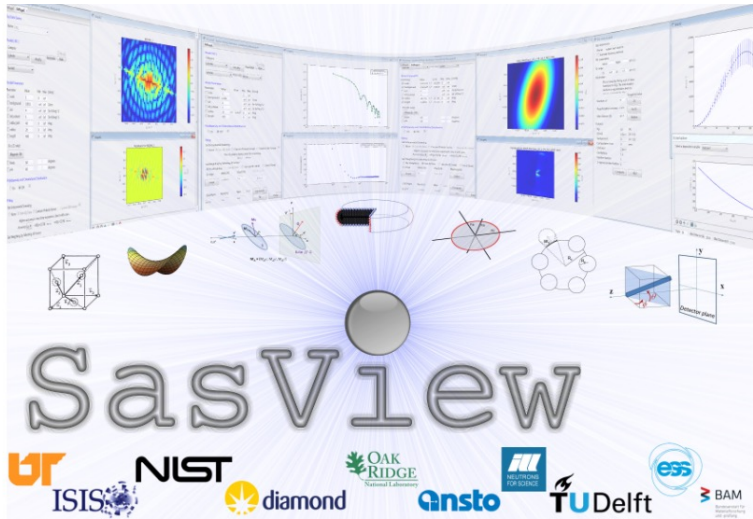
SasView Marketplace

Search [] Log In

Model Name	Description	Shape	Date	Author	Downloads	Rating	Category
OrientedMagneticChains	with the option of adding a magnetic SLD to each layer. The chain scattering is the incoherent sum of a user-defined combination of sin...	Sphere	21 May 2021	krycket	0	✖	Ellipsoid, Lamellae, Other
Magnetic vortex in a disc	This model describes the approximated scattering of a magnetic vortex in a flat ferromagnetic cylinders made of isotropic material [Metov2016]. The circular cylinder with radius SRS and length SLS...	Cylinder	10 Mar 2021	dehoni	0	✖	Paracrystal, Parallelepiped, Shape-Independent
Field-dependent magnetic SANS of misaligned magnetic moments in bulk ferromagnets	For bulk ferromagnets, this model allows to analyze the field-dependent purely magnetic SANS. The misalignment scattering is obtained by subtracting the reference scattering at a high (saturating) ...	Sphere	17 Feb 2021	dehoni	0	✖	Sphere, Structure Factor
SANS of bulk ferromagnets	This model is a micromagnetic approach to analyse the SANS that arises from nanoscale variations in the magnitude and orientation of the magnetization in bulk ferromagnets in the approach to magnet...	Sphere	17 Feb 2021	dehoni	0	✖	All Models
core_shell_ellipsoid_tied and core_shell_ellipsoid_repar	Two methods, both requiring sasview v5, to produce a core_shell_ellipsoid with solvent in the shell. Parameters include the dry_shell / core volume ratio, the local fraction of solvent in the she...	Ellipsoid	16 Feb 2021	richardh	0	✖	

Plugin models tutorial

Available at <https://www.sasview.org/download/>



SasView Tutorials

Creating Custom Fitting Models
in SasView Version 5.x

www.sasview.org

Contents

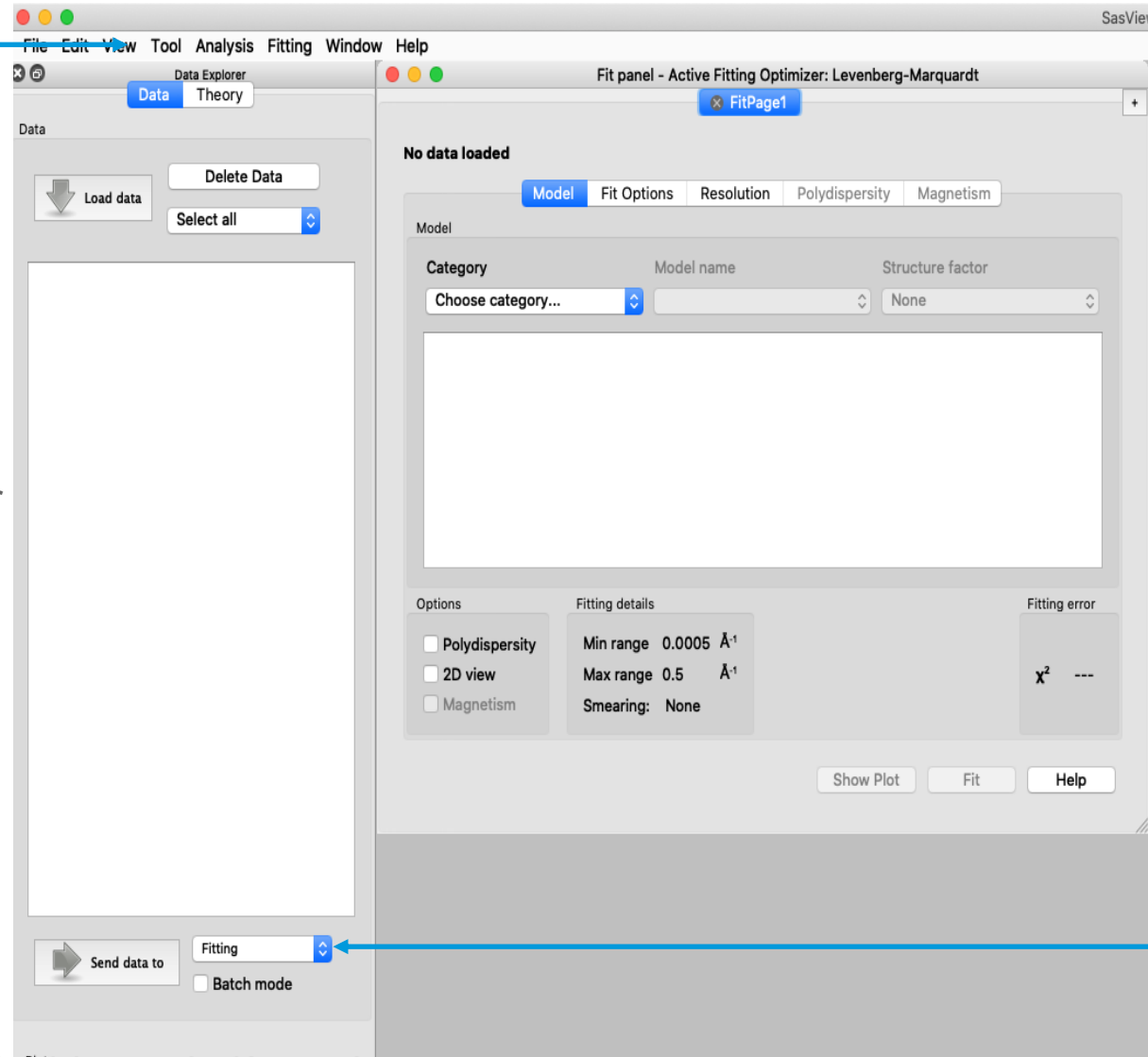
	Page
Running SasView	4
Example 1 – Combining Two Library Models	5
Example 2 – Combining More Than Two Models	8
Example 3 – Creating A Simple Model With The Model Editor	11
Example 4 – Repurposing An Existing Model	17
Example 5 – Reparameterising An Existing Model	23
Example 6 – Getting Creative	27

Other SasView functionality

Various utility tools and calculators

Tools

- Data Operation
- SLD calculator
- Density/Volume calculator
- Slit Size Calculator
- Kiessig Thickness Calculator
- Q Resolution Estimator
- Generic Scattering calculator
- Orientation Viewer
- Python Shell/Editor
- Image Viewer
- File Converter

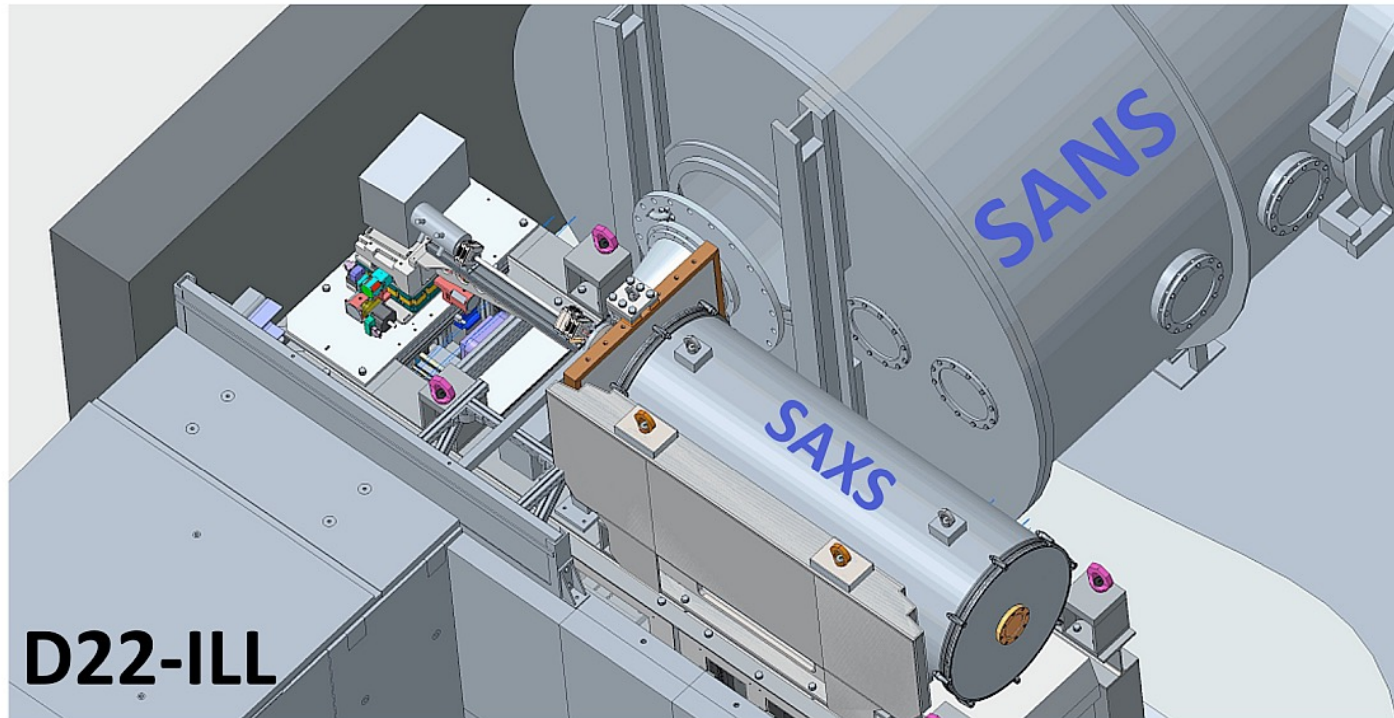


Analysis

- Fitting
- Invariant
- Pr Inversion
- Correlation Function

Combined SAXS and SANS

Simultaneous measurements on the same sample

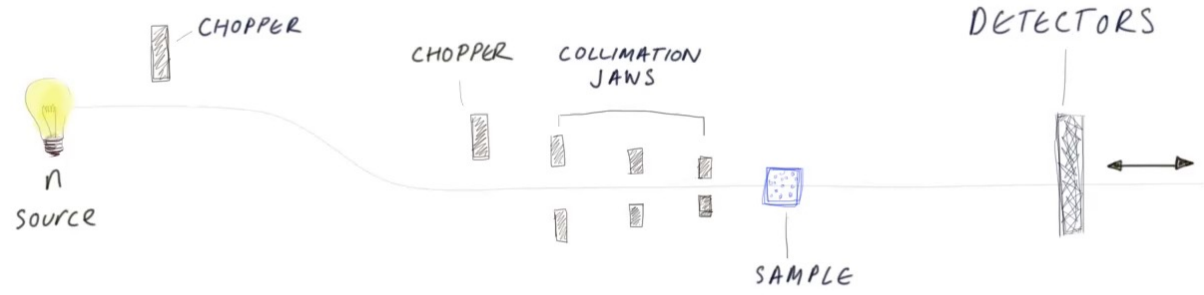
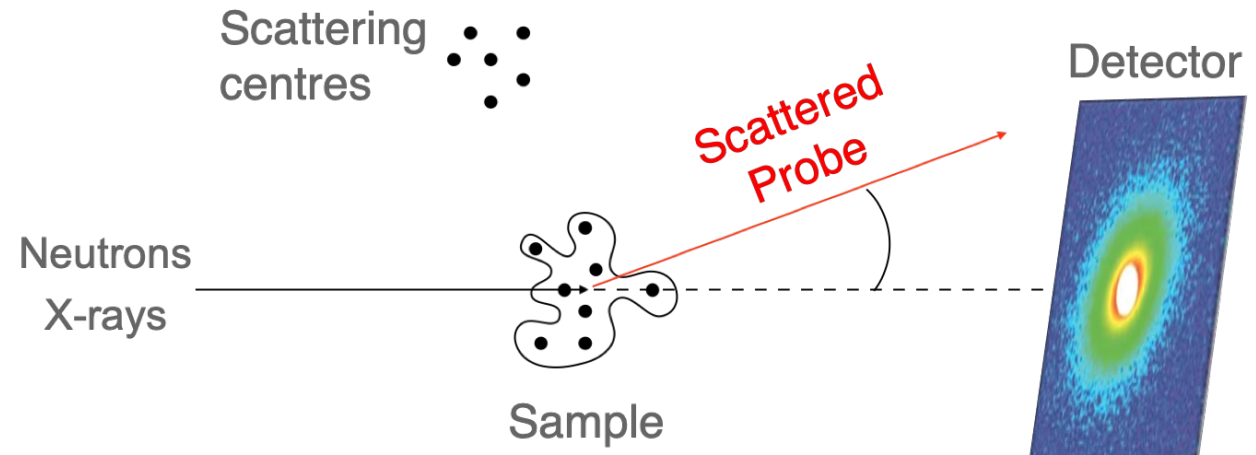


- Running at D22 instrument at ILL
- Low-flux SAXS source
- Specialized sample environment
- Non-trivial data analysis
- SasView (6.0.0) provides a weighting mechanism in simultaneous fitting

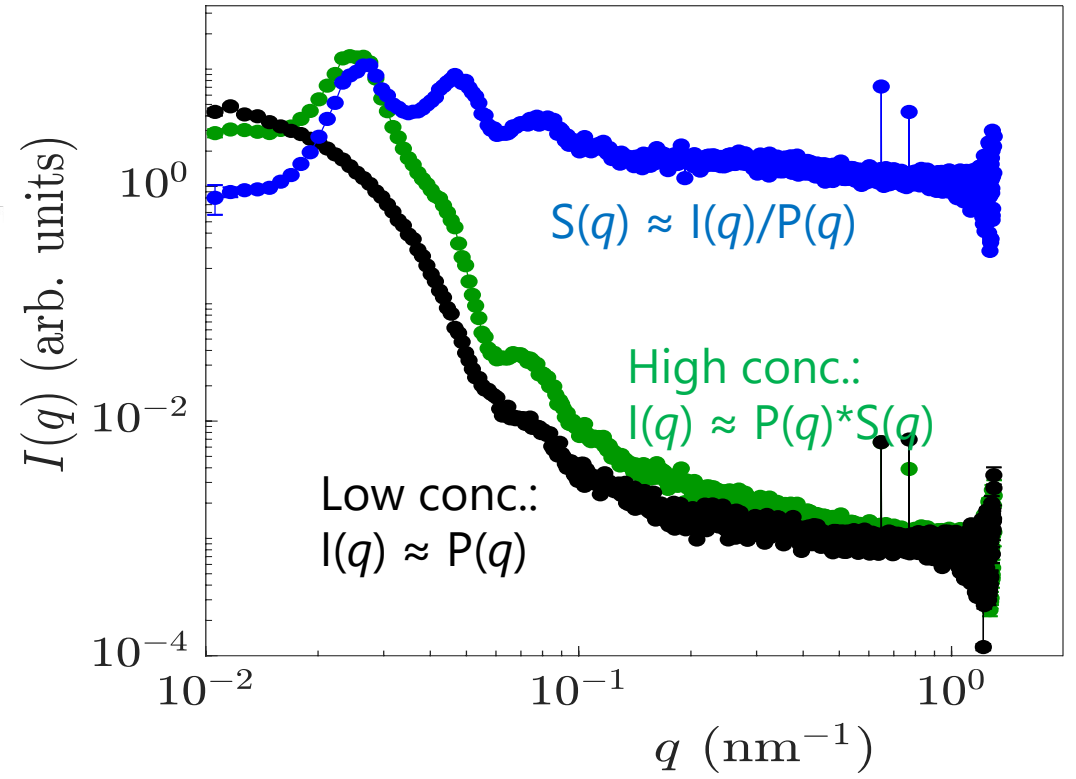
6

Small-angle scattering instruments

Small-angle scattering



$$I_{exp}(q) = n\Delta\rho^2V^2P(q)S(q)$$



SAXS: synchrotron vs. benchtop



synchrotron
High brightness
High time resolutions: measurements in ms
Risk of damage to biomaterials
Large dynamic q-range often due to multiple detectors

SAXS: synchrotron vs. benchtop



synchrotron	Benchtop
High brightness	Low brightness – low risk of damage to bio materials, but poor time resolution
High time resolutions: measurements in ms	Poor time resolution: measurements in min-h
Risk of damage to biomaterials	Low risk of damage to biomaterials
Large dynamic q-range often due to multiple detectors	Limited dynamic q-range at one detector

SANS: Continuous vs. time-of flight

We need to probe the wavevector, Q with neutrons....

$$q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$



Continuous

Fixed wavelength (monochromatic)

Fixed λ , varying θ

Need several measurements at different detector distances to cover adequate q -range

Typically reactor sources (exceptions: TOF instruments in monochromatic mode)

SANS: Continuous vs. time-of flight

We need to probe the wavevector, Q with neutrons....

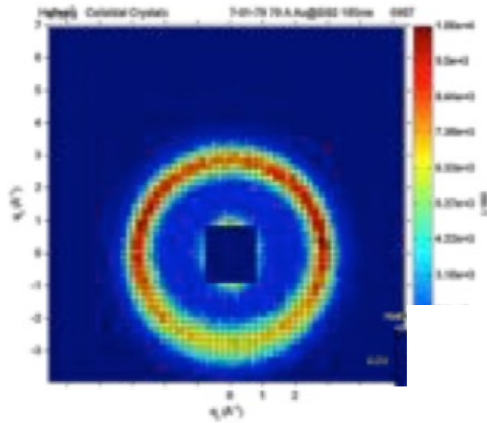
$$q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$



Continuous	Time-of-flight
Fixed wavelength (monochromatic)	Wavelength band
Fixed λ , varying θ	Varying θ , varying λ
Need several measurements at different detector distances to cover adequate q -range	Large dynamic q -range at one detector distance, q_{\max}/q_{\min}
Typically reactor sources (exceptions: TOF instruments in monochromatic mode)	Typically spallation sources (exceptions: ILL D33 and ANSTO Bilby)

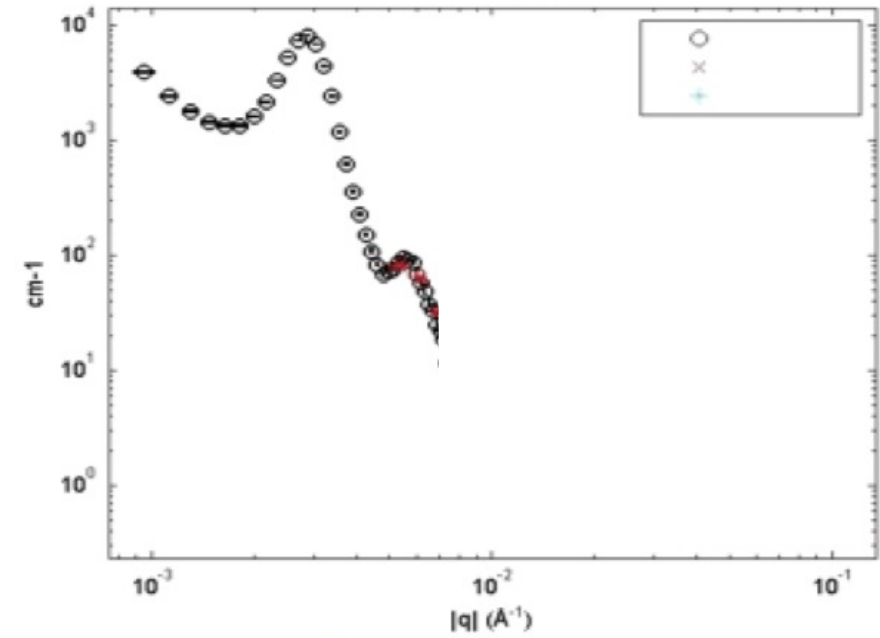
SANS: Continuous vs. time-of flight

High flux but often need several measurements at different distances to cover an adequate Q-range



Low q:
Largest
sample-to-
detector
distance

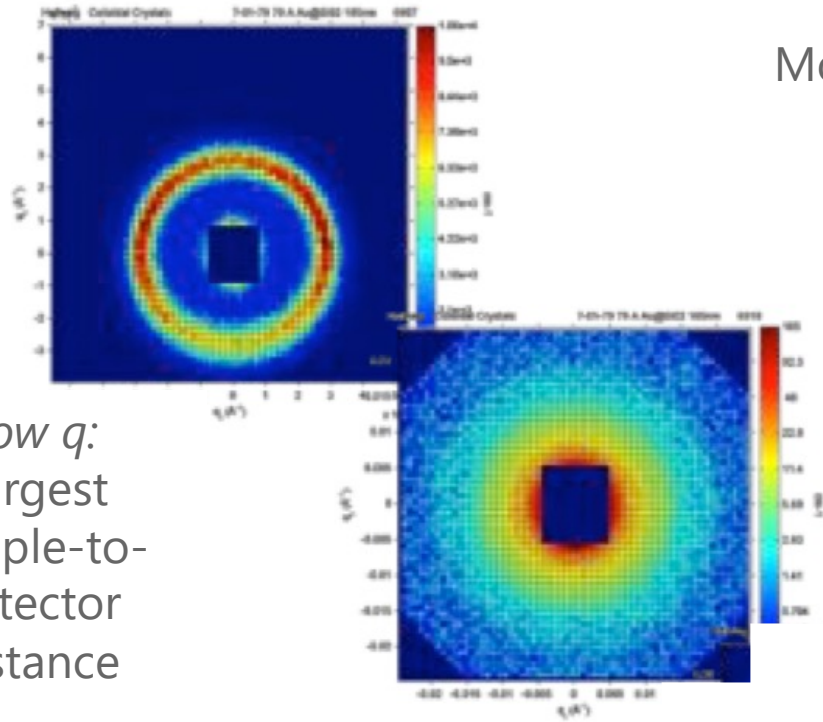
Monochromatic
beam



Figures from ILL

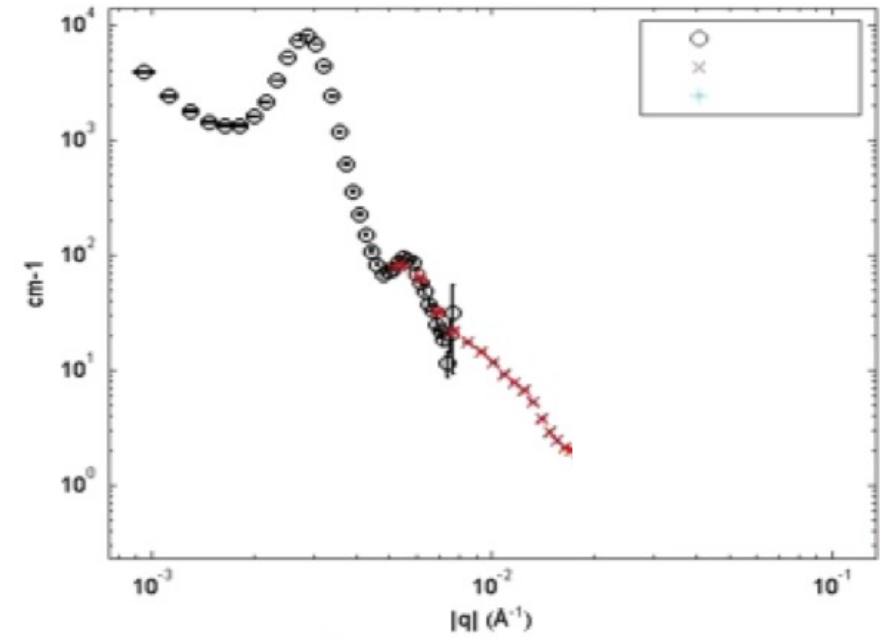
SANS: Continuous vs. time-of flight

Need several measurements at different distances to cover an adequate Q-range



Monochromatic beam

Low q:
Largest sample-to-detector distance

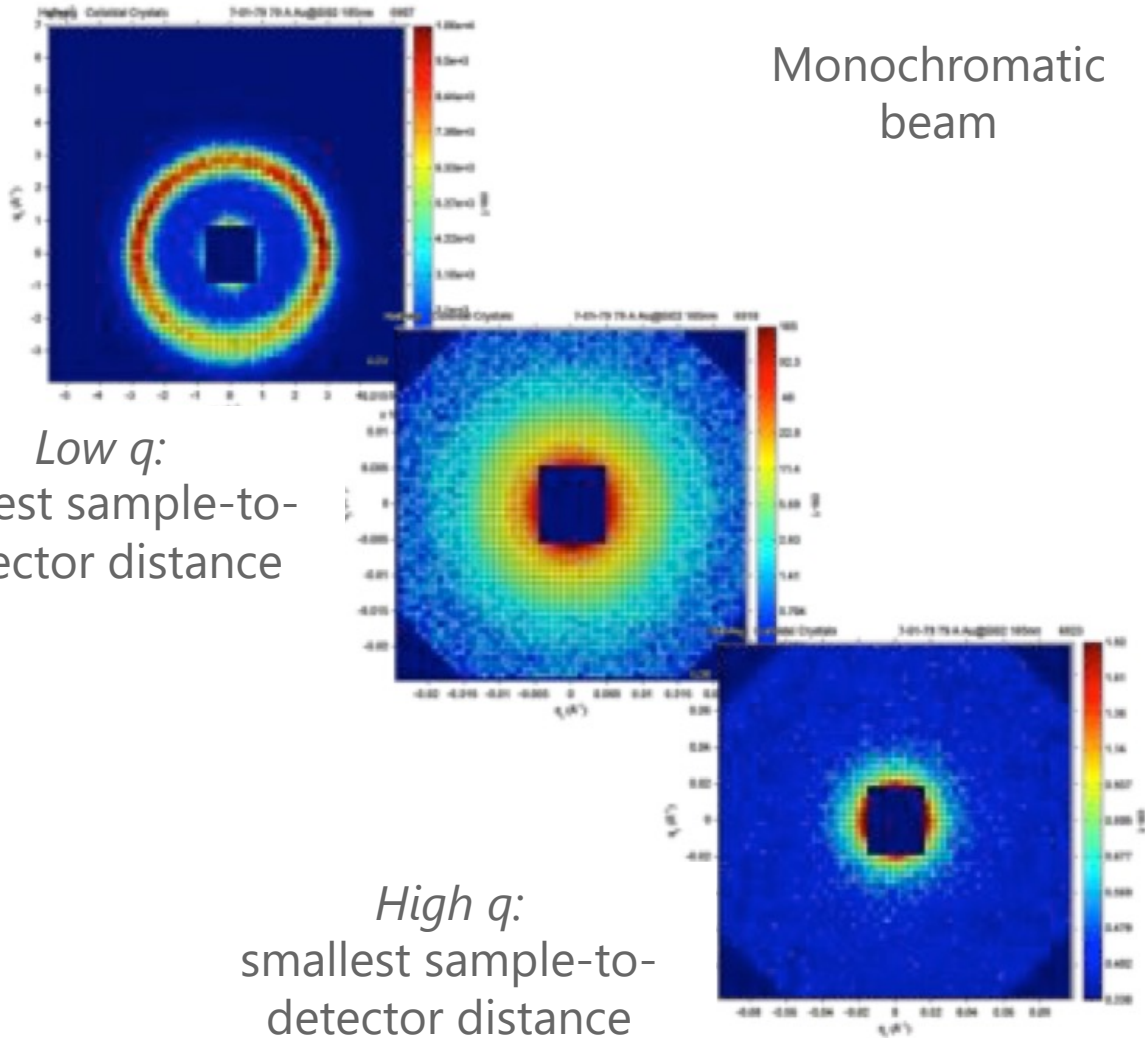


Figures from ILL

SANS: Continuous vs. time-of flight

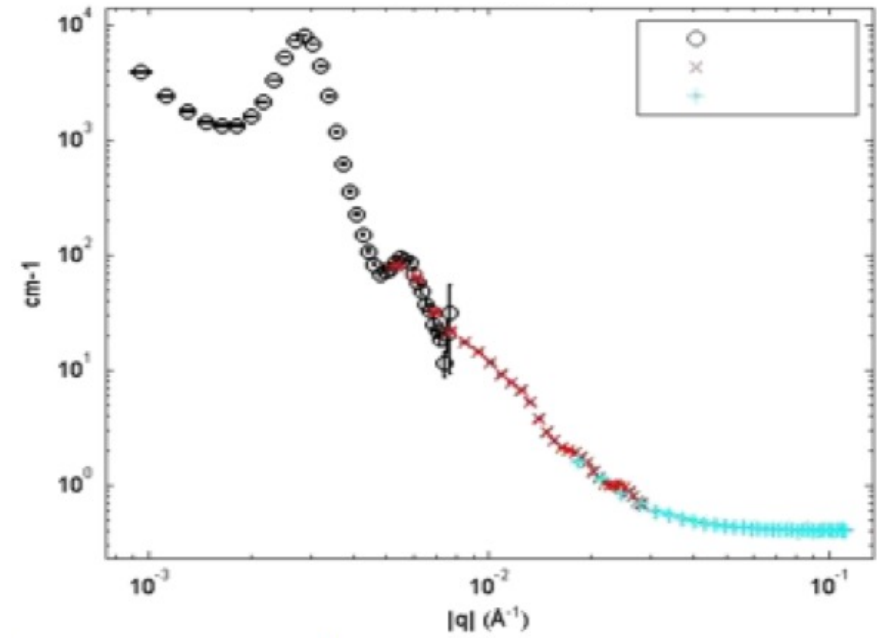
Need several measurements at different distances to cover an adequate Q-range

Monochromatic beam



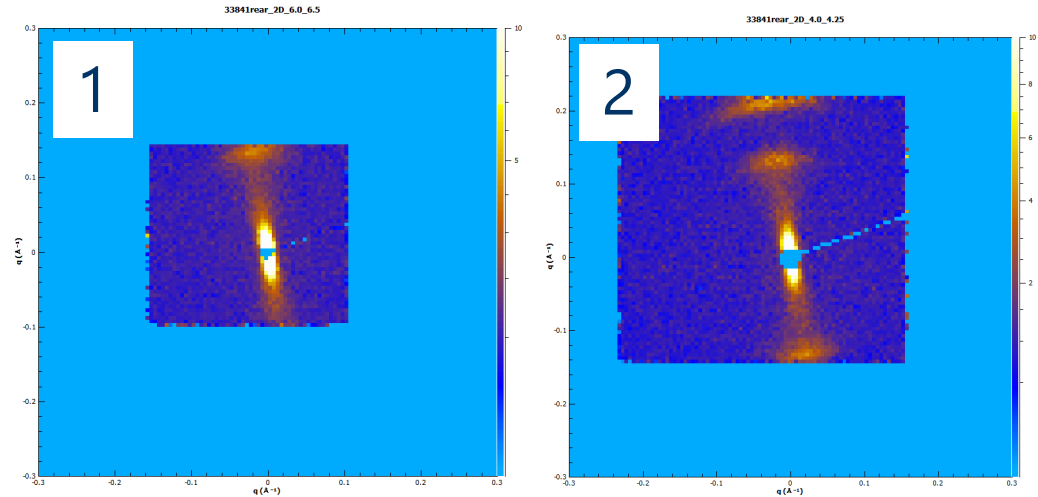
Low q :
Largest sample-to-detector distance

High q :
smallest sample-to-detector distance



Figures from ILL

SANS: Continuous vs. time-of flight

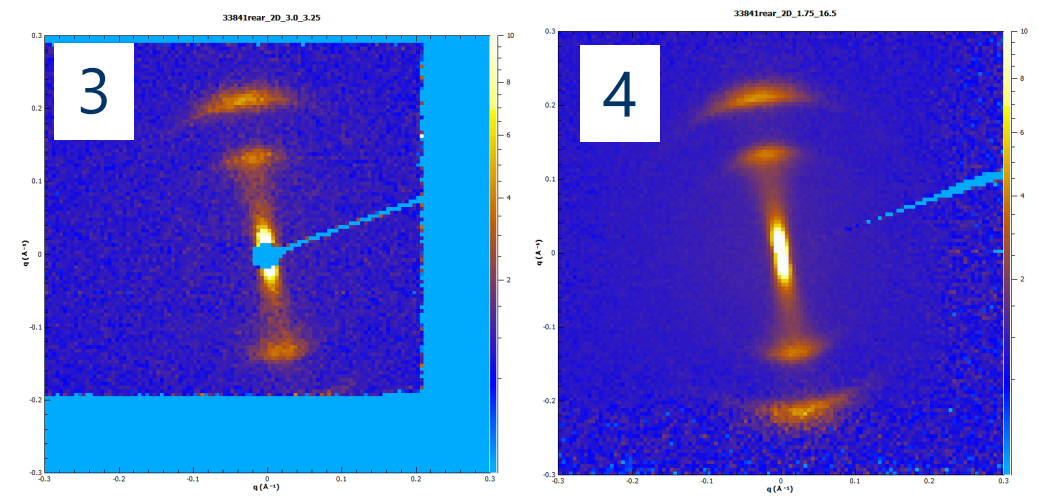


1

2

"fixed wavelength"
~6.25 Å

Shorter wavelengths
expand Qmax

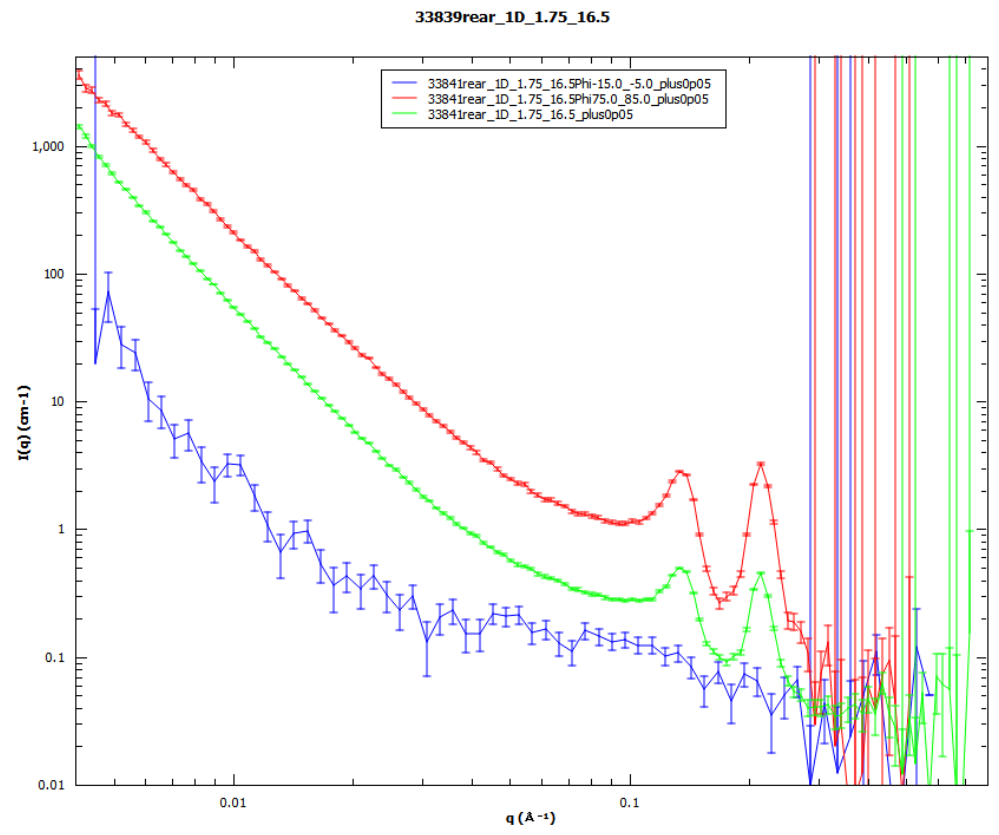


3

4

Even shorter wavelengths
expand Qmax further

Full 1.75 to 16.5 Å gives a
wide simultaneous Q range.



Courtesy of R. K. Heenan and M. Hollamby

SANS: So you have a choice reactor vs. spallation...



e.g. D11 or D33 @ ILL, France (reactor source)

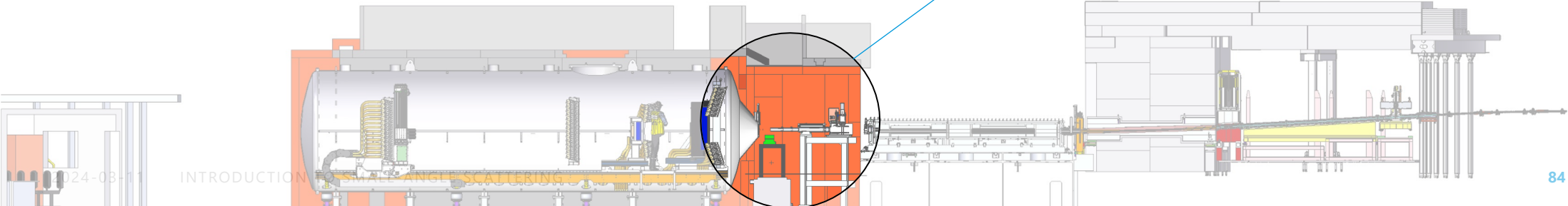
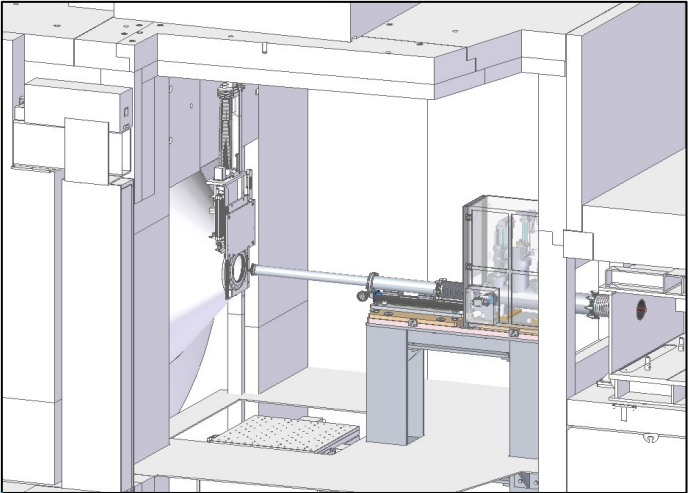


e.g. SANS2D @ ISIS, UK (spallation source)

Need to also consider the sample environment!

Sample environment

How do we control the positioning and conditions of our samples in the neutron beam?



Sample environment

The "off-the-shelf" variety

- **Thermostated cell/capillary holder**
- Rheometer
- Flow cell with HPLC pumps
- Rotating cell holder
- Couette shear (higher shear rates)
- Plate-plate shear (for e.g. polymers)
- 2.5T electromagnet
- Humidity chamber
- Stopped-flow equipment
- Stress/strain rig (load capacity for stretching polymers)
- Cryostats

Custom-built sample environments

NuRF set-up

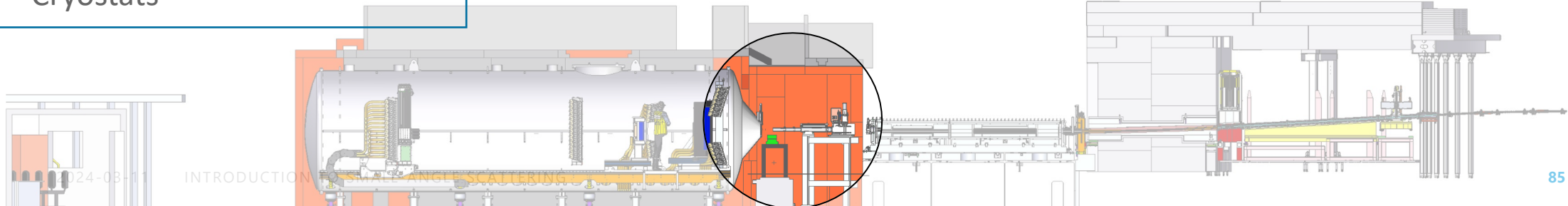
(b)

Size-Exclusion Chromatography-SANS

(a)

Microfluidics

in situ fluorescence, UV/vis absorption, densitometry on a continuous flow cell





Sample cells for biological solutions

Things to consider before selecting a cell:

1. How much hydrogen is in my sample? How concentrated is my sample?
2. Is my sample easy to pipette? super viscous? a film? solid?
3. How much sample do I have?
4. What cells are available and/or used at the beamline?

Sample cells

- Quartz cells - **no SAS signal** and low background
- **Cell thickness** may depend on the H content of the sample
 - 1 mm for samples with more than 50% H
 - 2 or 5 mm for predominantly deuterated samples
- **Stopper or no stopper?**
- **Cell shape:**
 - 10 mm width rectangular cell
 - Cylindrical cell (banjo)
 - 20 mm width rectangular cell (tank)
 - Sandwich cell
- **Sample volume** for standard cells: 200 μ L to 1 mL
- Some sample environments require specific cells (Al, TiZr...)

Capillaries



Quartz cuvettes



Sandwich cells



- ✓ Highly reproducible
- ✓ Low scattering
- ✓ Low background

Conclusions

- Small-angle scattering is an experimental technique which uses elastic scattering at small angles to investigate the structure of substances at a mesoscopic scale of $\sim 1\text{--}200$ nm
- Neutrons are a non-destructive, penetrating probe of structure on the atomic to macroscopic scale.
- Neutrons provide chemical sensitivity being especially sensitive to light elements.
- Neutron scattering can be isotope dependent, so contrast variation using H/D substitution allows complex structures to be more easily understood



Thanks for listening!

Any questions please ask!

(or email judith.houston@ess.eu)

2024-03-11