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- Liquid scattering

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Homework Assignment #03:
Chapter 3:1,3,4,6,8
due Thursday, February 27, 2020

Scattering from molecules

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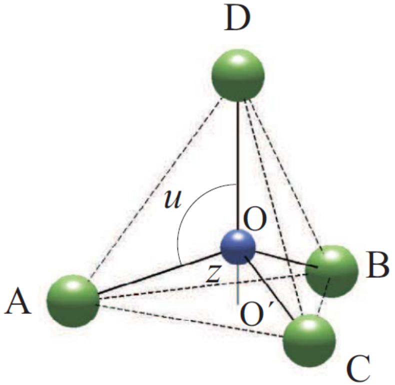
As an example take the CF_4 molecule



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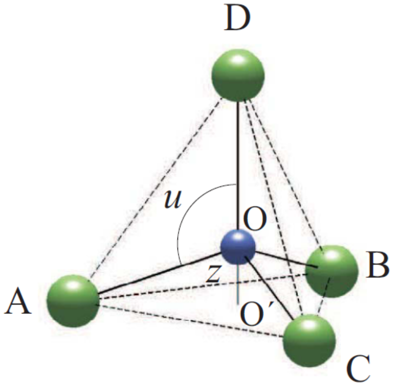

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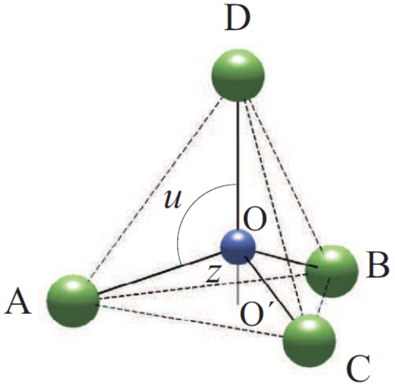

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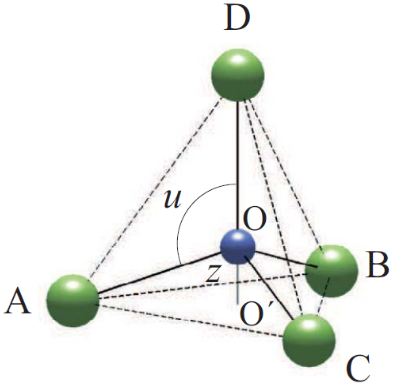

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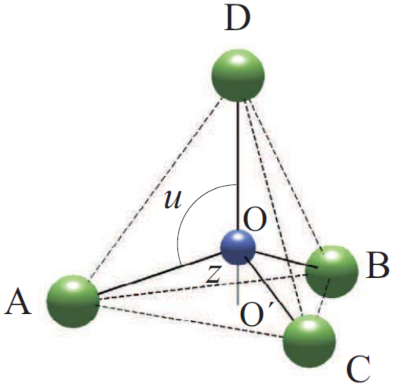

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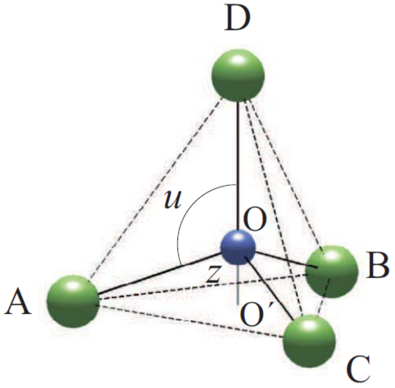

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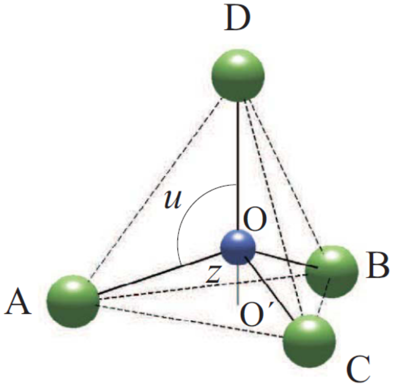

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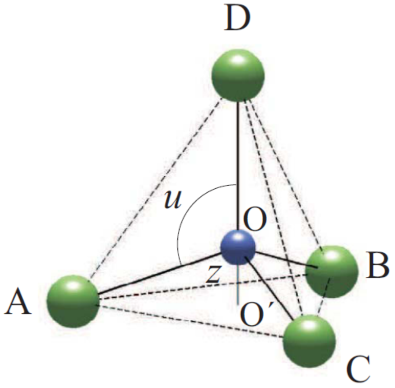

$$\overline{OA} \cdot \overline{OD} = 1 \cdot 1 \cdot \cos u$$

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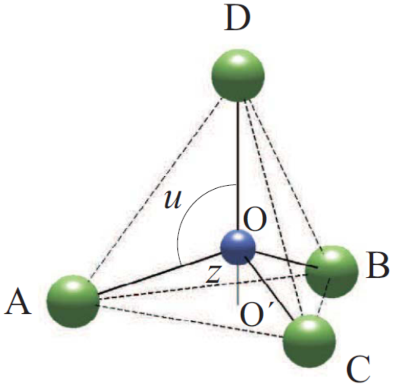

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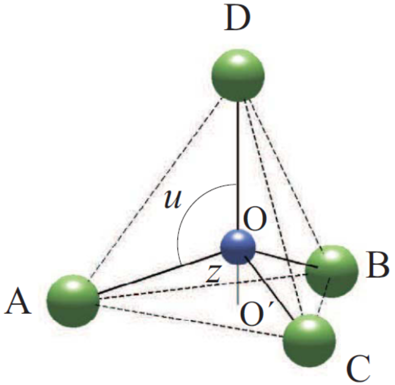

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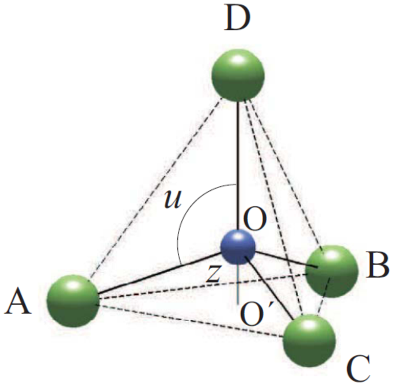

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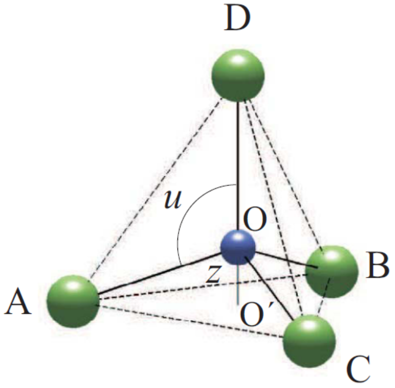

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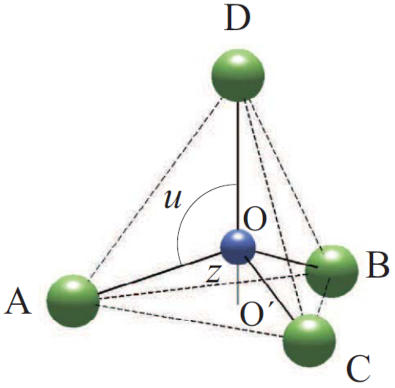
$$-z = (\overline{OO'} + \overline{O'A}) \cdot (\overline{OO'} + \overline{O'B})$$



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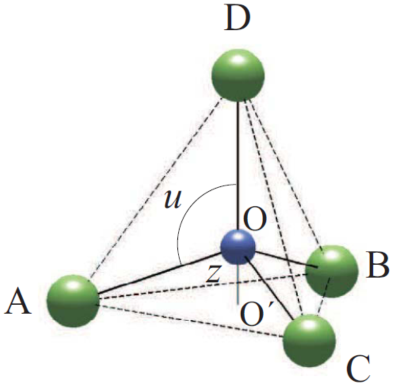

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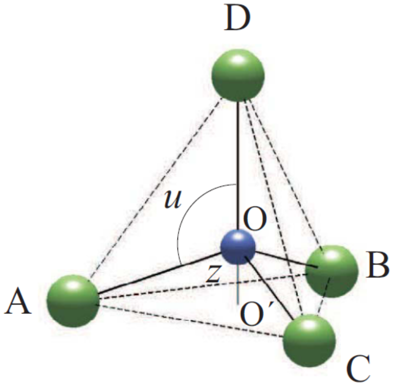

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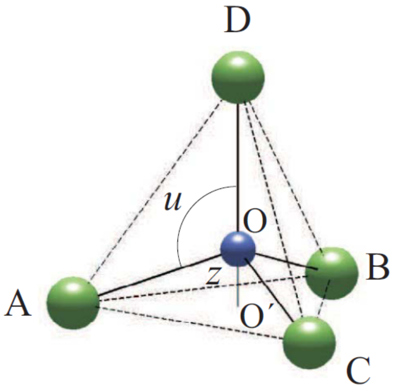

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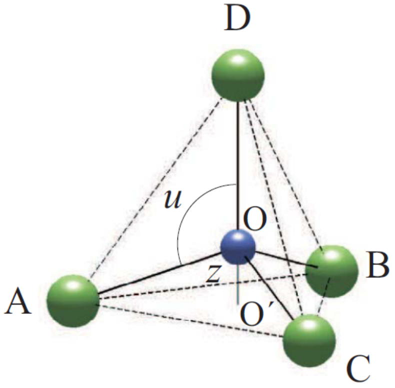

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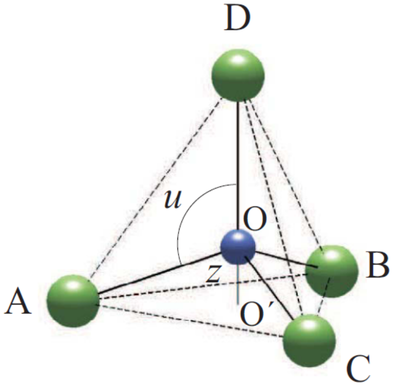

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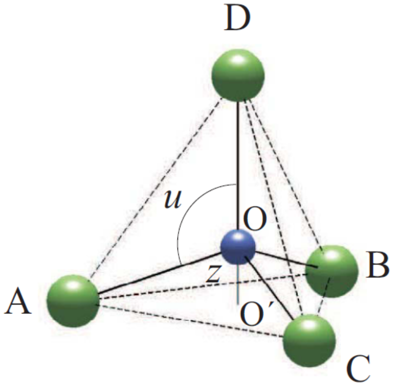

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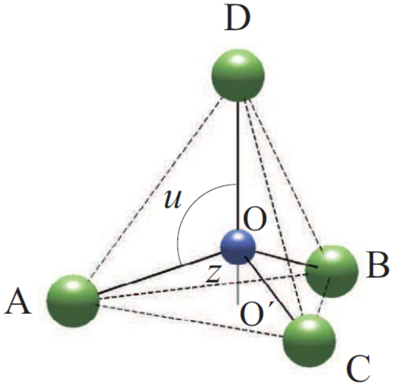

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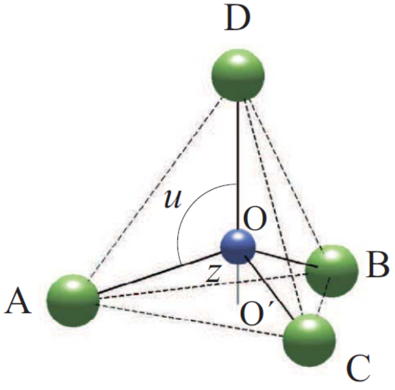

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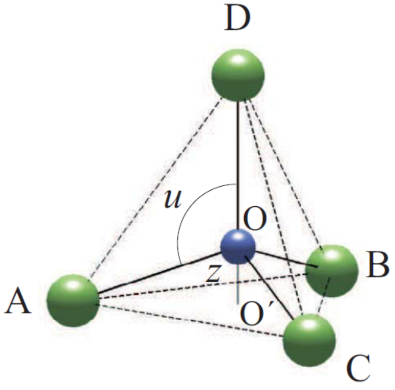

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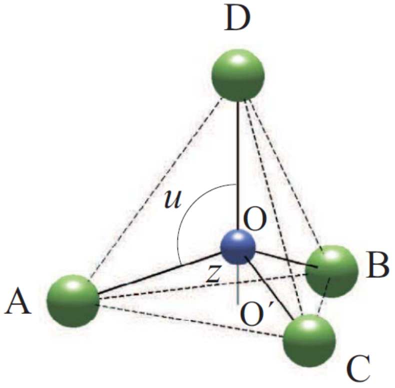

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$$F_{\pm}^{mol} = f^C(Q) + f^F(Q)\left[3e^{\mp iQR/3} + e^{\pm iQR}\right]$$

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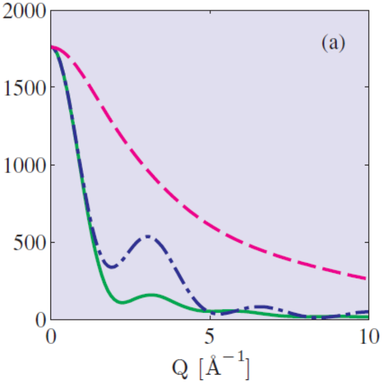
The plot shows the structure factor of CF_4,



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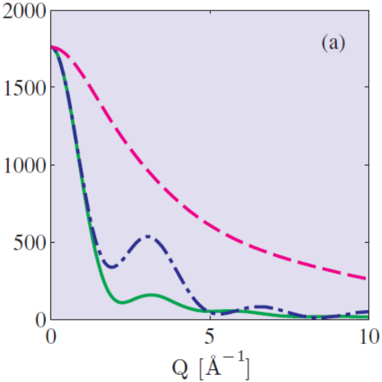
$$|F^{mol}|^2 = |f^C|^2 + 4|f^F|^2 + 8f^Cf^F\frac{\sin(QR)}{QR} + 12|f^F|^2\frac{\sin(Q\sqrt{8/3}R)}{Q\sqrt{8/3}R}$$

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



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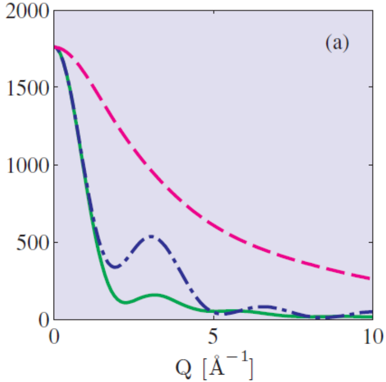
The plot shows the structure factor of CF_4, its orientationally averaged structure factor, and the form factor factor of Mo which has the same number of electrons as CF_4



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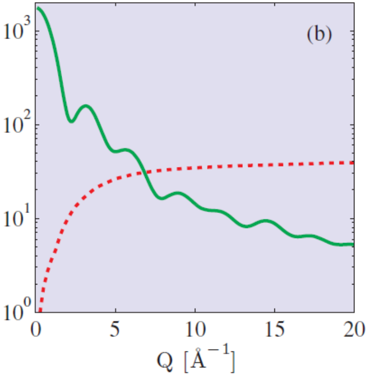

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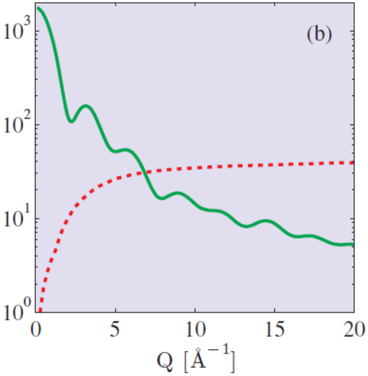
The logarithmic plot shows the spherically averaged structure factor compared to the inelastic scattering for CF_4



The radial distribution function

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Ordered 2D crystal

Amorphous solid or liquid

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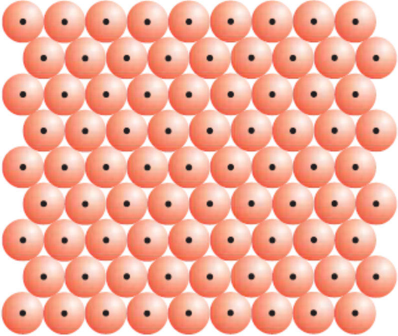

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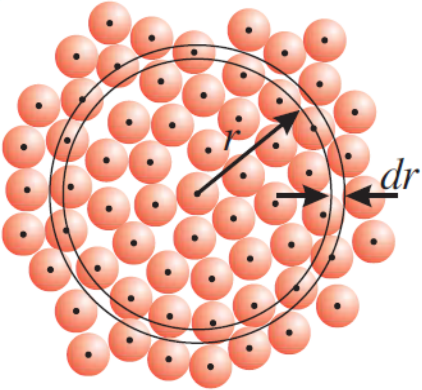

The radial distribution function

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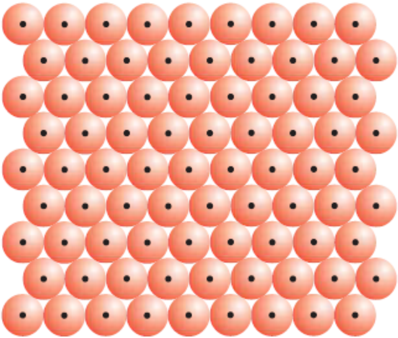

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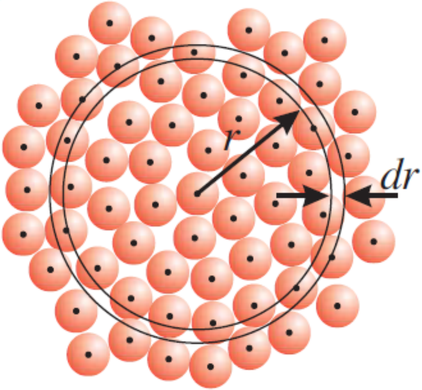

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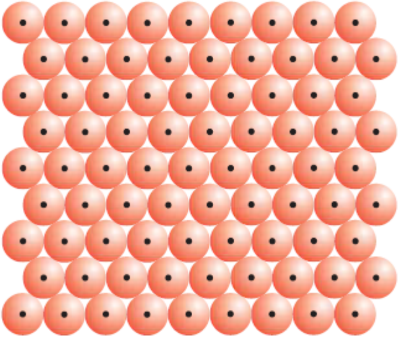
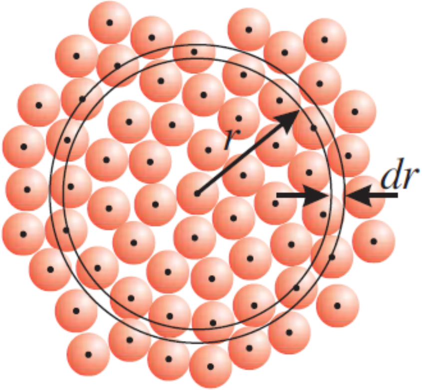
The radial distribution function





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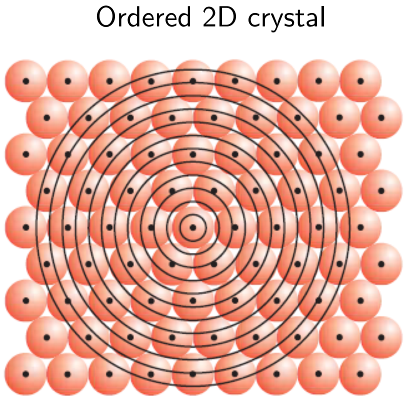

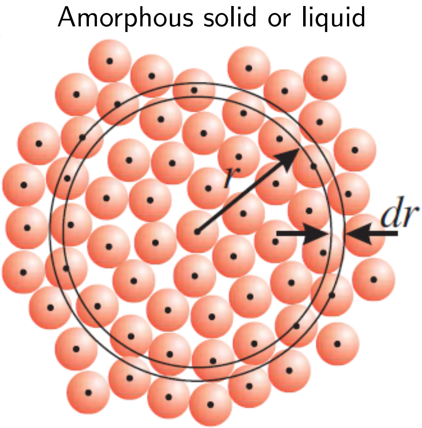

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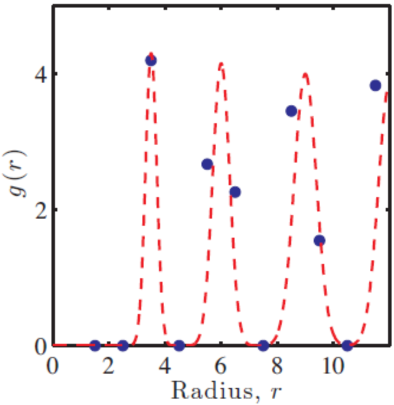

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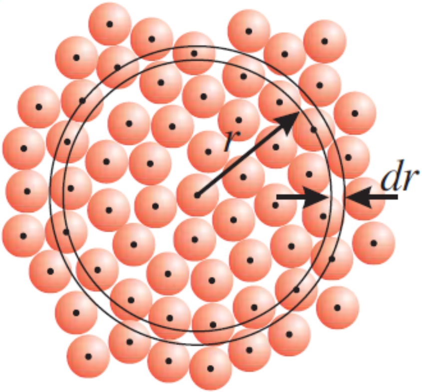

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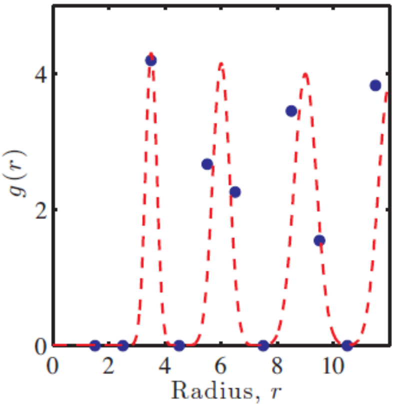

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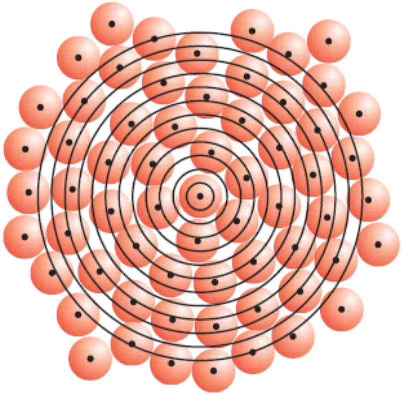

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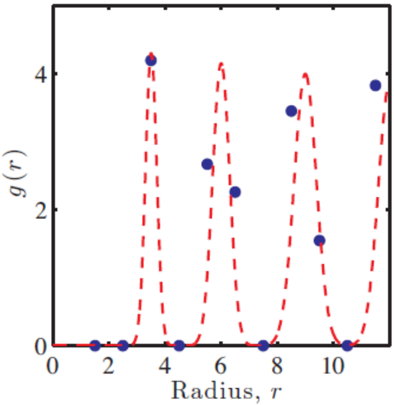

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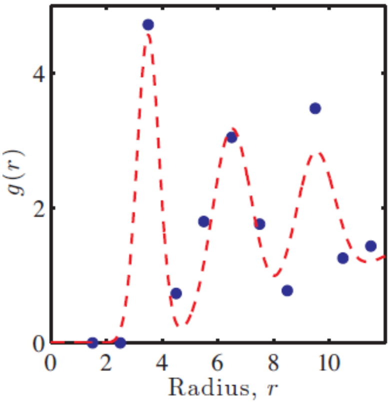

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The relation between radial distribution function and structure factor can be extended to multi-component systems where $g(r) \rightarrow g_{ij}(r)$ and $S(Q) \rightarrow S_{ij}(Q)$.

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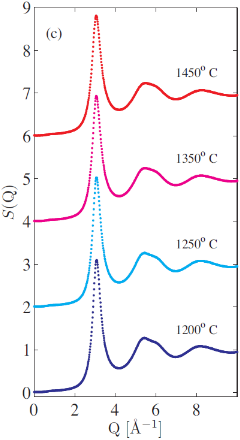

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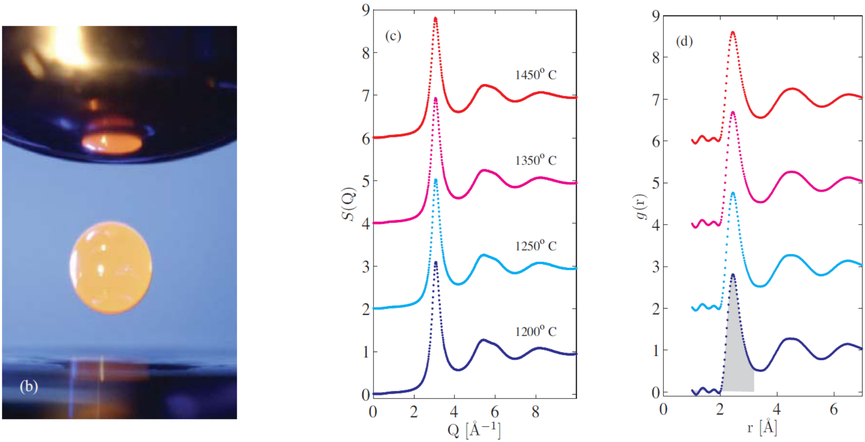

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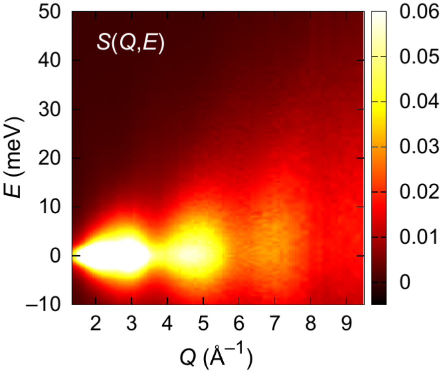

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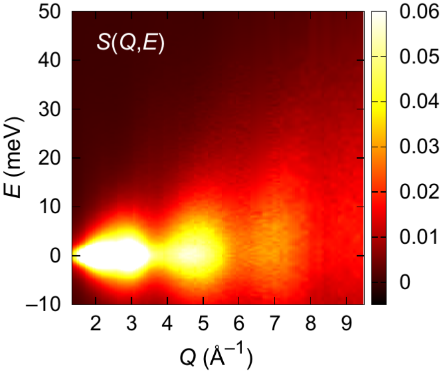

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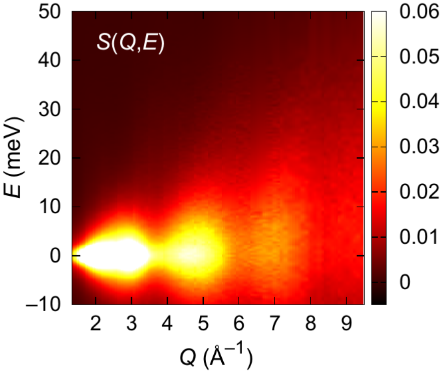
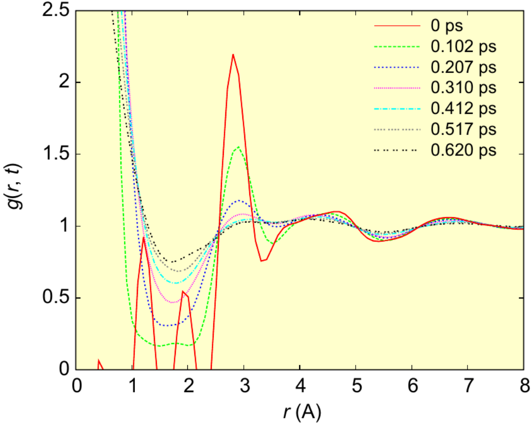


The Van Hoff function can be obtained by a double Fourier transform

$$g(r,t) - 1 = \frac{1}{2\rho\pi^2 r} \int\int e^{i\omega t} \sin(Qr) QS(Q,E) dQ\, dE$$

"Seeing real-space dynamics of liquid water through inelastic x-ray scattering," T. Iwashita et al. *Sci. Adv.* **3**, e1603079 (2017).

Water dynamics



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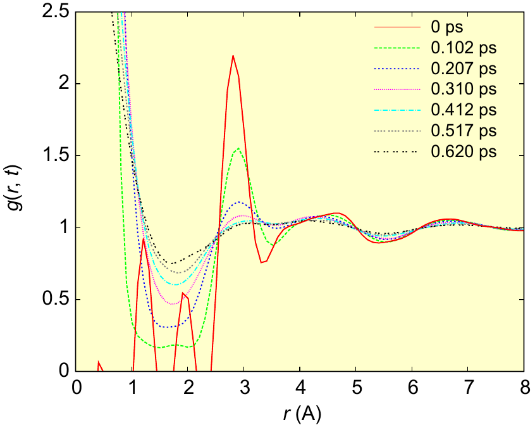

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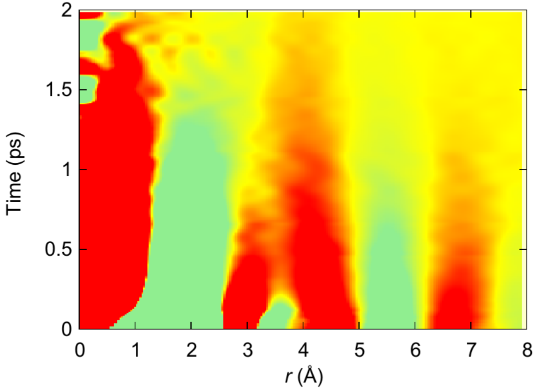

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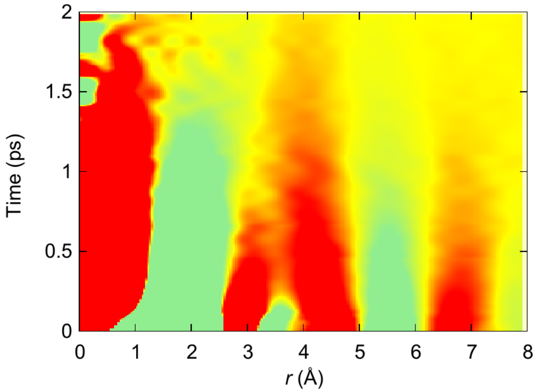

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The first and second peaks are highly coupled in space and time and merge within 0.8 ps. This behavior is different from liquid metals and leads to the viscosity of water.

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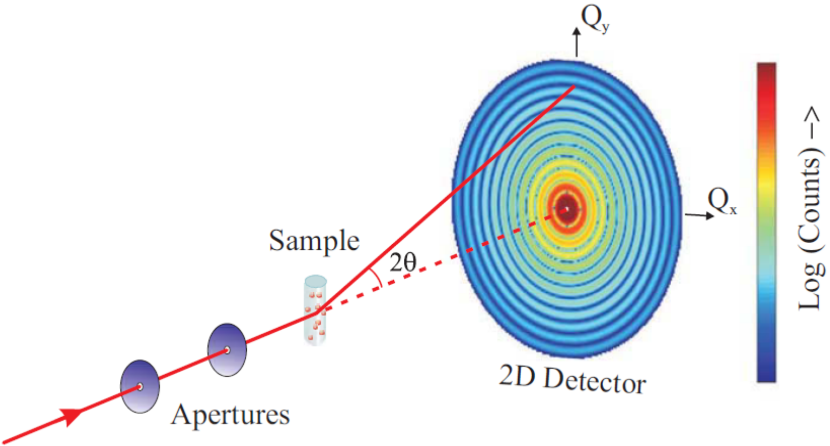
The SAXS experiment



Scattering from a dilute solution

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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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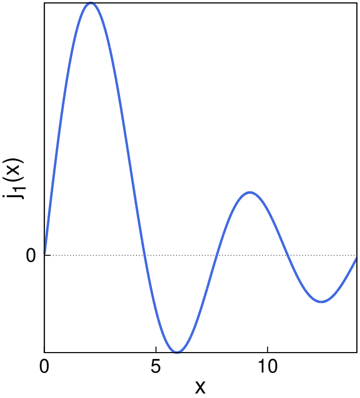

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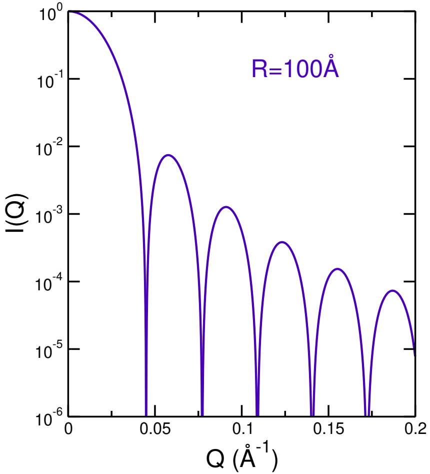

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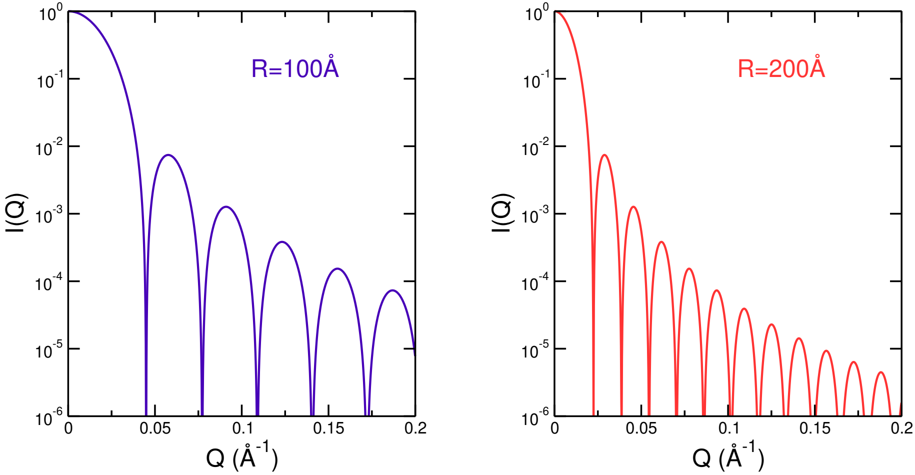

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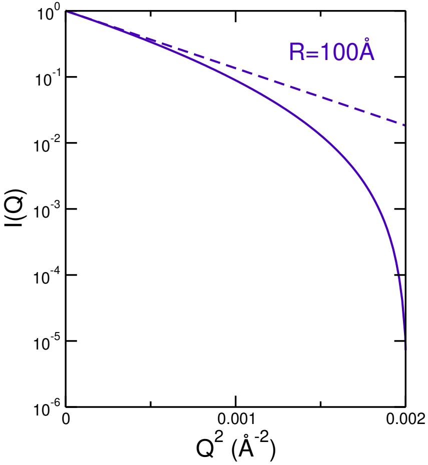

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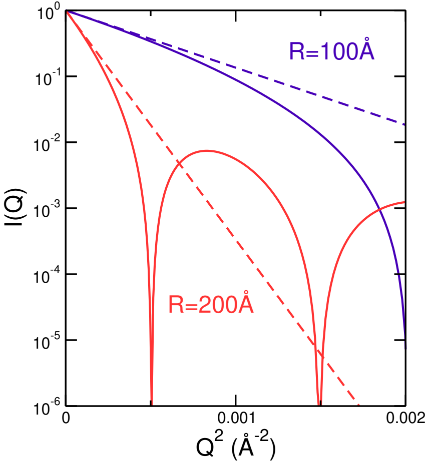

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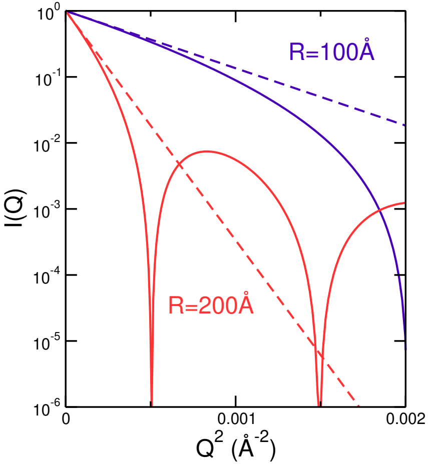

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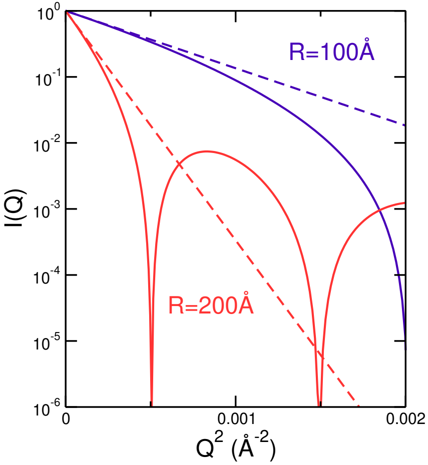

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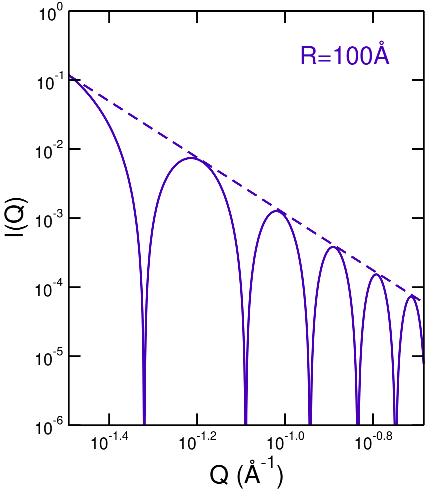

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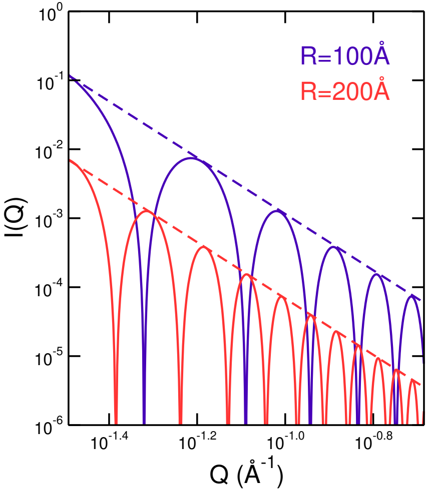

power law drop as Q^{-4} for spheres

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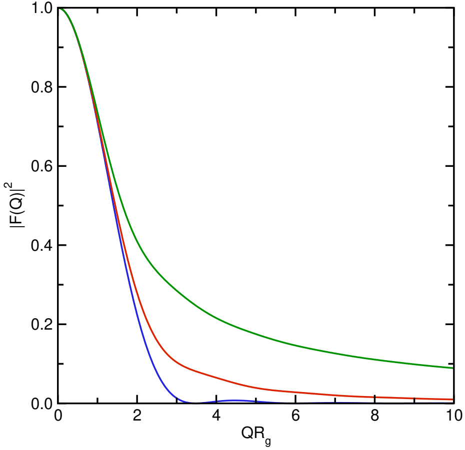

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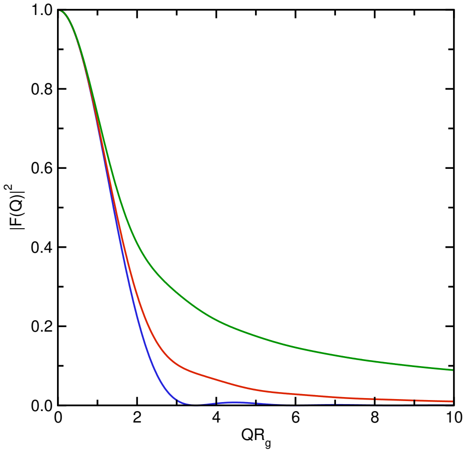

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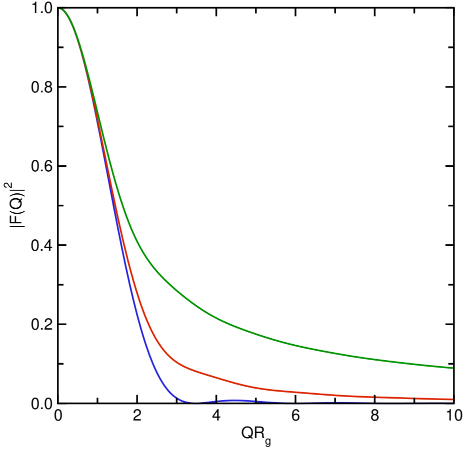

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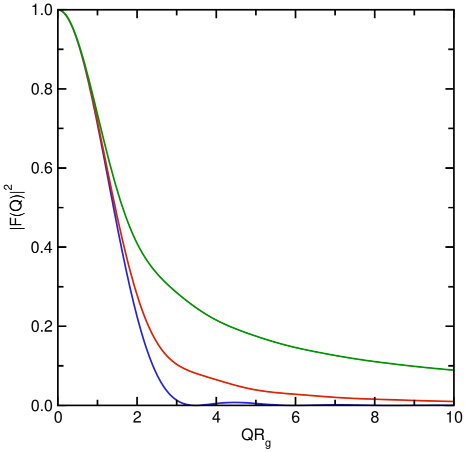

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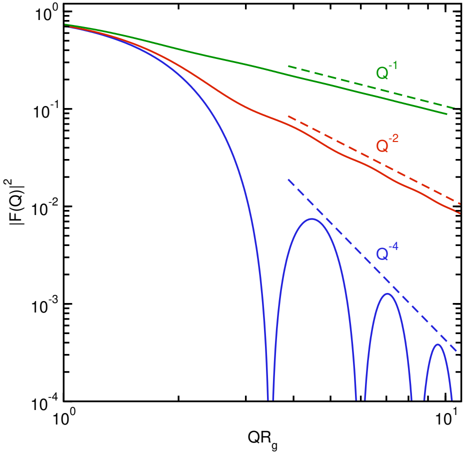

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p = 0

p = 10%

p = 20%