SANS DATA ANALYSIS

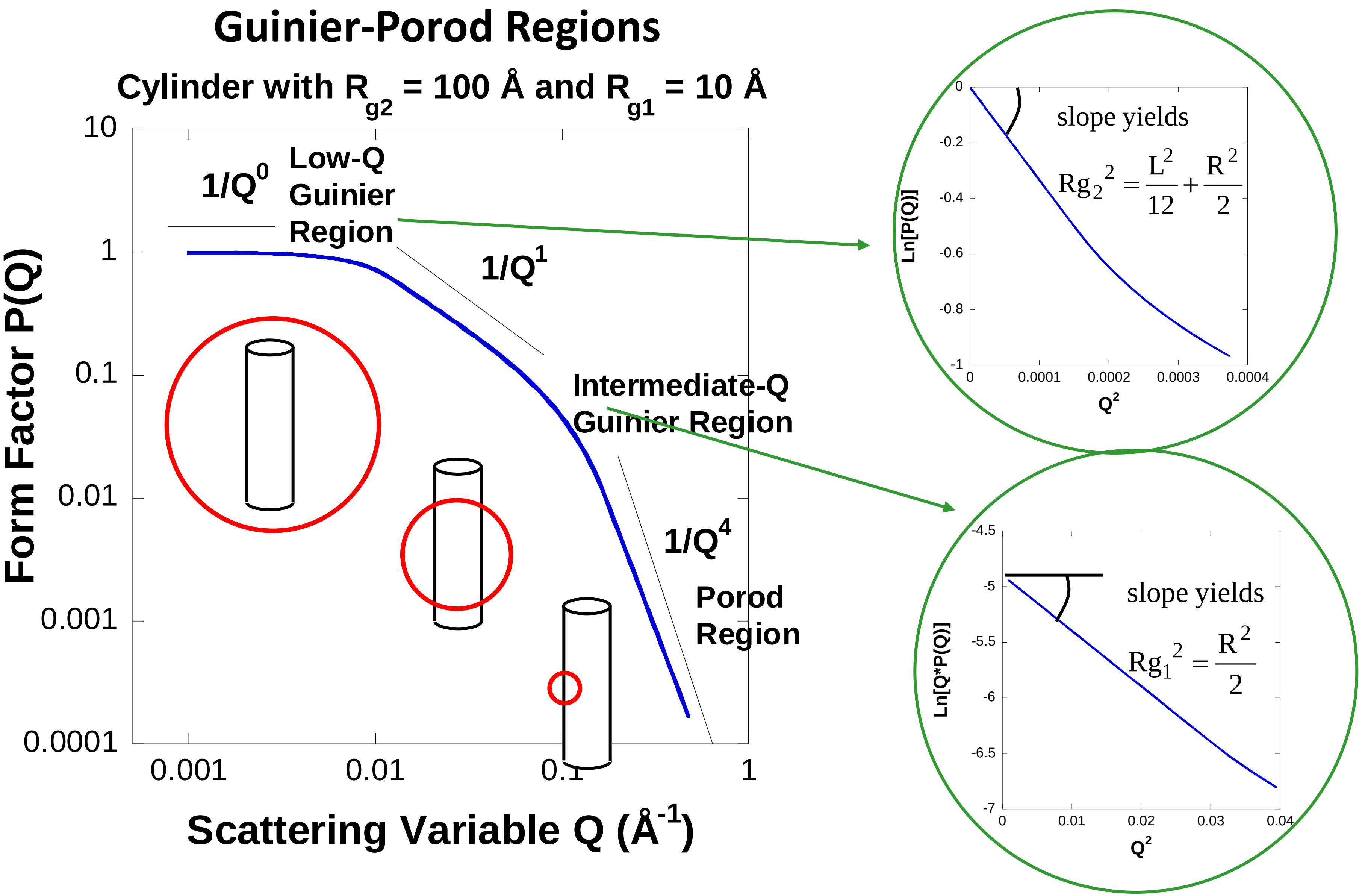
Boualem Hammouda

National Institute of Standards and Technology
Center for Neutron Research

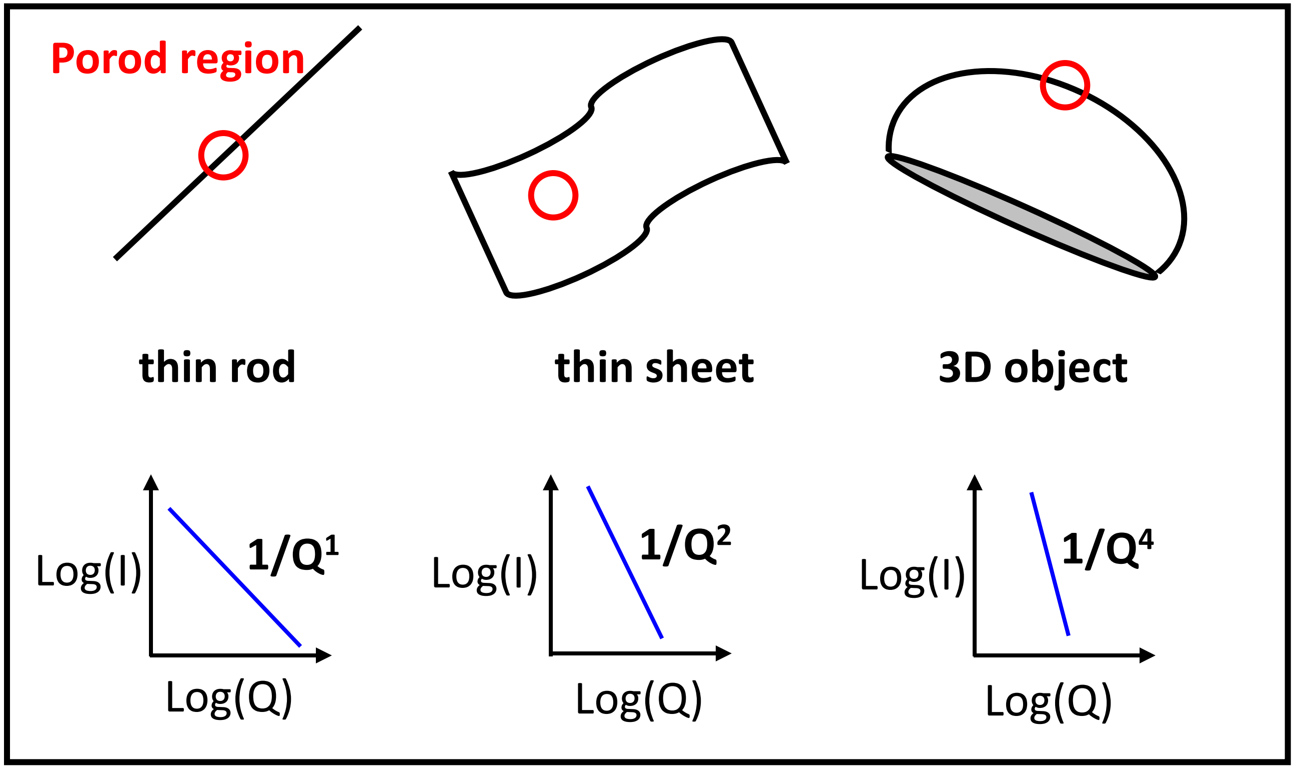
- 1. Standard Plots (Guinier Plot, Porod Plot)
- 2. SANS Models
- 3. Inverse Fourier Transform
- 4. Shape Reconstruction Method

1. Standard Plots

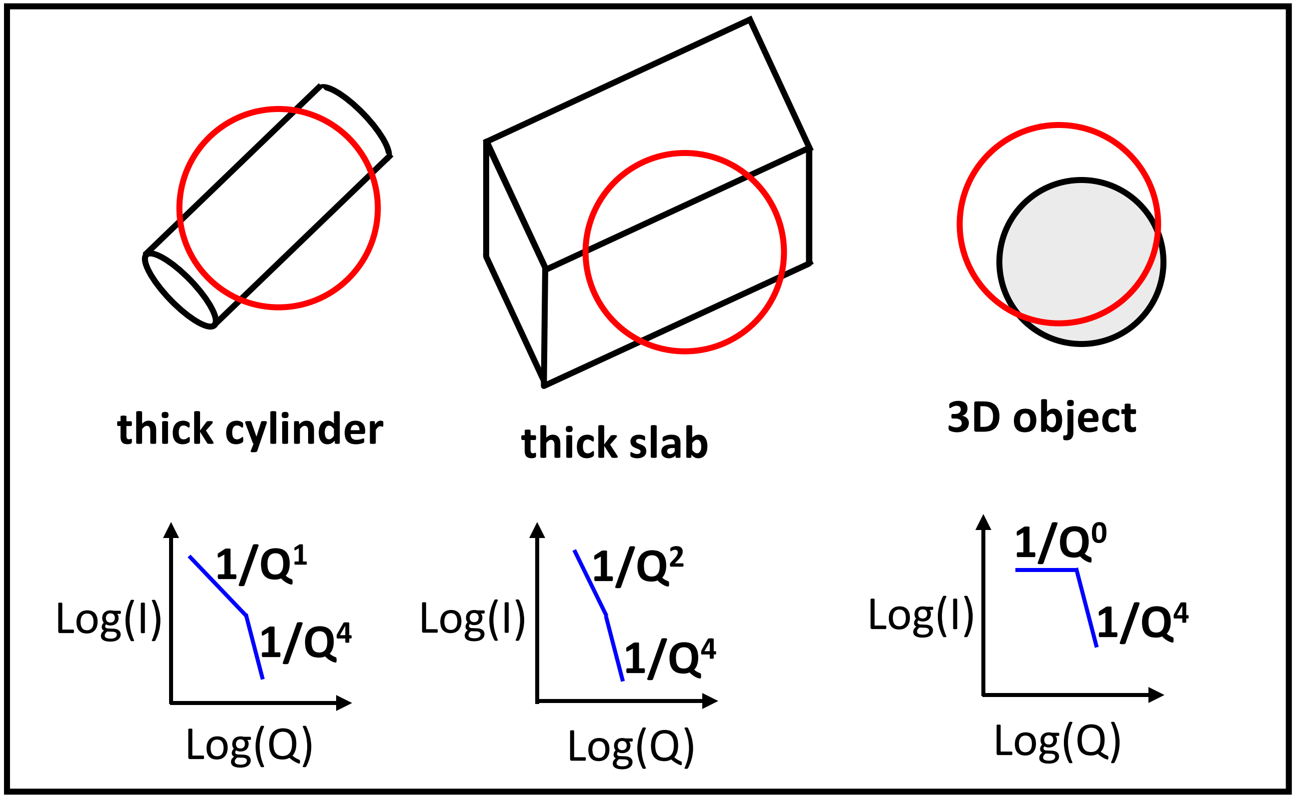
Guinier Plots



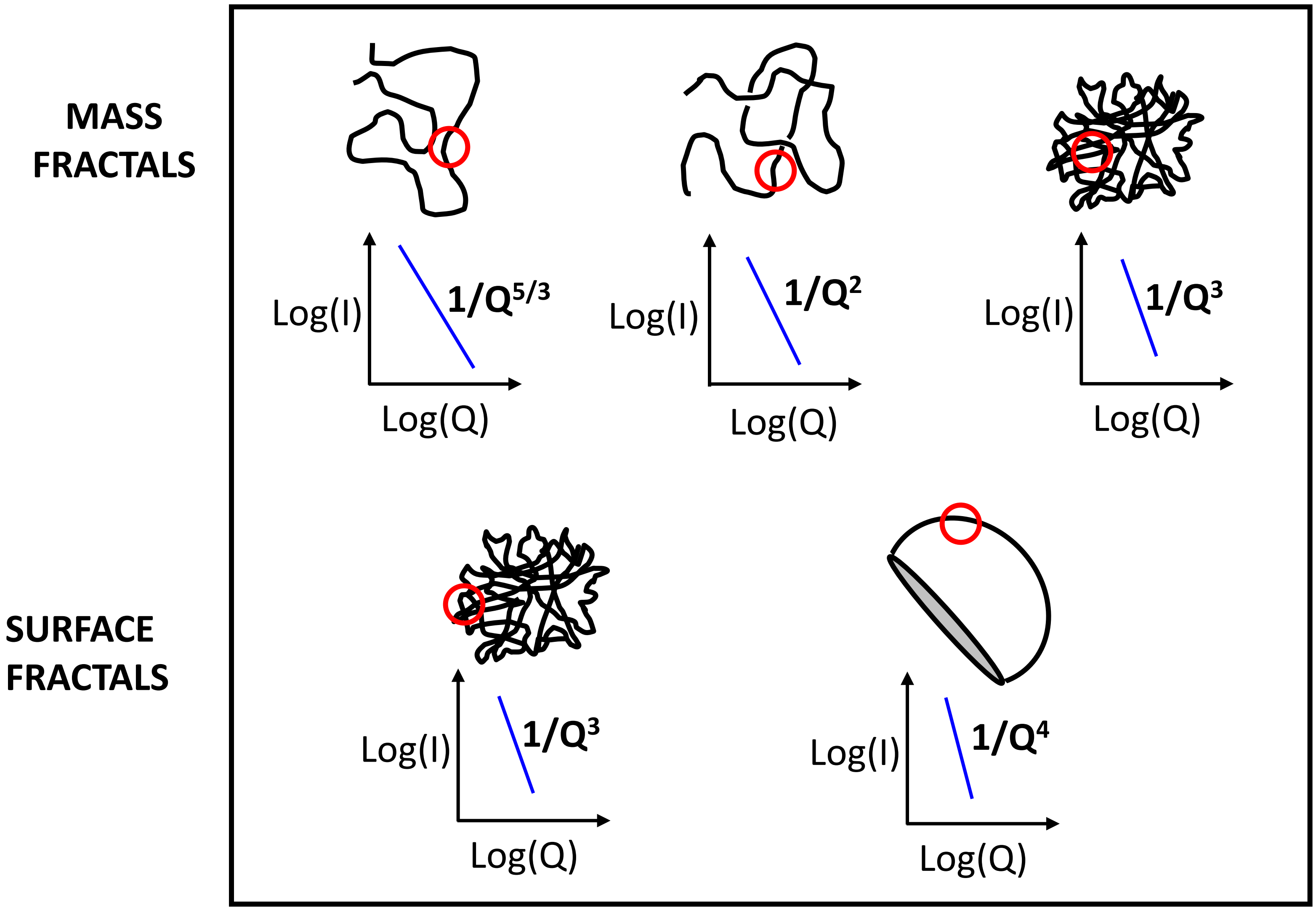
Assortment of Porod Exponents



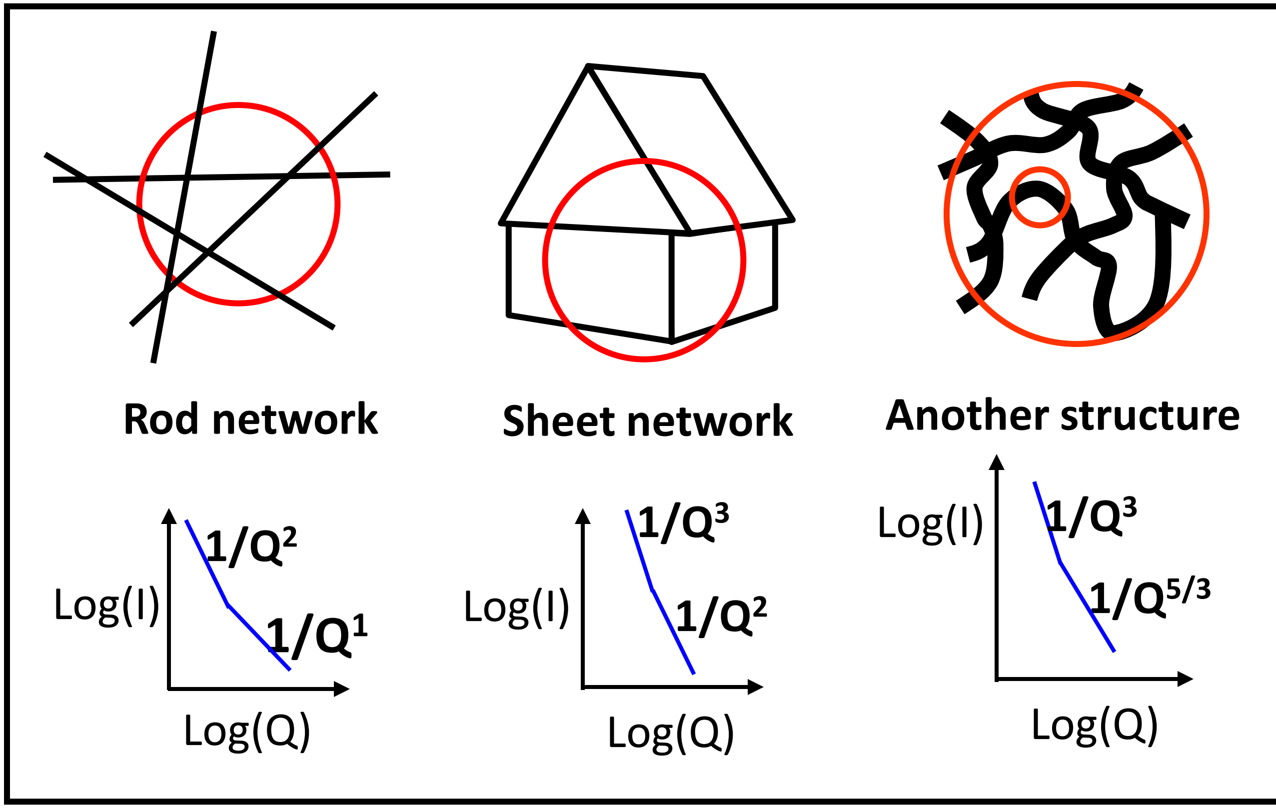
More Porod Exponents



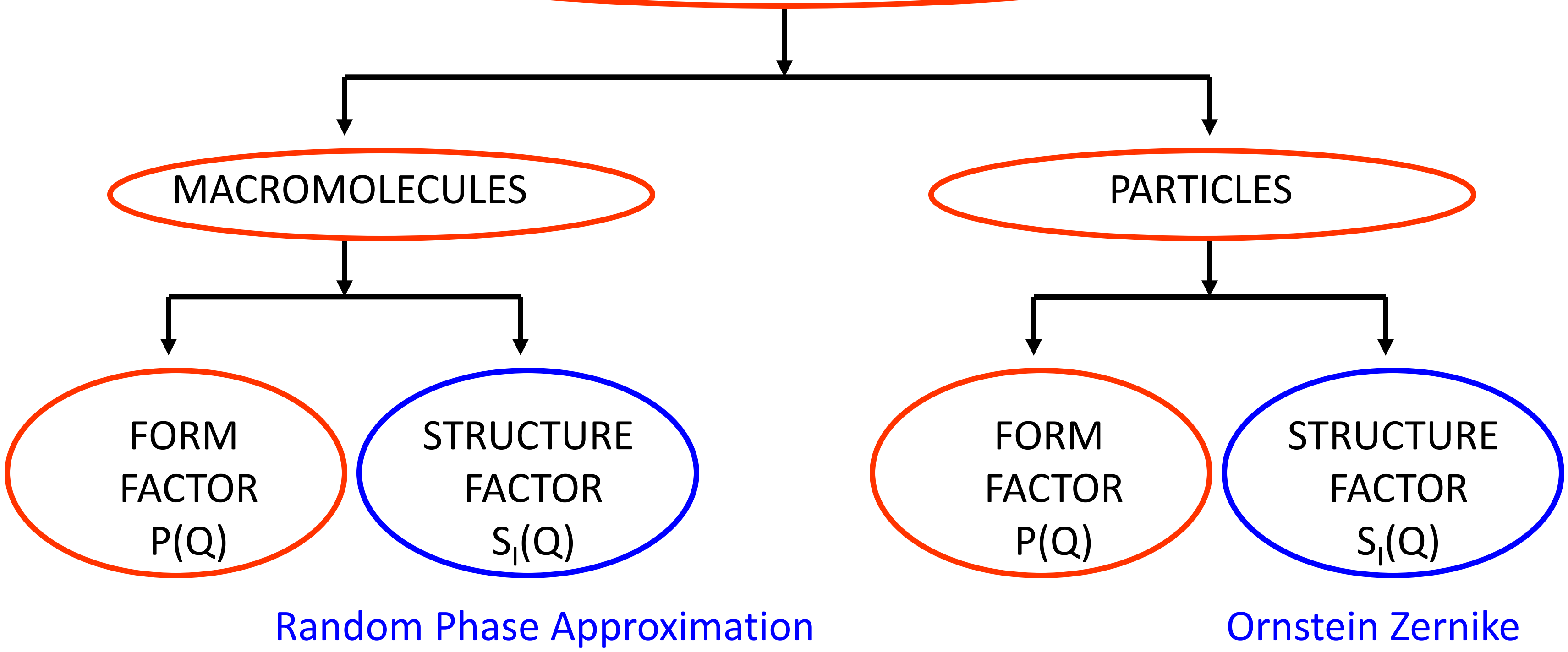
More Porod Exponents



More Porod Exponents



2. SANS Models



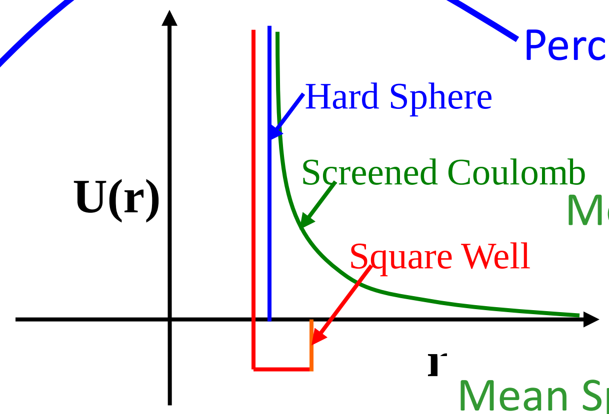
$$\frac{d\Sigma(Q)}{d\Omega} = \phi_A (\rho_A - \rho_B)^2 V_A P(Q) S_I(Q)$$

cross section — volume fraction — contrast factor — particle volume — form factor — structure factor

The Ornstein-Zernike Equation

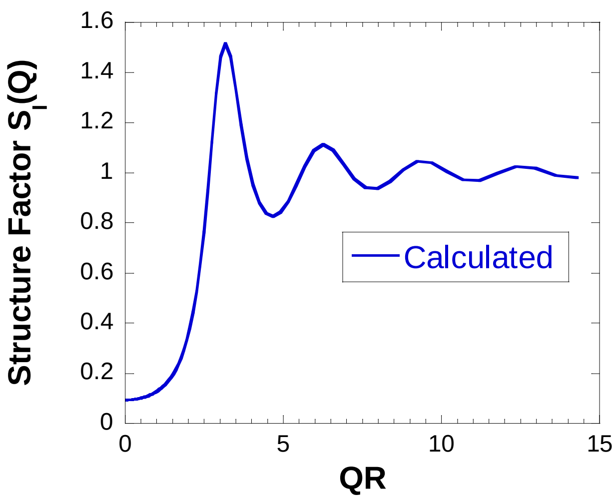
Interaction Potentials

Percus-Yevick

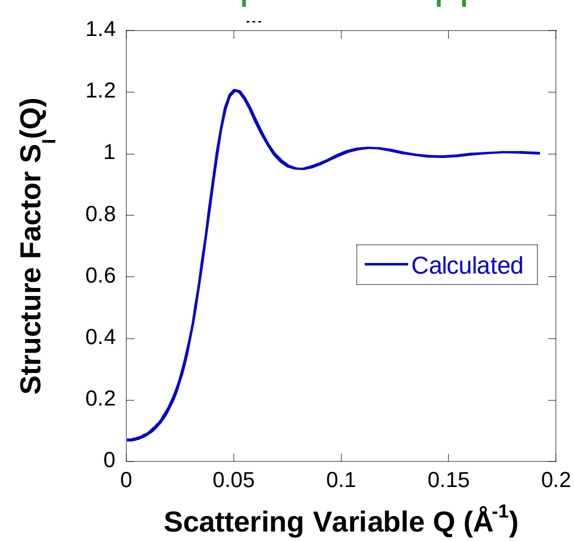


Mean Spherical Approximation

Percus-Yevick

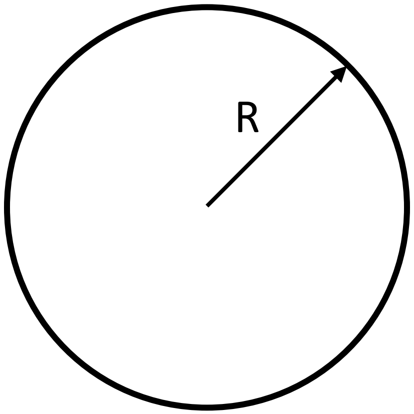


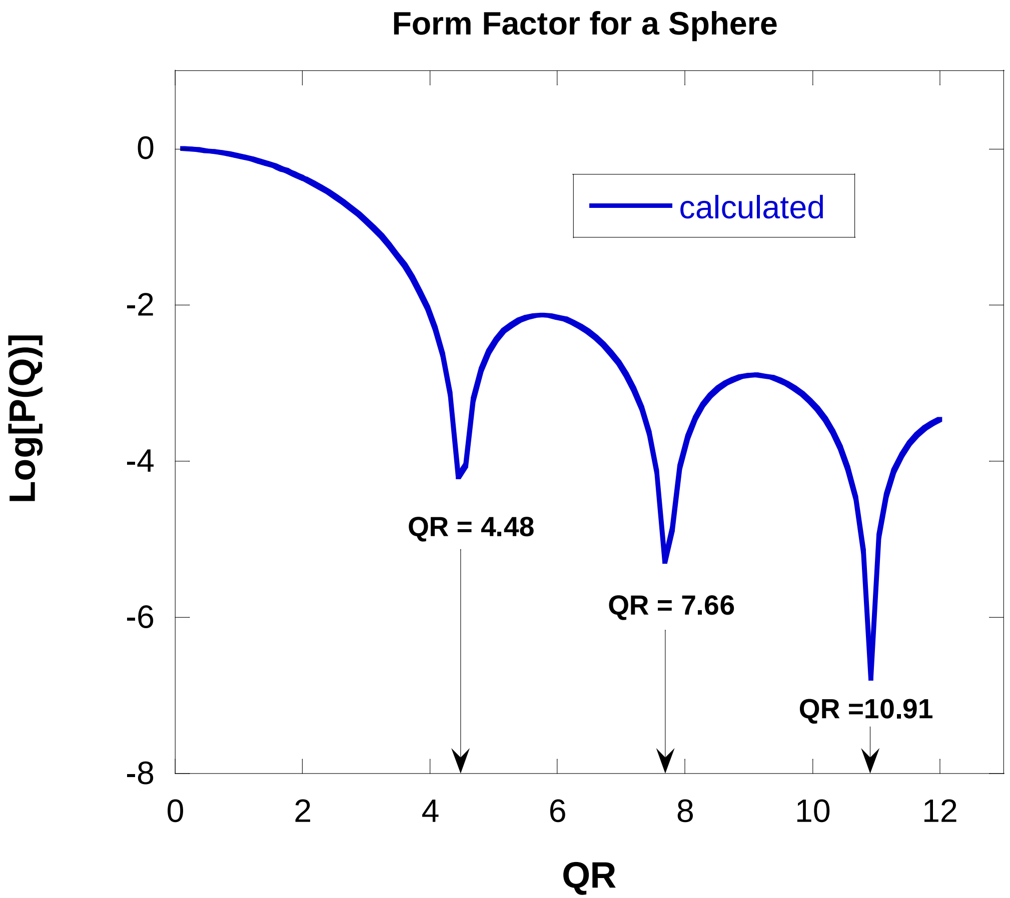
Mean Spherical Approximation



FORM FACTOR FOR A SPHERE

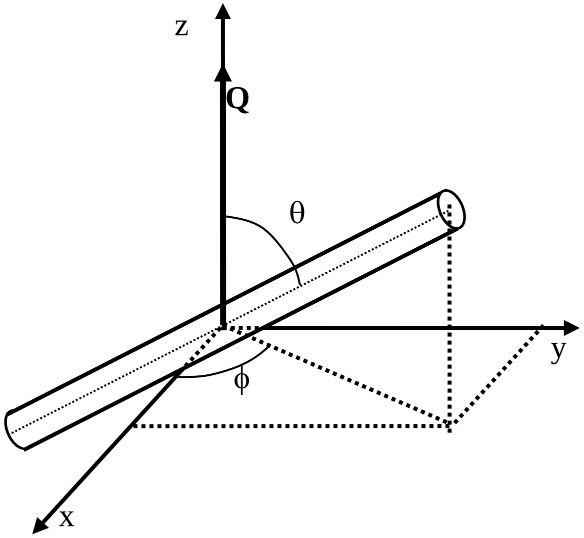
$$P(Q) = \left[\frac{3j_1(QR)}{QR}\right]^2 = \left[\frac{3}{QR}\left(\frac{\sin(QR)}{(QR)^2} - \frac{\cos(QR)}{QR}\right)\right]^2$$

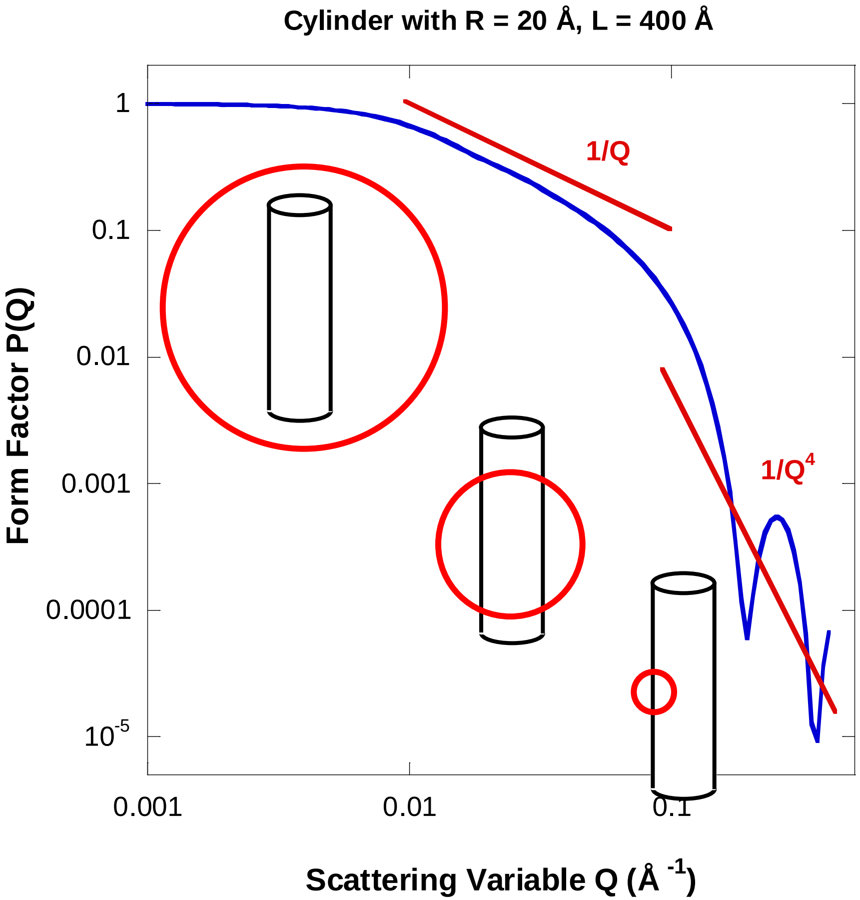




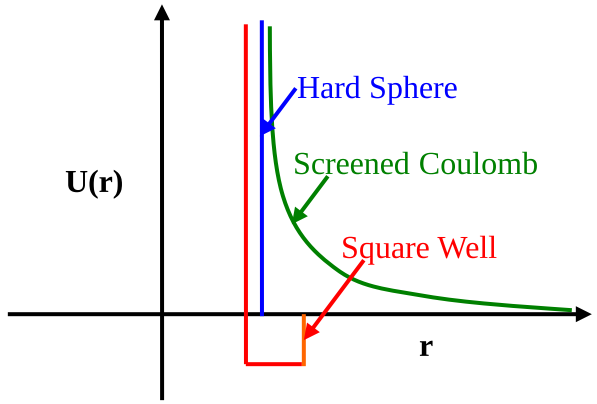
FORM FACTOR FOR A CYLINDER

$$P(Q) = \frac{1}{2}\int_{-1}^{1} d\mu \left[\frac{\sin(Q\mu L/2)}{Q\mu L/2}\right]^2 \left[\frac{2J_1(Q\sqrt{1-\mu^2}R)}{Q\sqrt{1-\mu^2}R}\right]^2$$

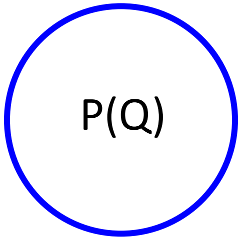


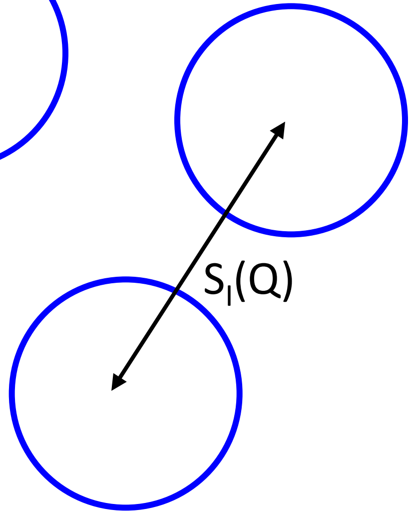


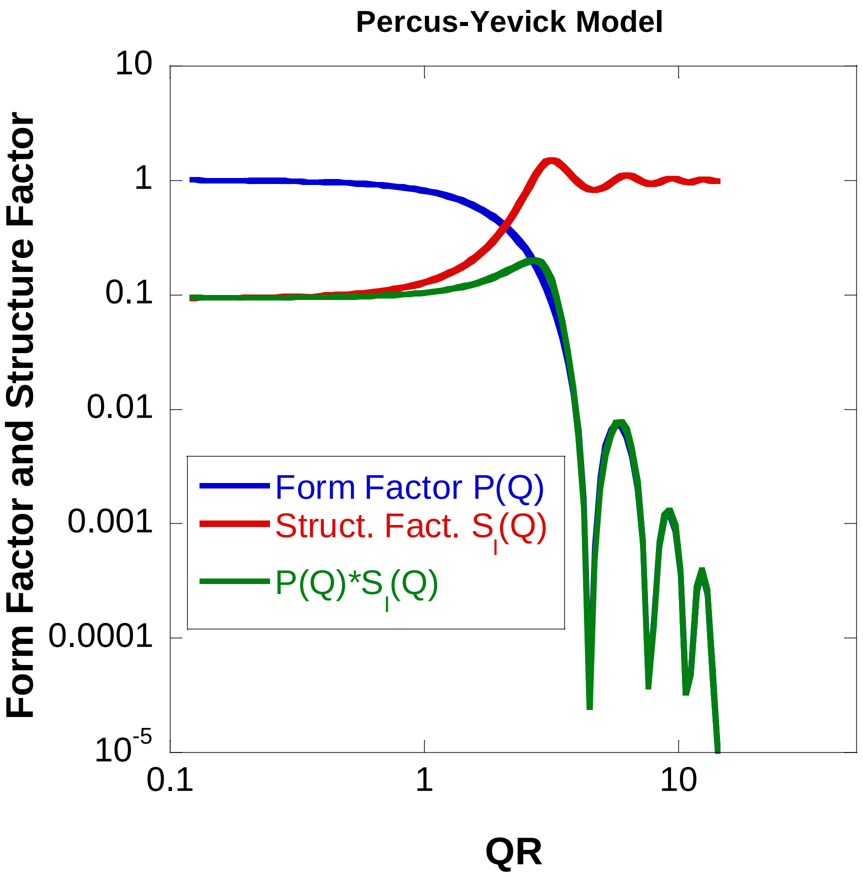
STRUCTURE FACTOR –
THE ORNSTEIN-ZERNIKE EQUATION



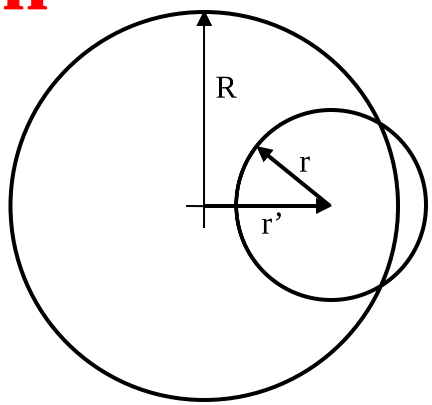
$$\frac{d\Sigma(Q)}{d\Omega} = \phi_A \left(\rho_A - \rho_B\right)^2 V_A \, P(Q) \, S_I(Q)$$







3. Fourier Transform



Density-density correlation function:

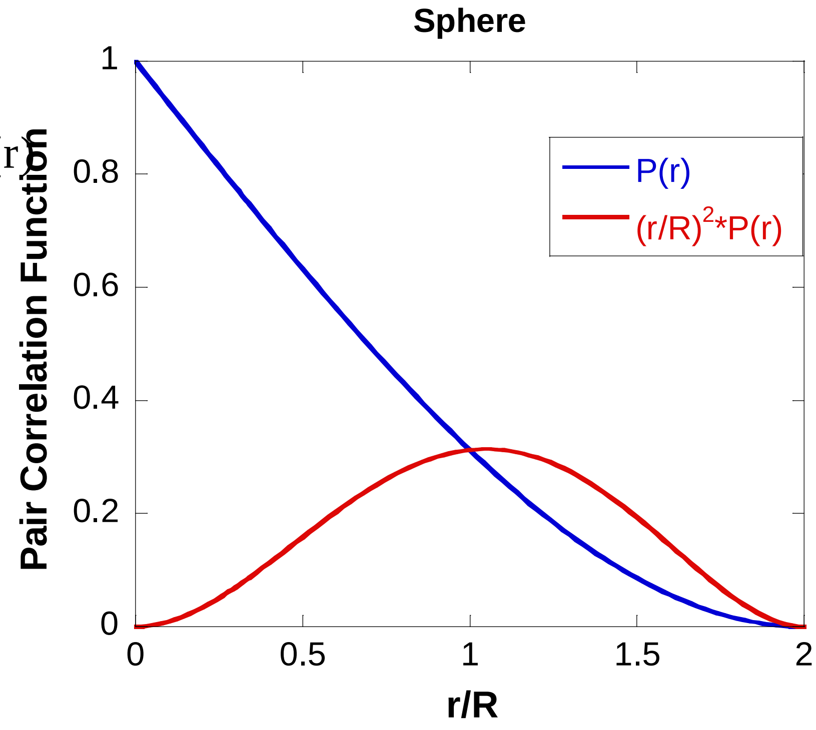
$$P(Q) = \frac{< n(-Q)n(Q) >}{n^2} = \int d\vec{r} \int d\vec{r}' \frac{< n(r)n(r') >}{n^2} \exp[i\vec{Q}.(\vec{r}'-\vec{r})]$$

Fourier transform:

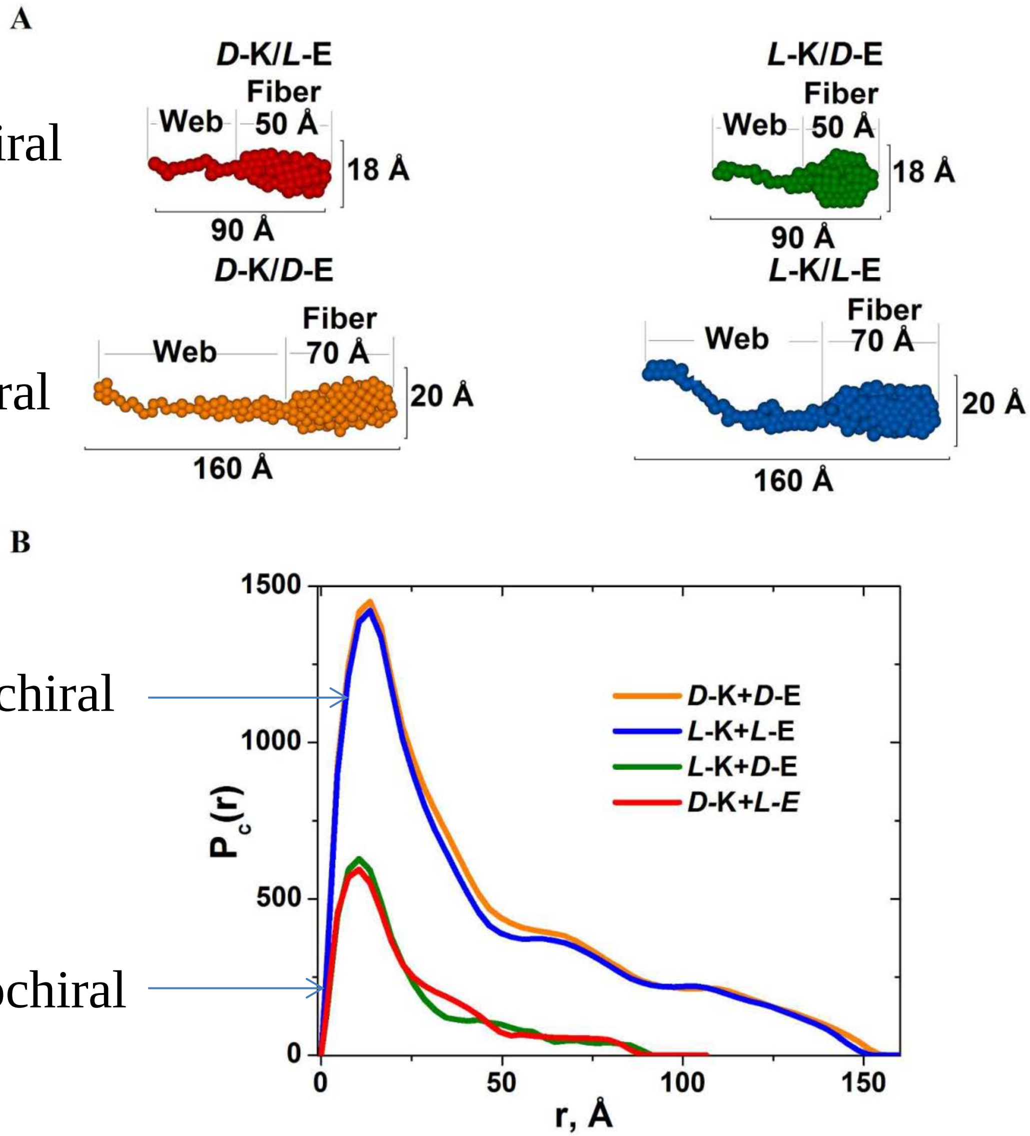
$$P(Q) = \int d^3 r \exp[-i\vec{Q}.\vec{r}]\, P(\vec{r}) = \frac{1}{V_P} \int_0^\infty dr 4\pi r^2 \frac{\sin(Qr)}{Qr} P(r)$$

Radial pair correlation function:

$$P(r) = 1 - \frac{3}{4}\left(\frac{r}{R}\right) + \frac{1}{16}\left(\frac{r}{R}\right)^3$$



SANS Data Analysis



Heterochiral

Homochiral

Shape Reconstruction

Fiber cross sections

Homochiral

Heterochiral

Inverse Fourier Transform

- Homochiral fibers are thicker and denser than heterochiral ones

SANS DATA ANALYSIS METHODS

- 1. Standard Plots (Guinier Plot, Porod Plot)
- 2. SANS Models

  - Igor Pro
  - SASVIEW