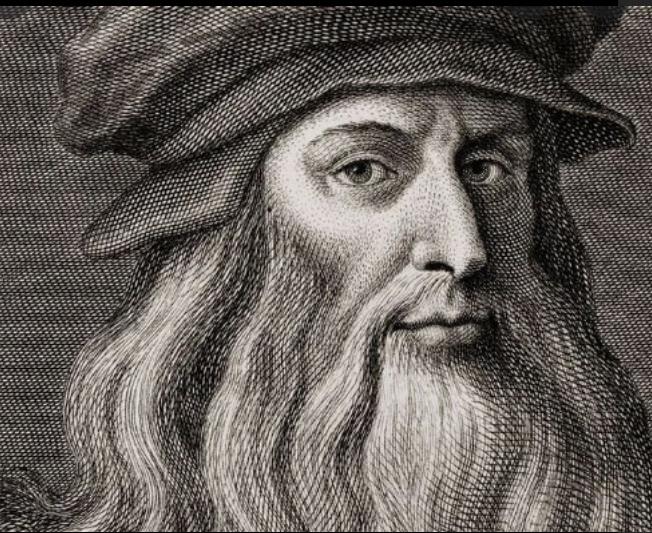


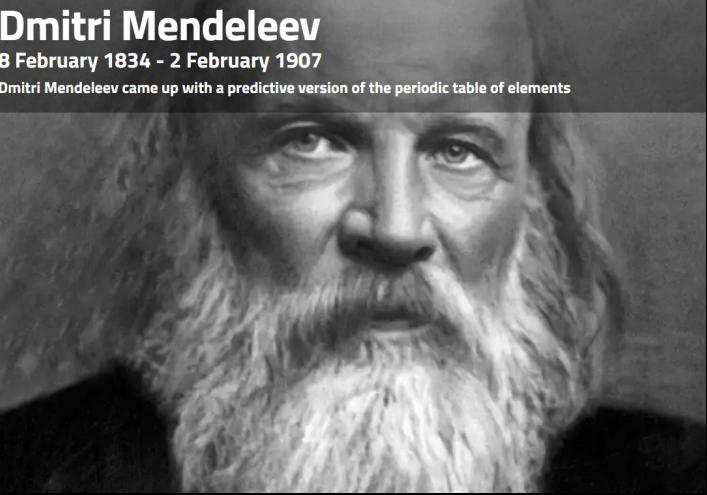
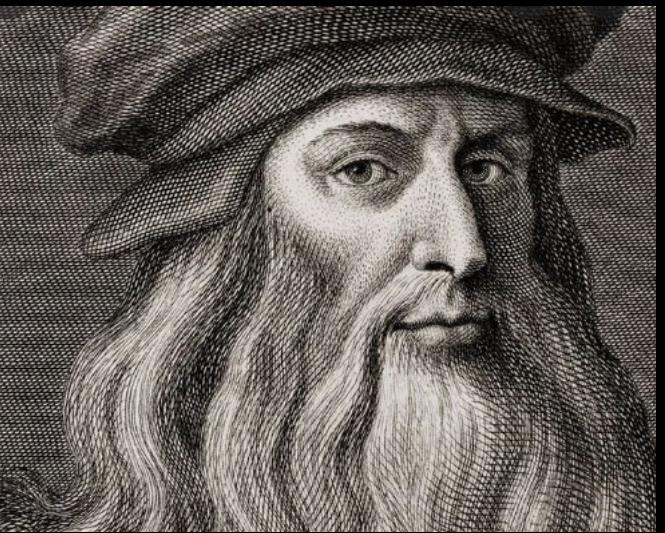
Chemistry is Imagination! Intuition!



THE ESSENCE OF CHEMICAL SCIENCE
THUS FINDS ITS FULL EXPRESSION IN
THE WORDS OF LEONARDO DA VINCI:
**"WHERE NATURE FINISHES
PRODUCING ITS OWN SPECIES, MAN
BEGINS, USING NATURAL THINGS AND
IN HARMONY WITH THIS VERY NATURE,
TO CREATE AN INFINITY OF SPECIES."**

- JEAN-MARIE LEHN -

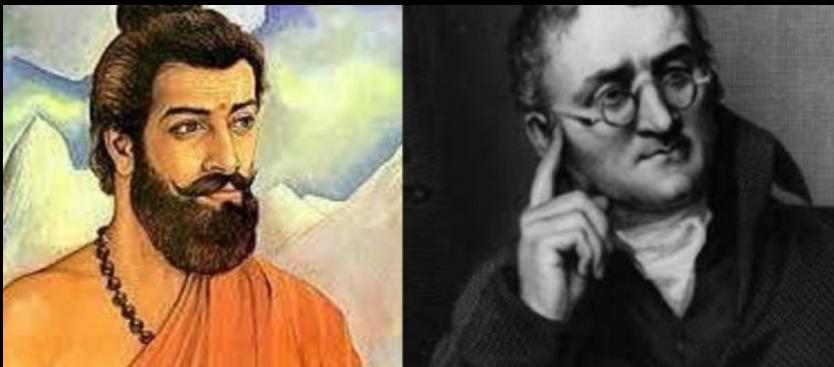




Welcome on board!

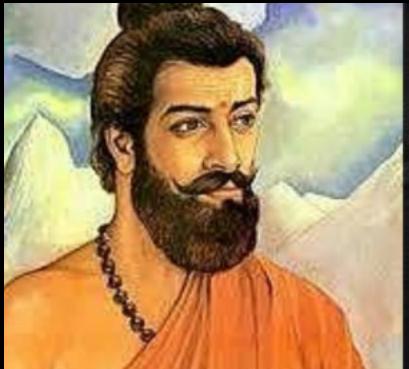
CH 1101

Now Begins!

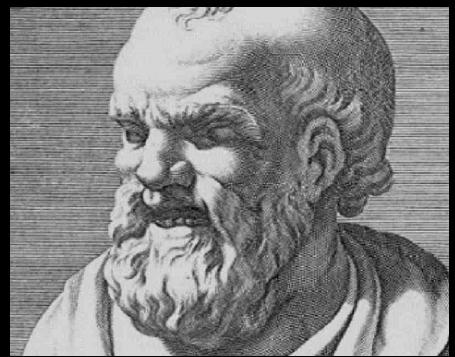


Questions?
E-mail: s.roy@iiserkol.ac.in

What is Matter?



Kanad
6th -2nd Century
BC



Democritus
3rd Century
BC



Dalton,
1801 AD

Part of an early table of atomic and molecular weights published by Dalton

Element	Weight
Hydrogen	1
Azot	4.2
Carbon (charcoal)	4.3
Ammonia	5.2
Oxygen	5.5
Water	6.5
Phosphorus	7.2
Nitrous gas	9.3
Ether	9.6
Nitrous oxide	13.7
Sulphur	14.4
Nitric acid	15.2

Adapted from J. Dalton, *Memoirs of the Literary and Philosophical Society of Manchester*, 2(1), 207, 1805, table on p. 287. (Azot is the old name for nitrogen.)

- Kanad, the Indian Philosopher ideated atoms as early as in 6th -5th Century BC, earlier than Democritus.
- In 1801, John Dalton, an English schoolteacher took the ancient Greek notion of Democritus' atoms and made it quantitative
- He proposed matter was composed of atoms that were indestructible and nonchangeable

What is Matter?

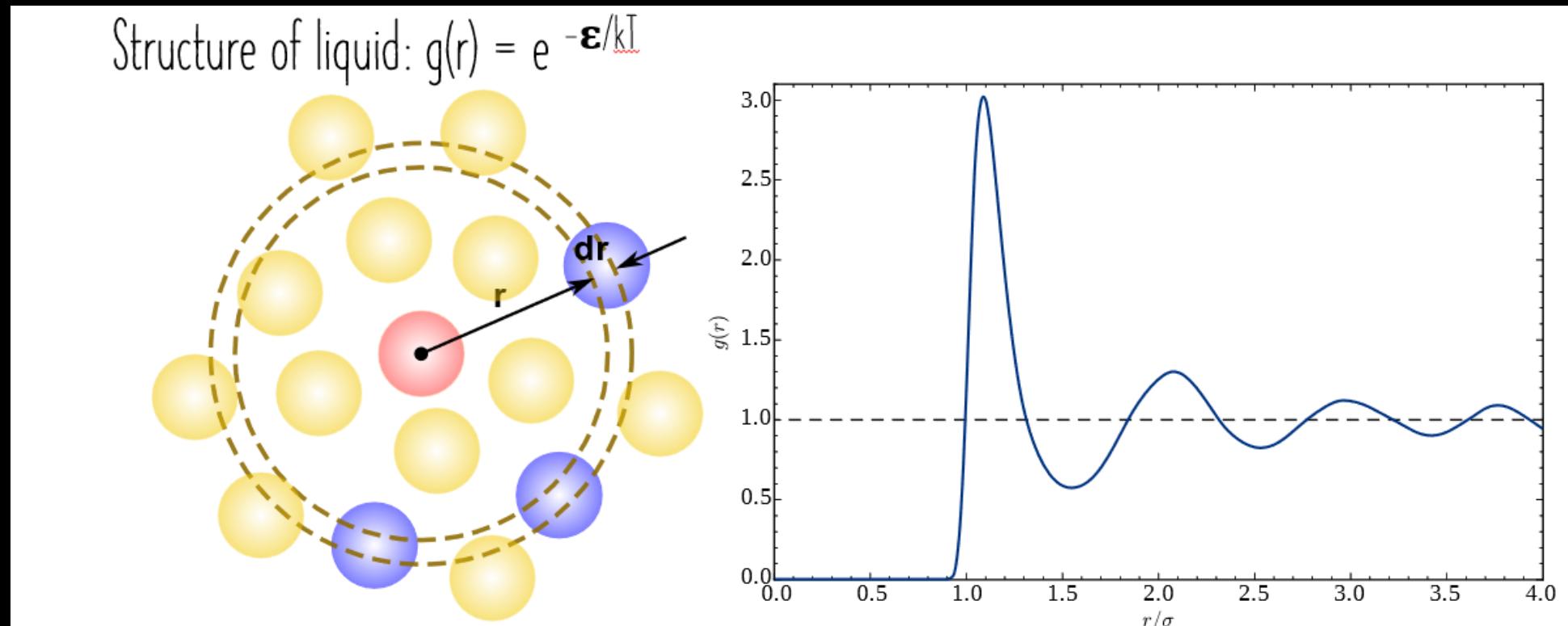
- What are liquids?
- Are liquids made of atoms?



- Is Crystallization then a phase transition?

On Liquid Models

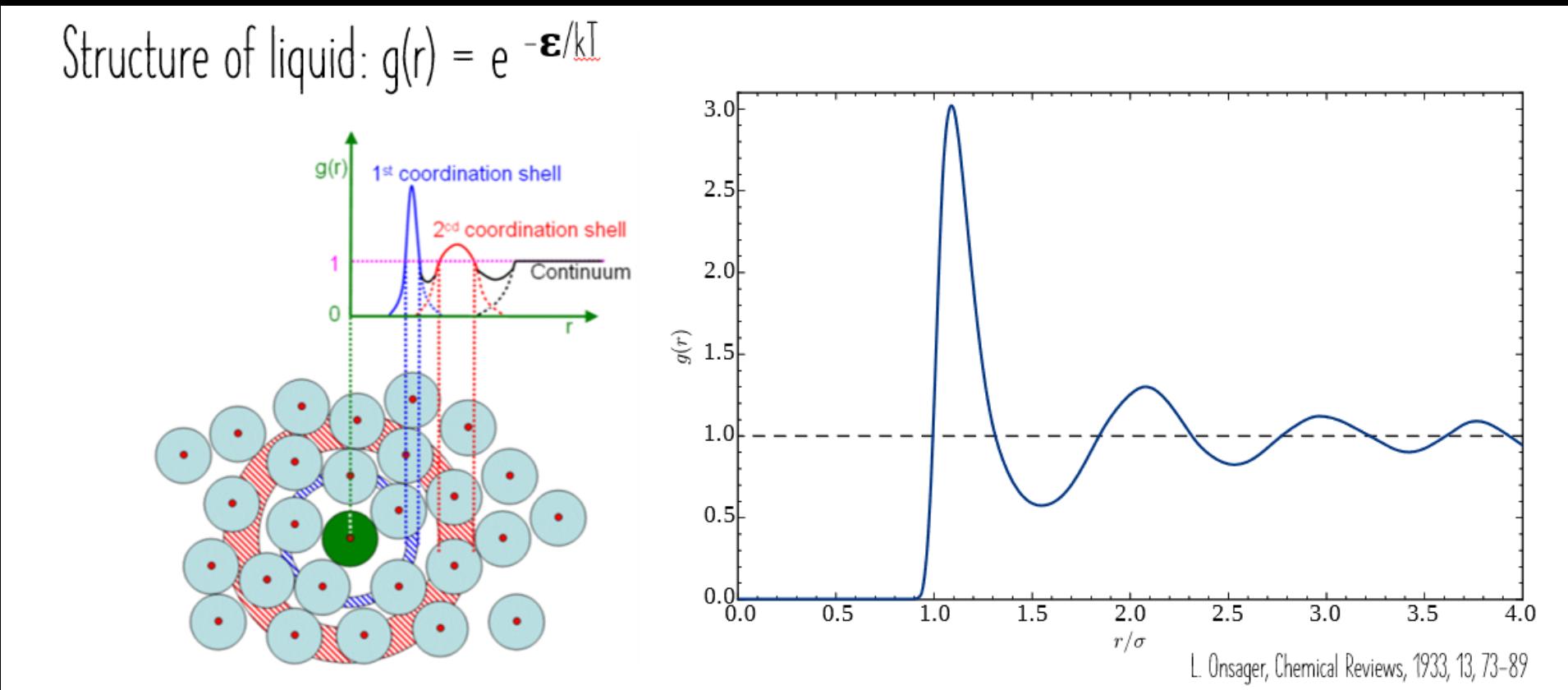
Structure of liquid: $g(r) = e^{-\epsilon/kT}$



L. Onsager, Chemical Reviews, 1933, 13, 73-89

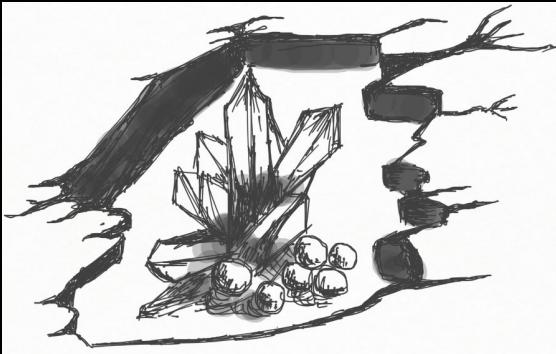
On Liquid Models

Structure of liquid: $g(r) = e^{-\epsilon/kT}$



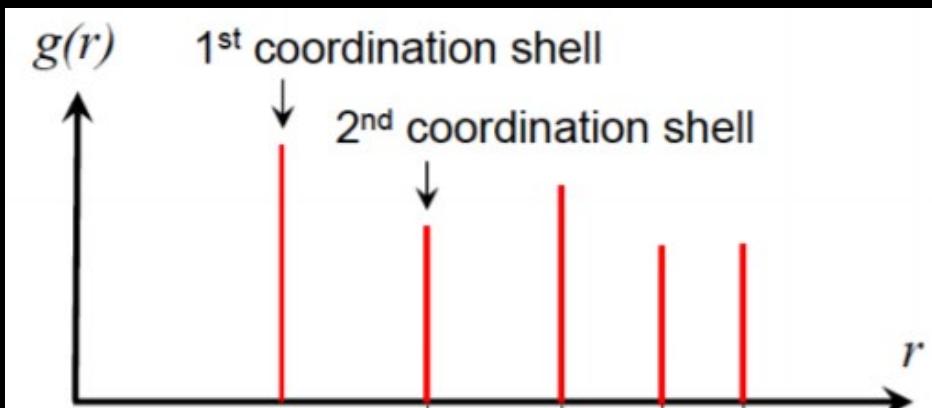
L. Onsager, Chemical Reviews, 1933, 13, 73-89

During Crystallization

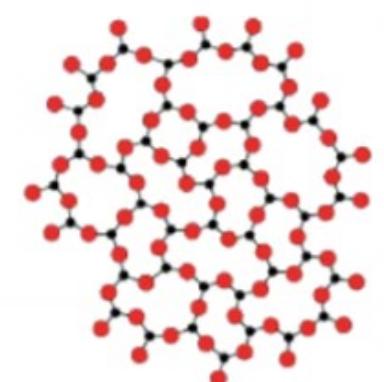
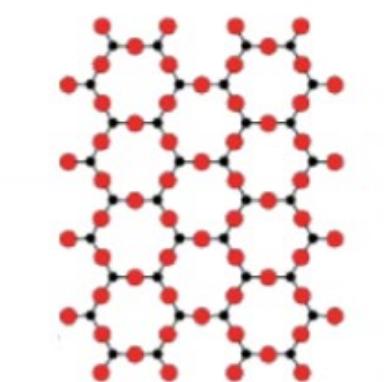
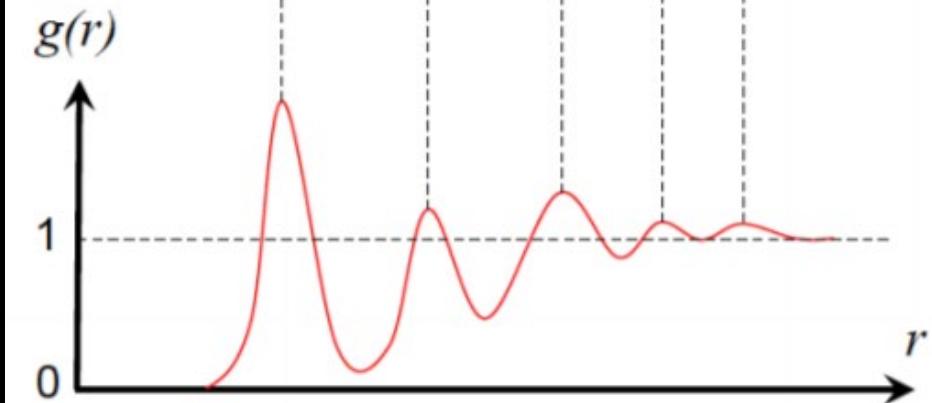


Change in: $g(r) = e^{-\epsilon/kT}$

Crystal



Liquid/
Glass



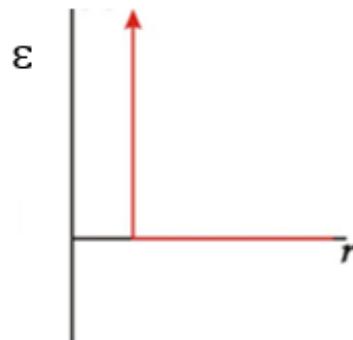
On Liquids & Crystallization

$$\text{Liquid: } g(r) = e^{-\frac{\epsilon}{kT}}$$

Hard sphere potential:

This is the simplest potential, given by:

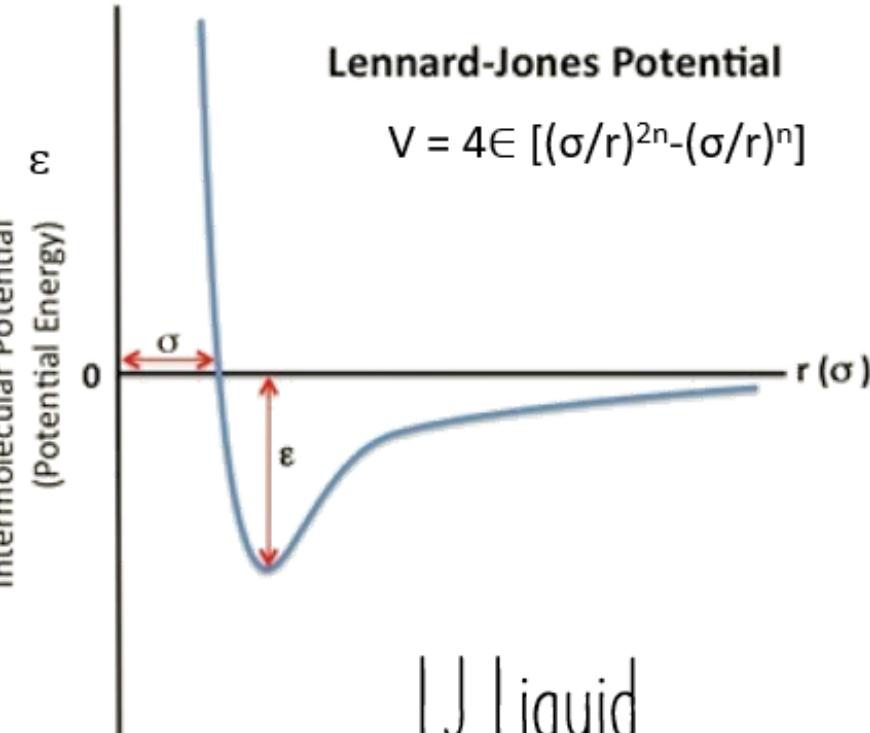
$$\epsilon = \begin{cases} \infty, r \leq \sigma \\ 0, r > \sigma \end{cases}$$



HS Liquid

B. Widom, Science, 1967, 157, 375-382.

H. Lekkerkerker, Physica A: Statistical Mechanics and its Applications, 1997, 244, 227-237.



LJ Liquid

Determine Crystallization!

In principle when there is a certain change in $g(r)$ we can find ϵ .

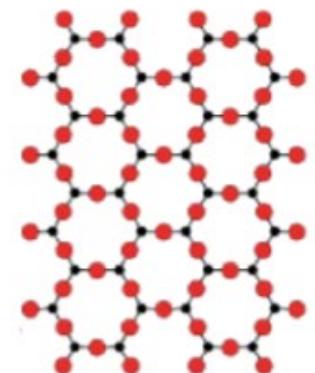
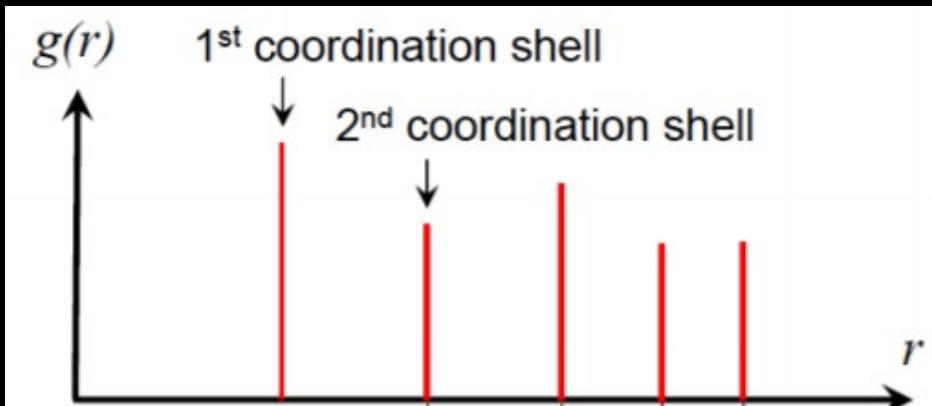
What is Matter?

Matter is particulate. Can be mapped.

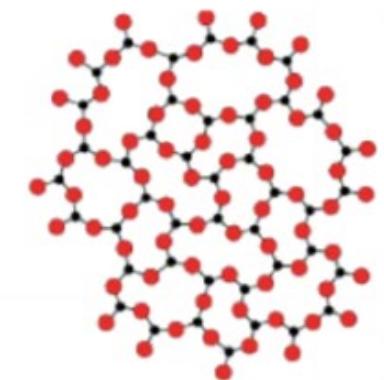
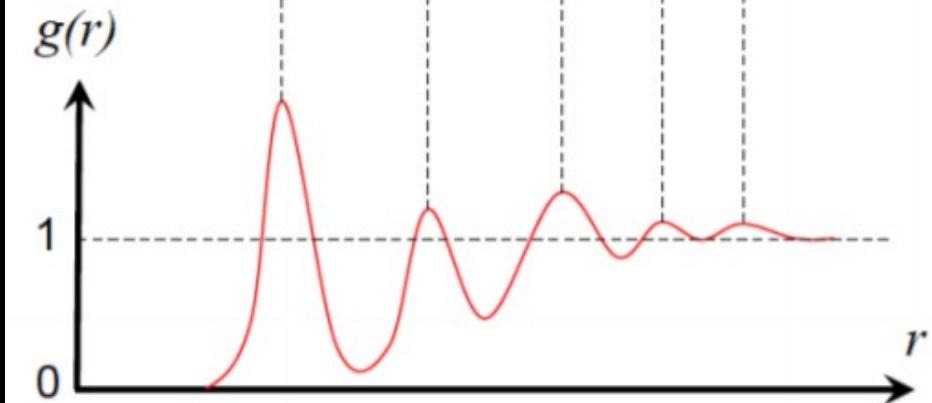


Change in: $g(r) = e^{-\epsilon/kT}$

Crystal

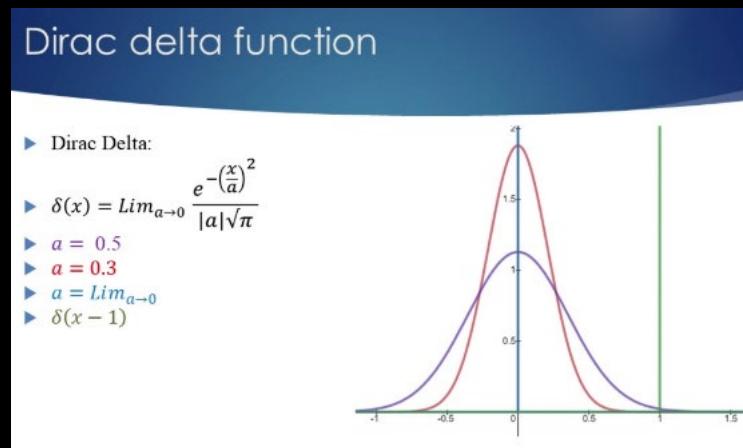
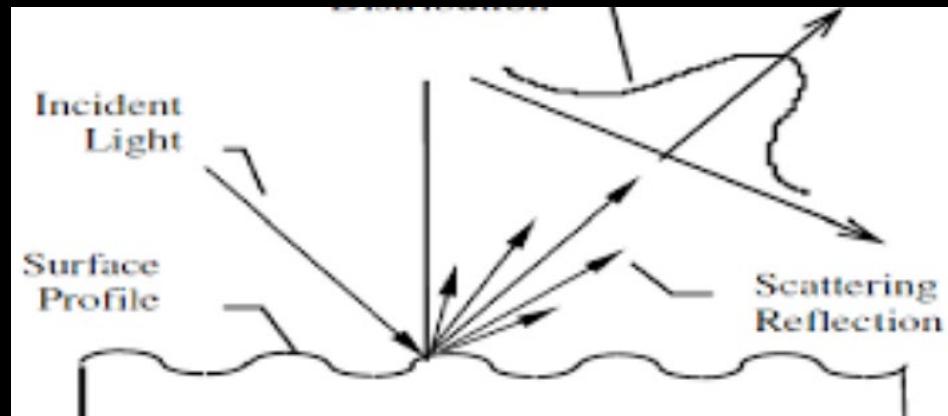


Liquid/
Glass



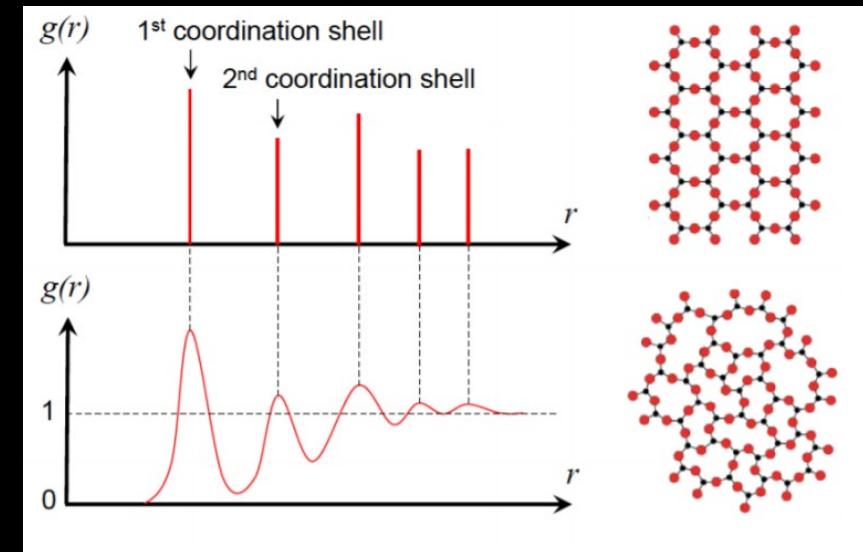
Using $g(r)$ to connect Structure and Property

Mapping Structure with Scattering using $g(r) = e^{-\varepsilon/kT}$



Crystal

Liquid



Tapping a surface with Light (I):
Scattering: Reciprocal (Structural
Info)

$$I: \xrightarrow{\text{FT}} g(r) = e^{-\varepsilon/kT}$$

What is Matter?

- What are liquids?
- Are liquids made of atoms?



- Is Crystallization then a phase transition? Today's Understanding with ICE-WATER

L. Onsager, Chemical Reviews, 1933, 13, 73-89

What is Matter?

An Information Theoretical Approach

- Information?
- Direction
- Bonds (Patches)
- Order
- Density
- Coding energy in above parameters

Crystals: As a solid/
Container of information

CODE NAME: SYMMETRY

The **Madelung constant** is a numerical constant used in determining the electrostatic energy of each ion in a crystal .

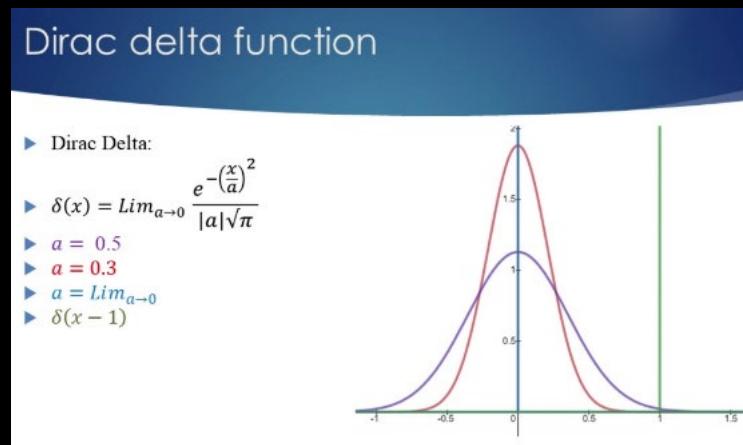
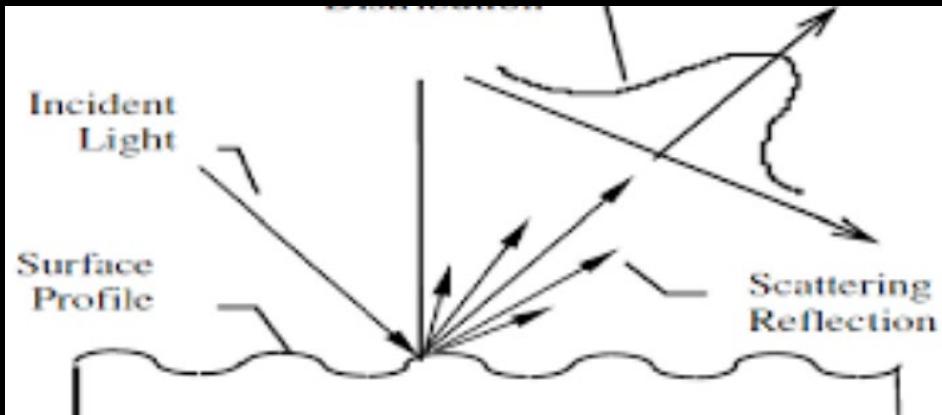
Summation of all the attraction and repulsion terms in a crystal lattice

$$E = A \frac{Z_+ Z_-}{r} \left[\frac{e^2}{4\pi\epsilon_o} \right]$$

↓
Madelung constant

Using $g(r)$ to connect Structure and Property

Mapping Structure with Scattering using $g(r) = e^{-\varepsilon/kT}$



Tapping a surface with Light (I):
Scattering: Reciprocal (Structural
Info)

$$I: \xrightarrow{\text{FT}} g(r) = e^{-\varepsilon/kT}$$

$$I = A + i\phi \quad \begin{matrix} \downarrow \\ \text{Phase Information (LOST!)} \end{matrix}$$

Amplitude Information

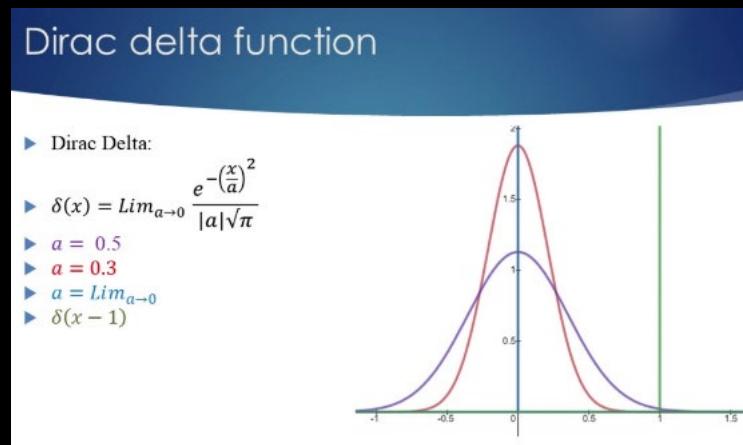
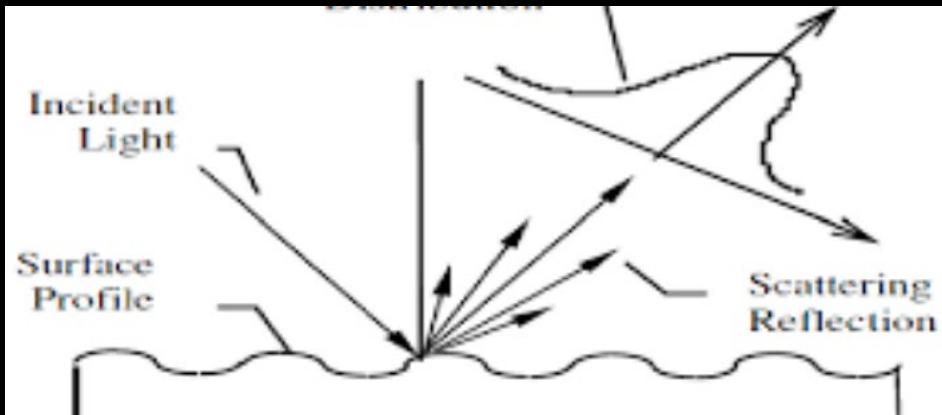
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Father of FT: Jean-Baptiste Fourier

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Fourier transform: Transforms Momentum Space into Position Space Wave Function

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

$$I: \xrightarrow{\text{FT}} S(q) \rightarrow 1 + \rho h^\sim(q) \rightarrow g(r) = e^{-\epsilon/kT}$$

Tapping a surface with Light (I):
Scattering: Reciprocal (Structural
Info)

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Phase Information (LOST!)

Amplitude Information

$$I = \psi(x) \times \psi^*(x)$$

$S(q)$: Structure Factor



Father of FT: Jean-Baptiste Fourier

Using $g(r)$ to connect Structure and Property

Mapping Structure with Scattering using $g(r) = e^{-\varepsilon/kT}$

$$I = \Psi(x) \times \Psi^*(x)$$

$$S(q) = I / \sum_{n=1}^{\infty} (f_n)^2$$

$$S(q) = 1 + \rho h^*(q)$$

$$h^*(q) = \text{FT}[h(r)]$$

$$h(r) = 1 - g(r)$$

Fourier transform: Transforms Momentum Space into Position Space Wave Function

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

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