Today's outline - September 30, 2024

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Reading Assignment: Chapter 4.5; Chapter 5.1

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Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Friday, October 05, 2024

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Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Friday, October 05, 2024

Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Monday, October 14, 2024

Scattering from molecules

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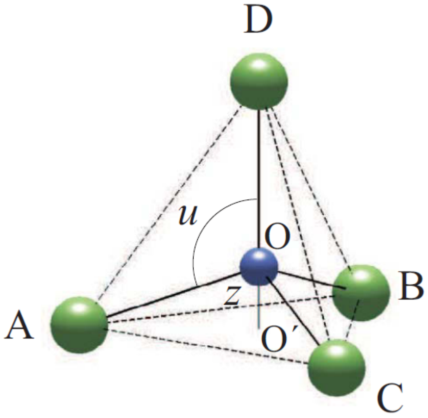
As an example take the CF_4 molecule



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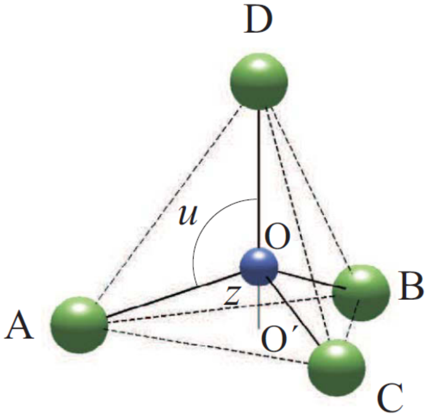

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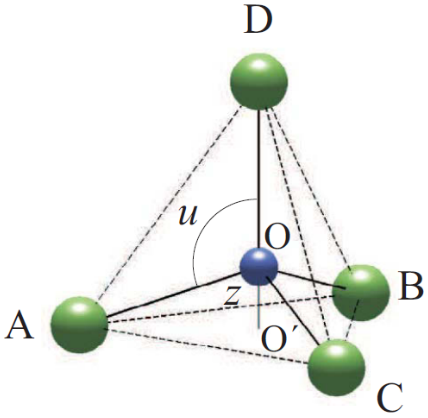

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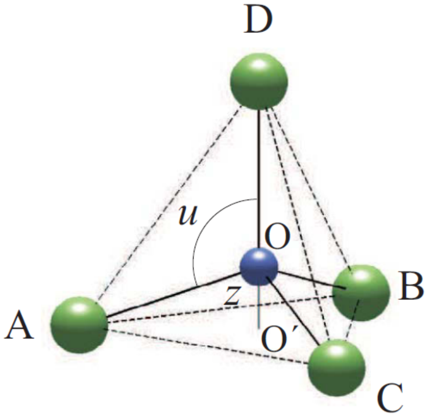

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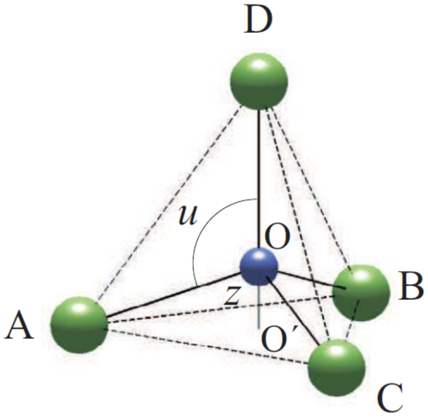

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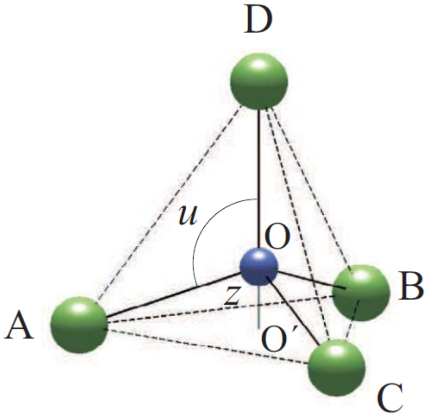

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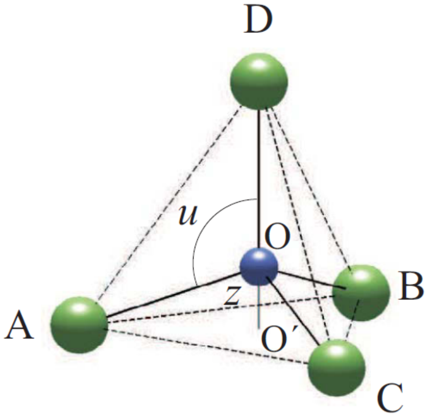

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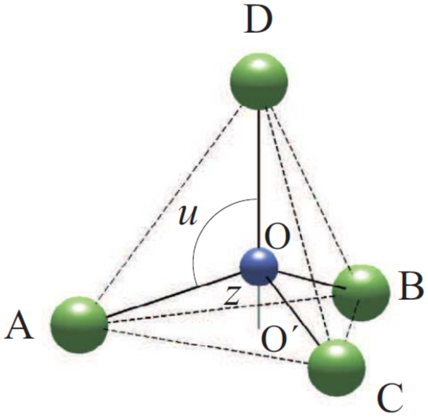

$$\overline{OA} \cdot \overline{OD} = 1 \cdot 1 \cdot \cos u$$

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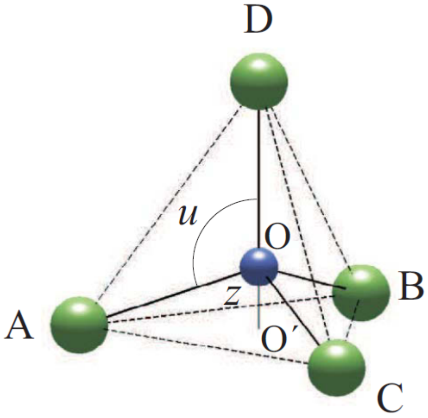

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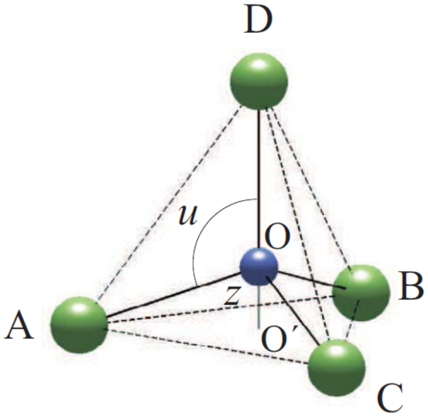

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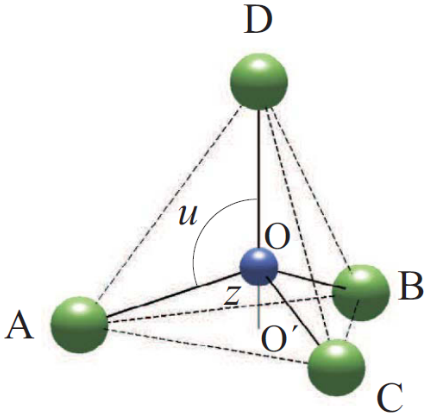

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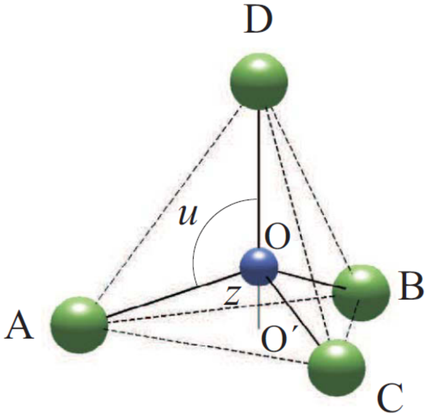

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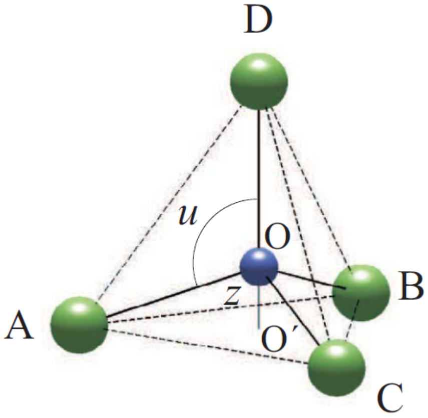
The CF_4 scattering factor

$$-z = (\overline{OO'} + \overline{O'A}) \cdot (\overline{OO'} + \overline{O'B})$$



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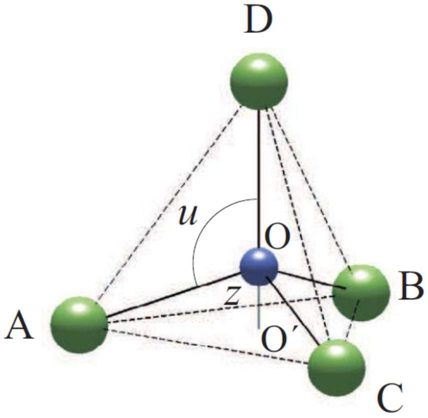

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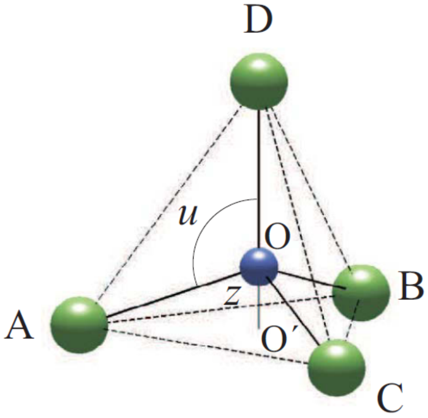

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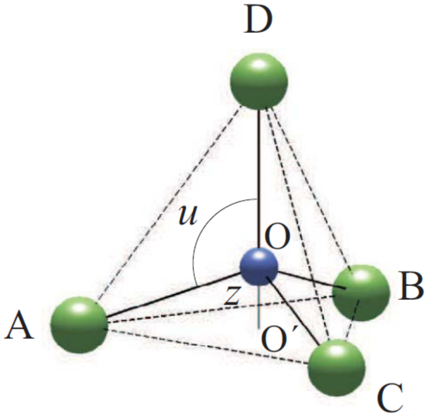

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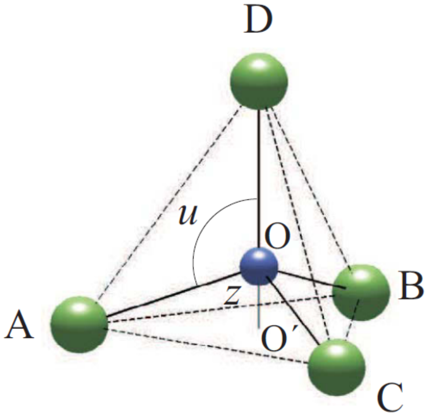

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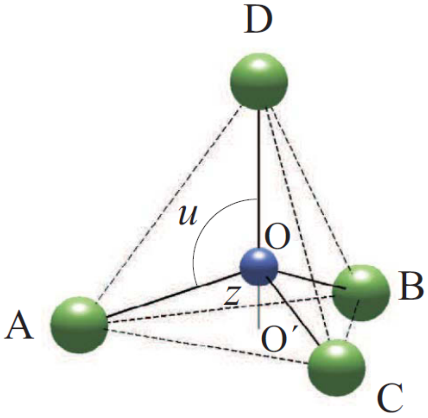

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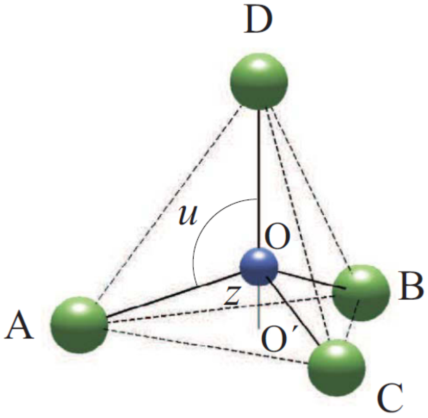

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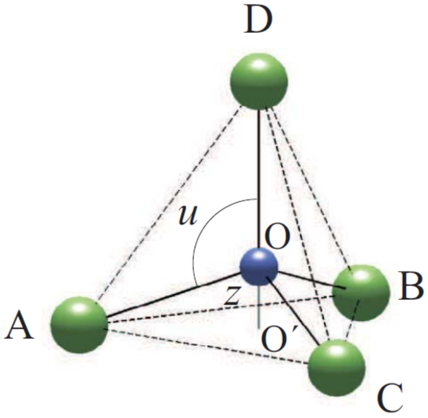

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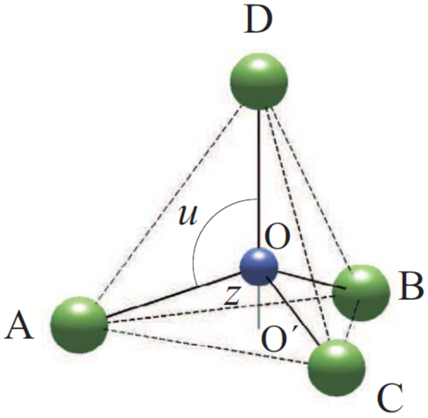

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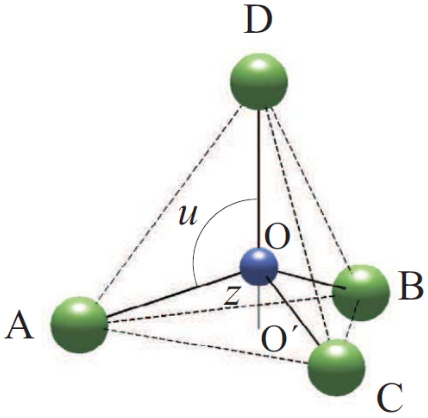

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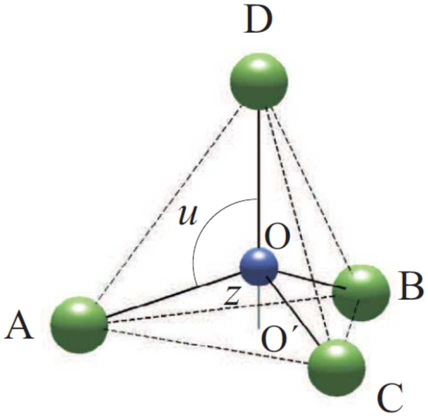

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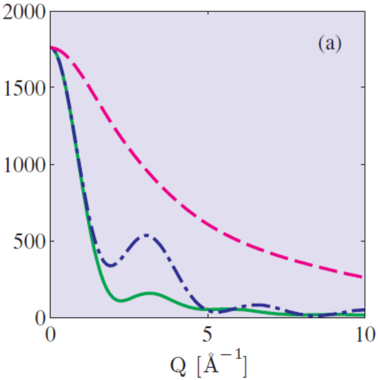

The plot shows the structure factor of CF_4,

The CF_4 scattering factor

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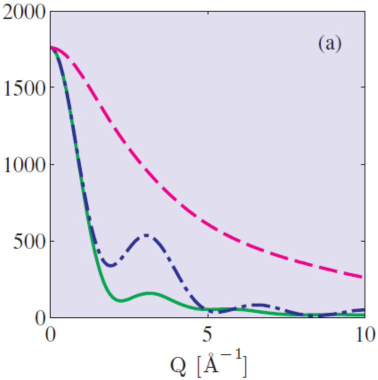

The plot shows the structure factor of CF_4, its orientationally averaged structure factor,

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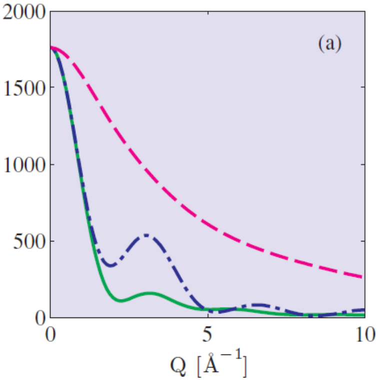

The plot shows the structure factor of CF_4, its orientationally averaged structure factor, and the form factor factor of Mo which has the same number of electrons as CF_4

The CF_4 scattering factor

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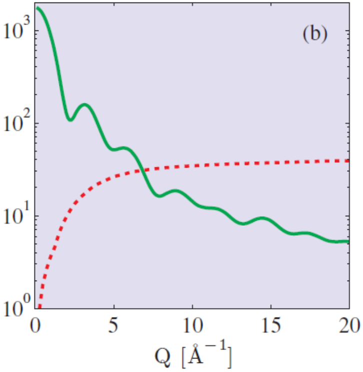

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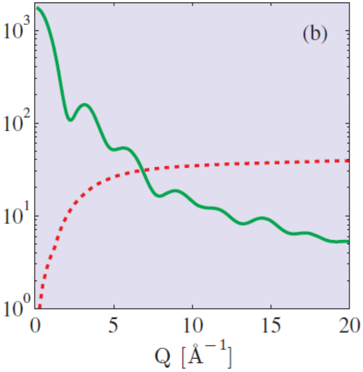


The plot shows the structure factor of CF_4, its orientationally averaged structure factor, and the form factor factor of Mo which has the same number of electrons as CF_4

The logarithmic plot shows the spherically averaged structure factor compared to the inelastic scattering for CF_4

The radial distribution function

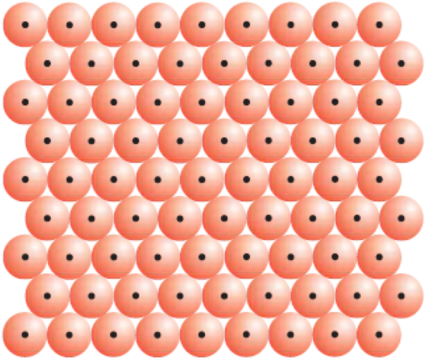
The radial distribution function

Ordered 2D crystal

Amorphous solid or liquid

The radial distribution function

Ordered 2D crystal



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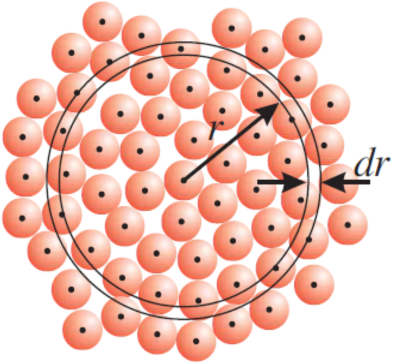
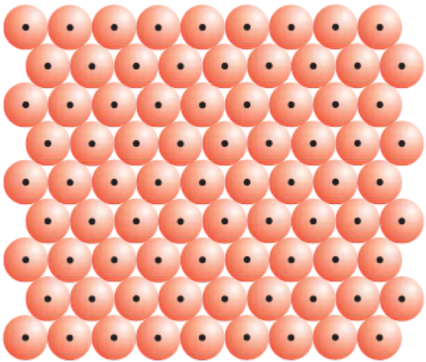


The radial distribution function

Ordered 2D crystal



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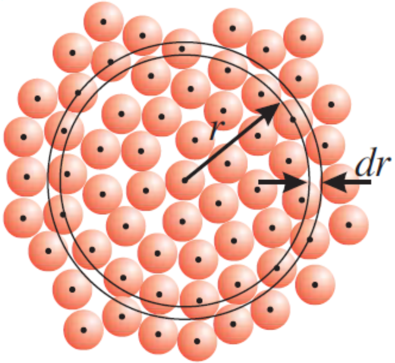

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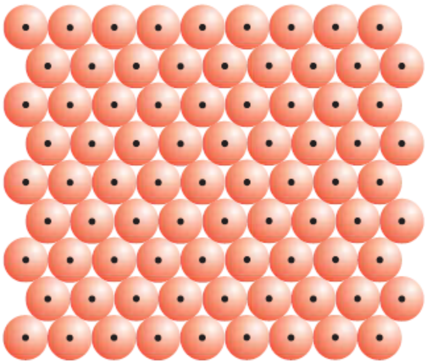
The radial distribution function

Ordered 2D crystal



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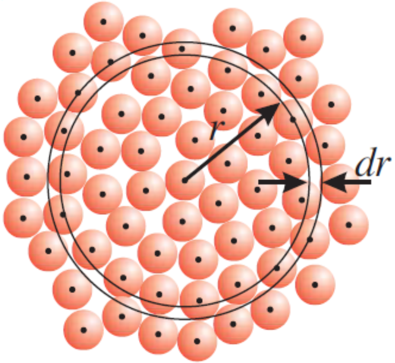

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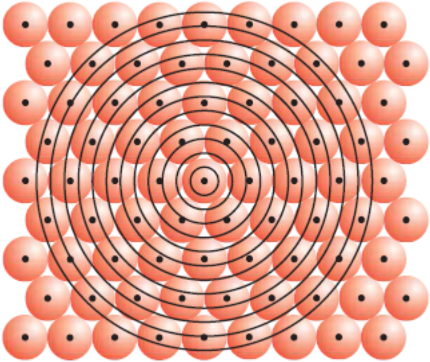

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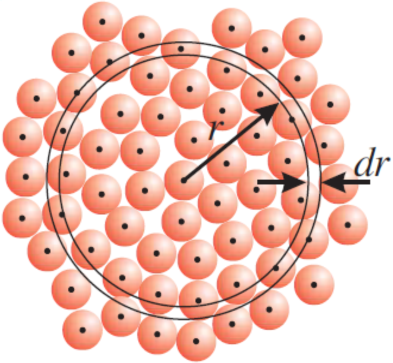

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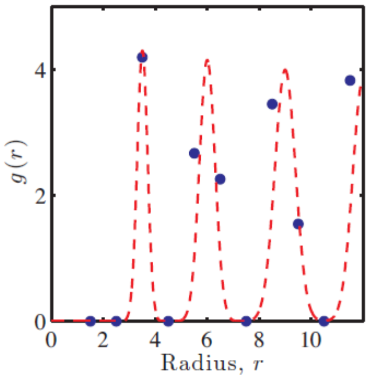

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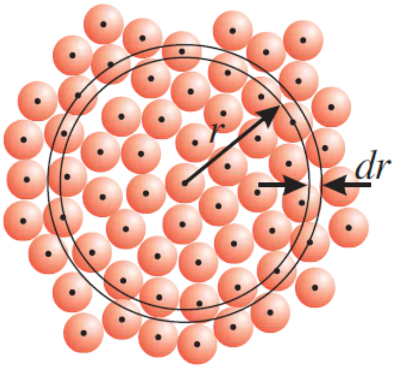

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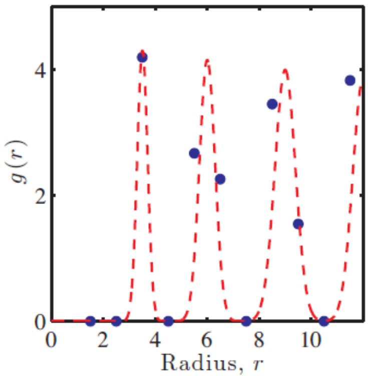

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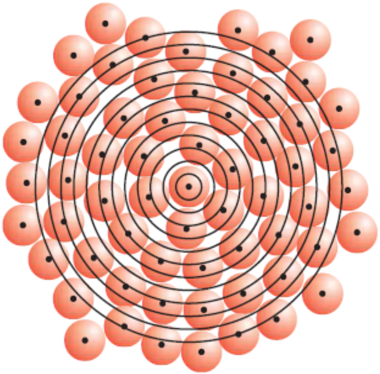

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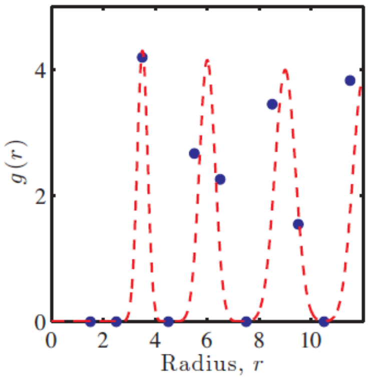

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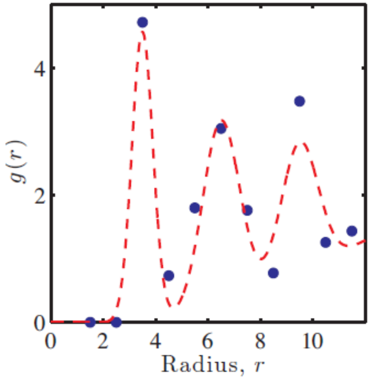

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The relation between radial distribution function and structure factor can be extended to multi-component systems where $g(r) \rightarrow g_{ij}(r)$ and $S(Q) \rightarrow S_{ij}(Q)$.

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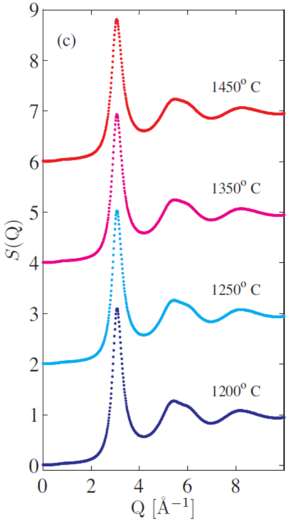

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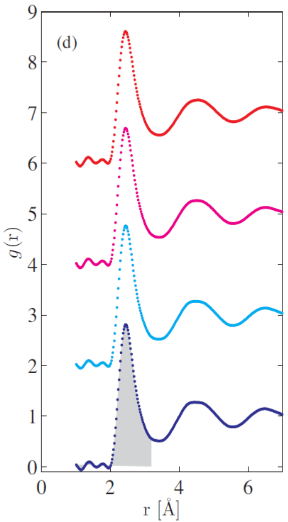

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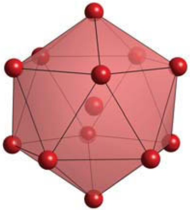

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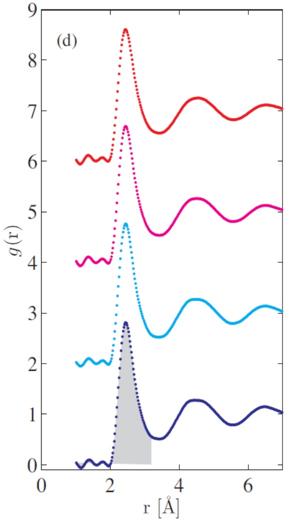

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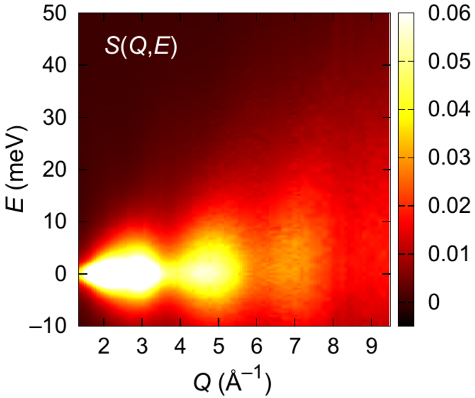

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Water dynamics

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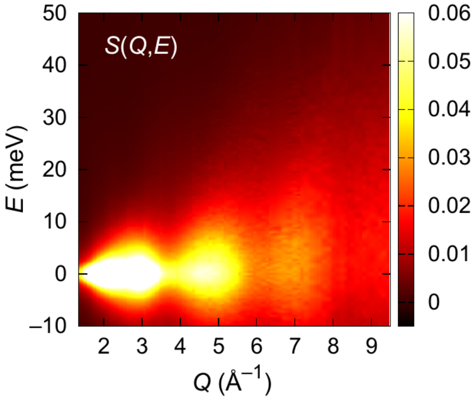

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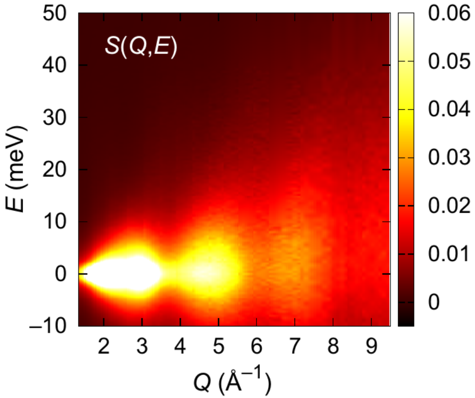

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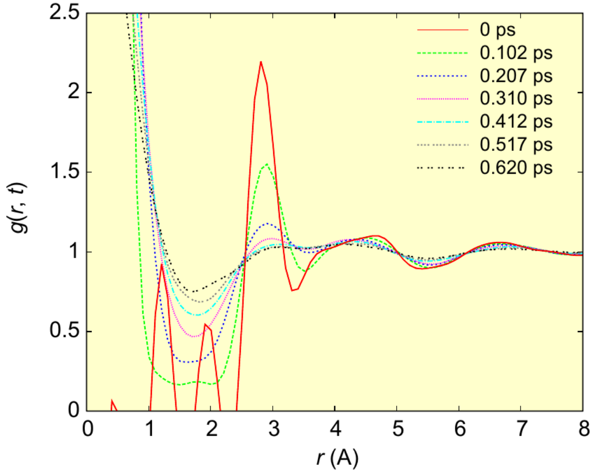

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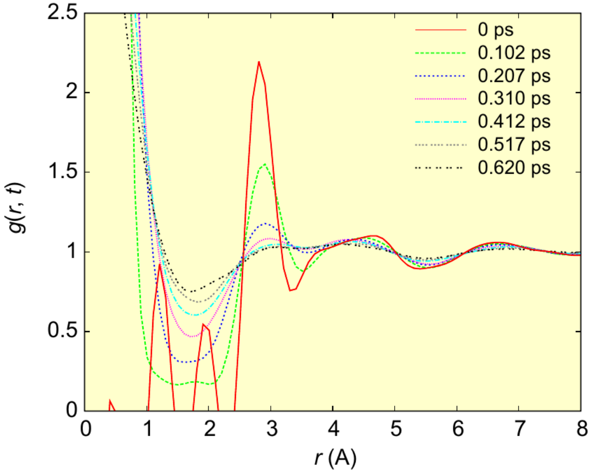

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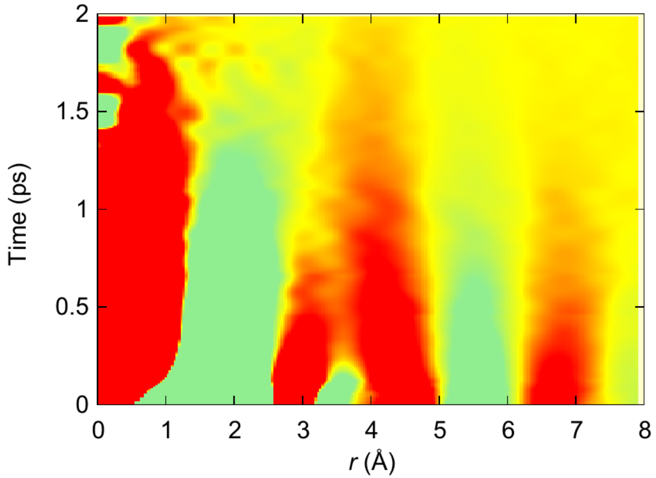

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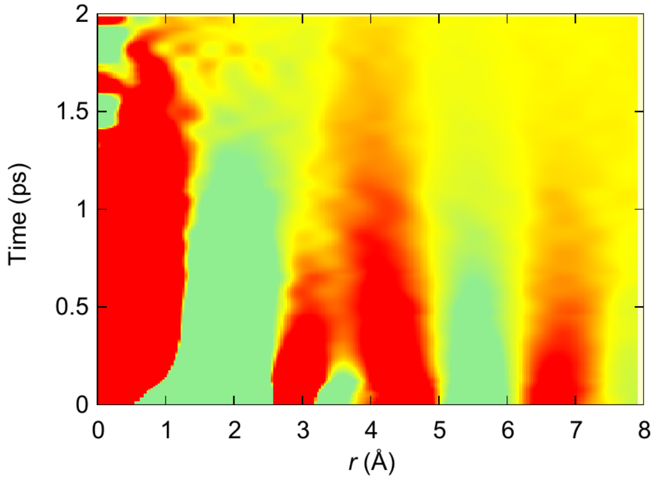

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The first and second peaks are highly coupled in space and time and merge within 0.8 ps. This behavior is different from liquid metals and leads to the viscosity of water.

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Small angle x-ray scattering

$$I(\vec{Q}) = Nf(\vec{Q})^2 + f(\vec{Q})^2 \sum_n \int_V [\rho_n(\vec{r}_{nm}) - \rho_{at}] e^{i\vec{Q}\cdot(\vec{r_n}-\vec{r_m})} \, dV_m + f(\vec{Q})^2 \rho_{at} \sum_n \int_V e^{i\vec{Q}\cdot(\vec{r_n}-\vec{r_m})} \, dV_m$$

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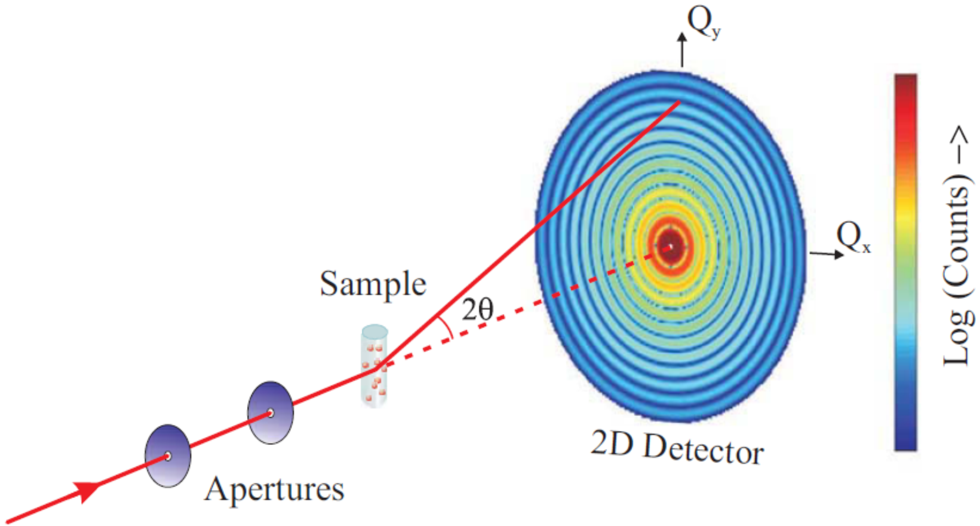
The SAXS experiment



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Where $\Delta\rho = (\rho_{sl,p} - \rho_{sl,0})$, and the form factor depends on the morphology of the particle (size and shape).

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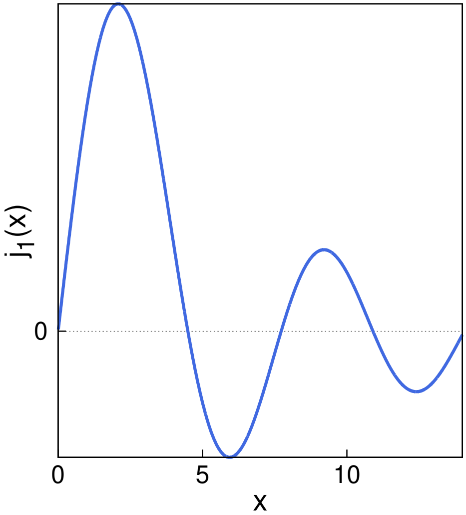

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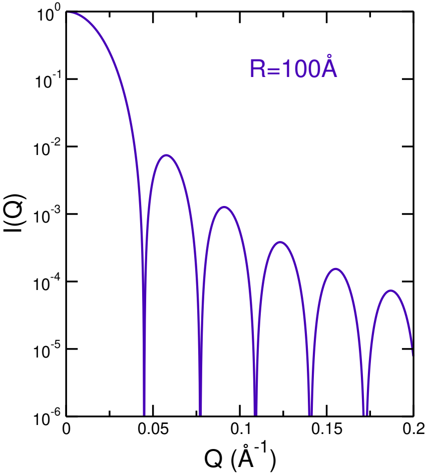

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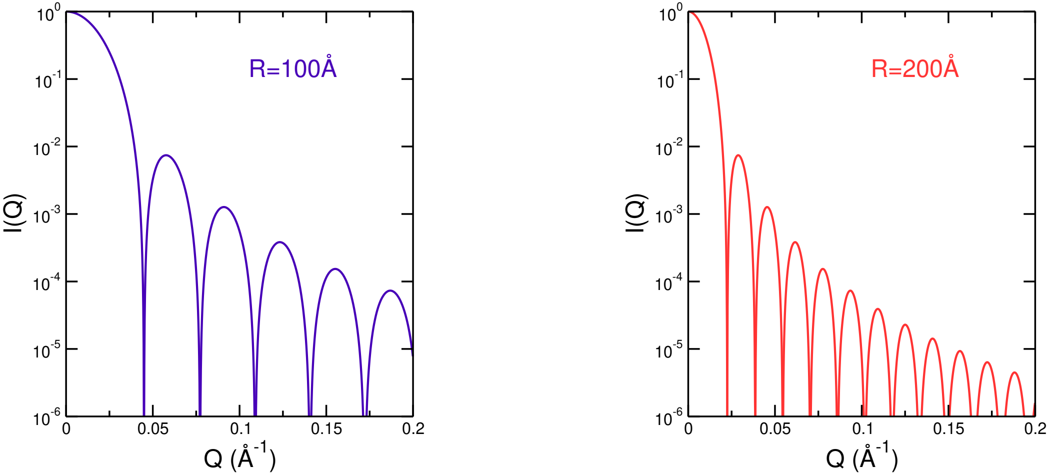

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$$I^{SAXS}(\vec{Q}) = \Delta\rho^2 V_p^2 |\mathcal{F}(\vec{Q})|^2, \qquad \mathcal{F}(\vec{Q}) = 3\left[\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3}\right]$$

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

this simplifies to $\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10} and$

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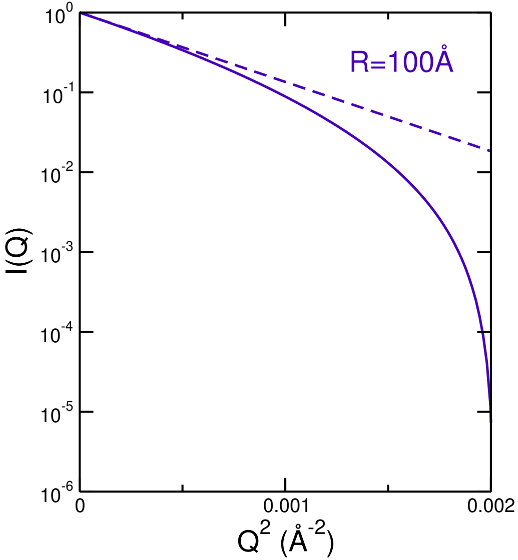

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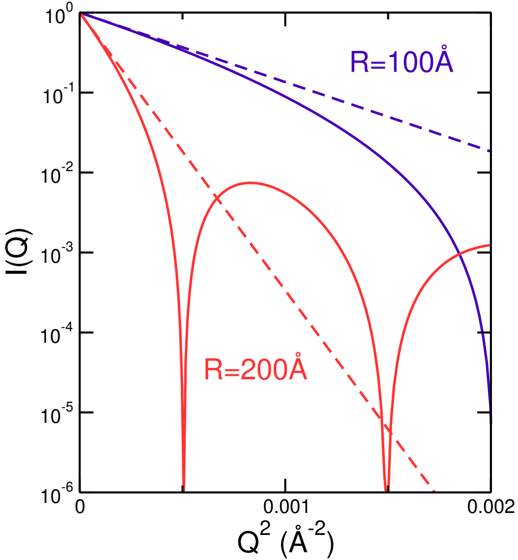

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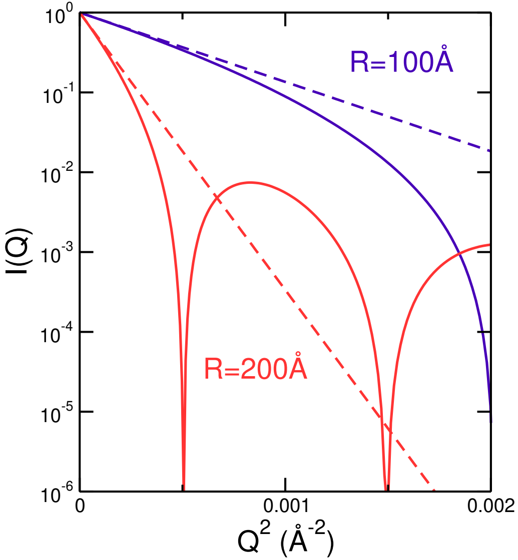

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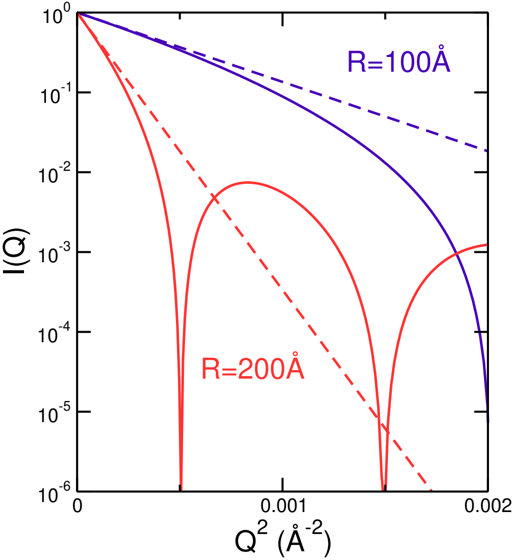

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