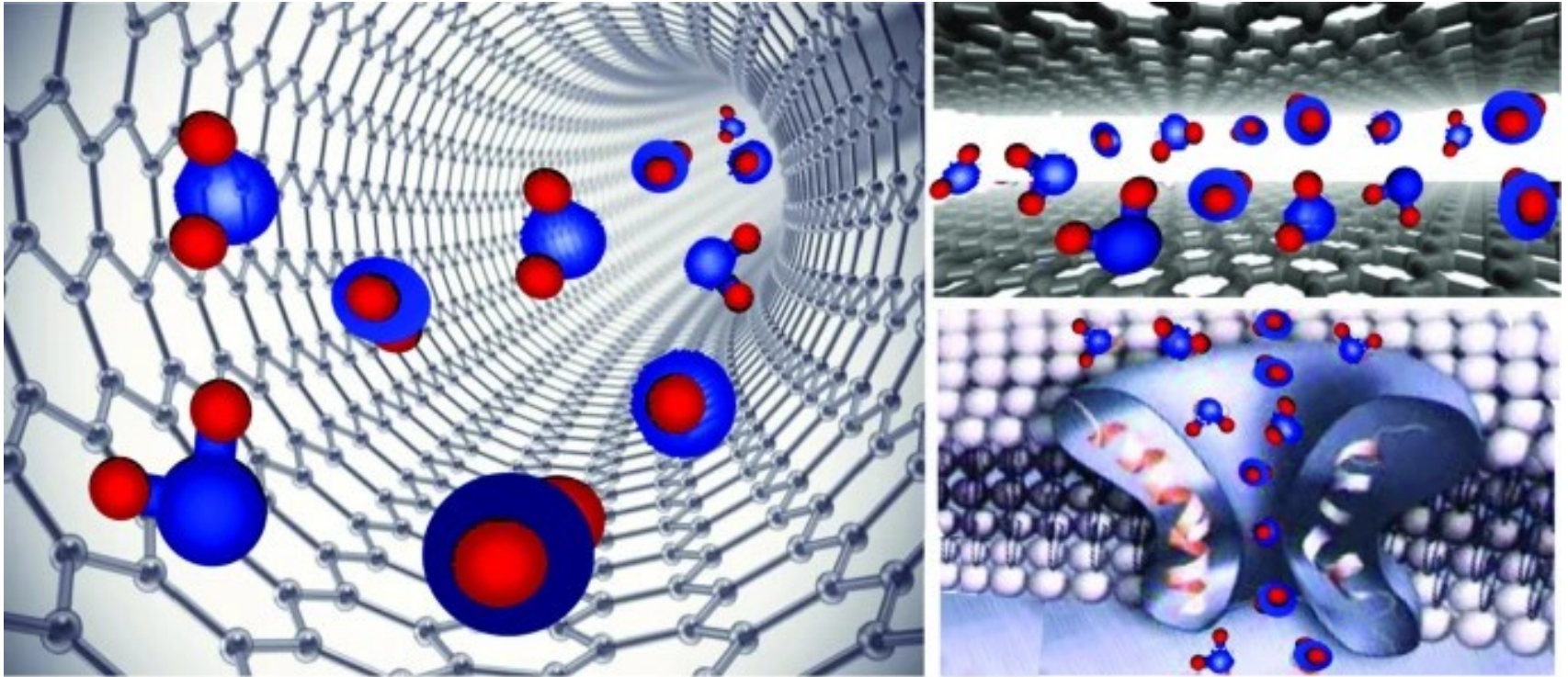


# Nanoconfined Water



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# Summary



## **Phase Transitions- Water Anomalies**

## **Nanoconfined Water in Solid State Materials**

## **Nanoconfined Water in Biology**

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# Criticality - Water Anomalies

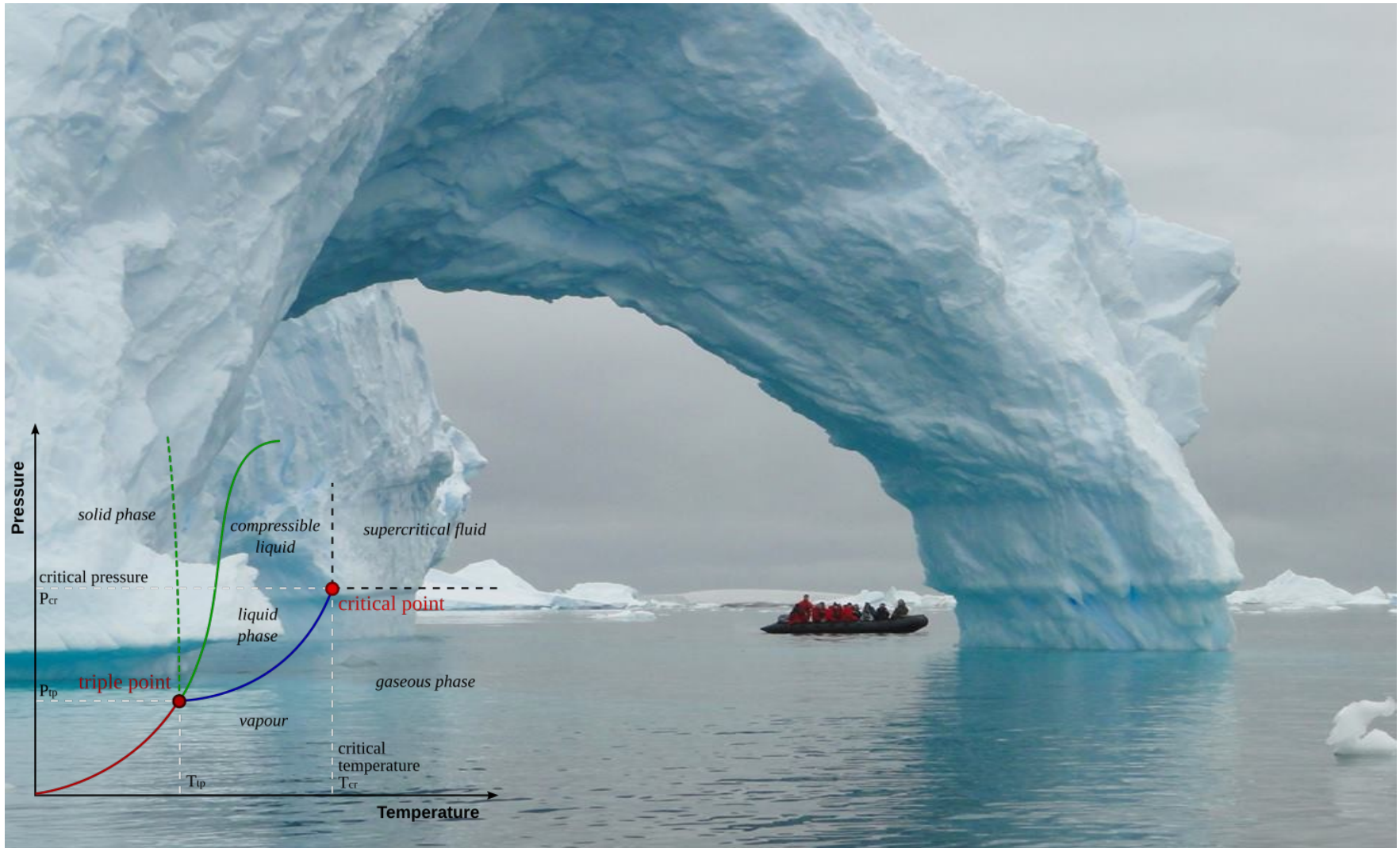


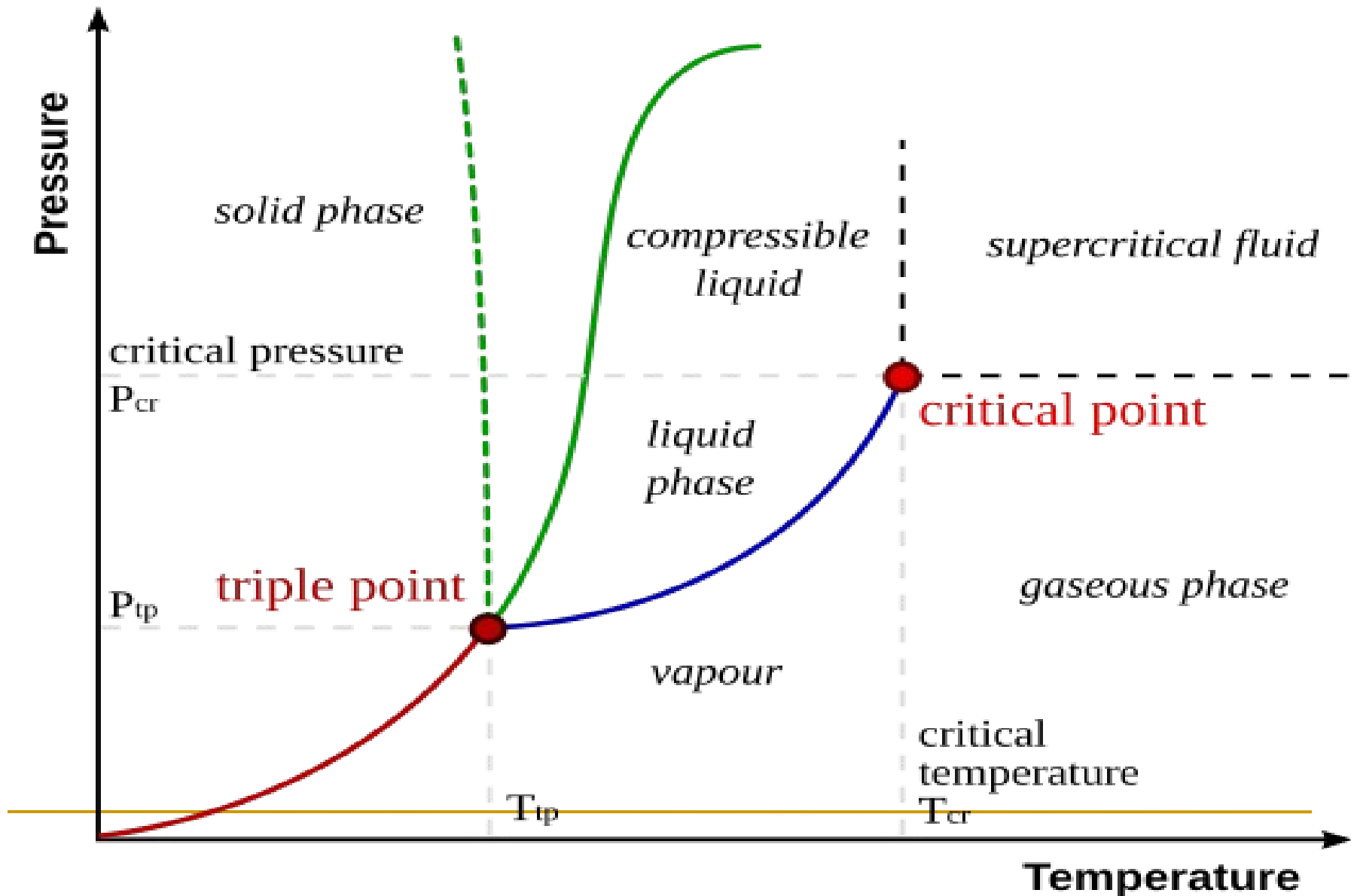
photo by Clóvis Jardim

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# **PHASE TRANSITIONS**

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# Phase Transitions



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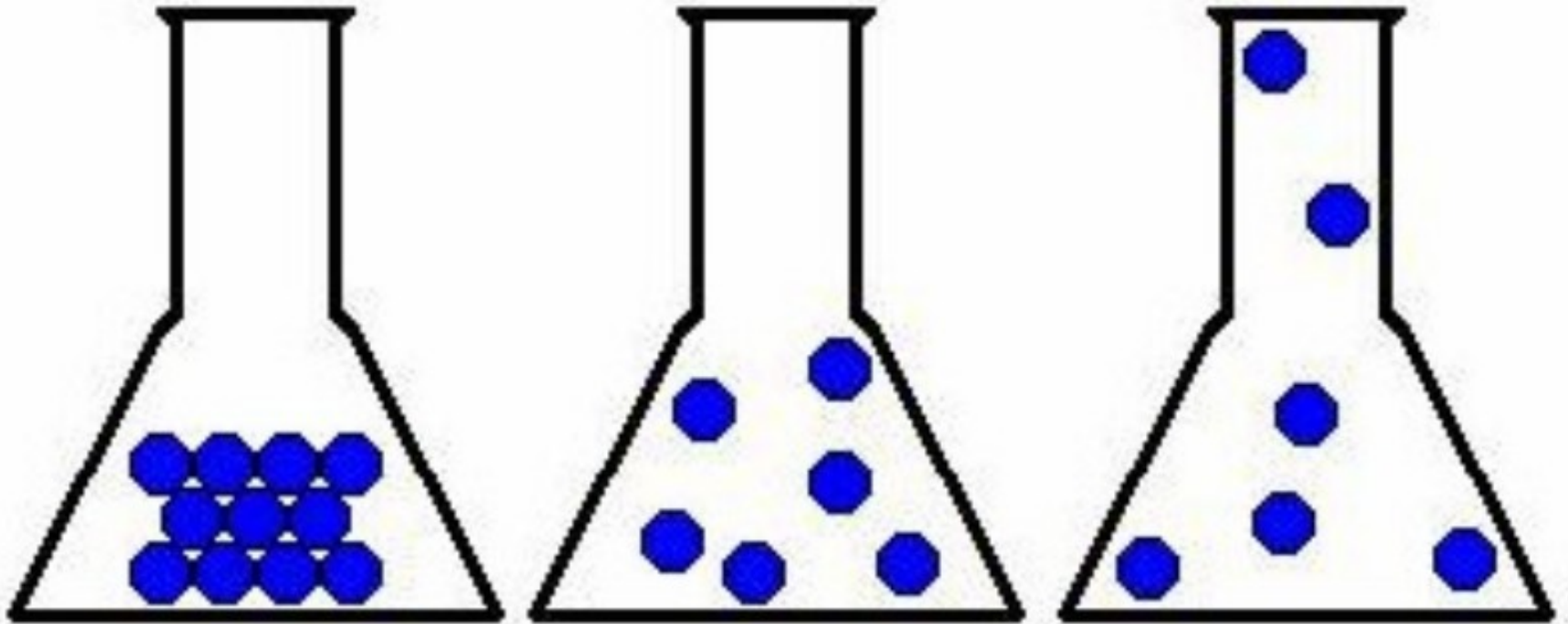
# **PHASES**

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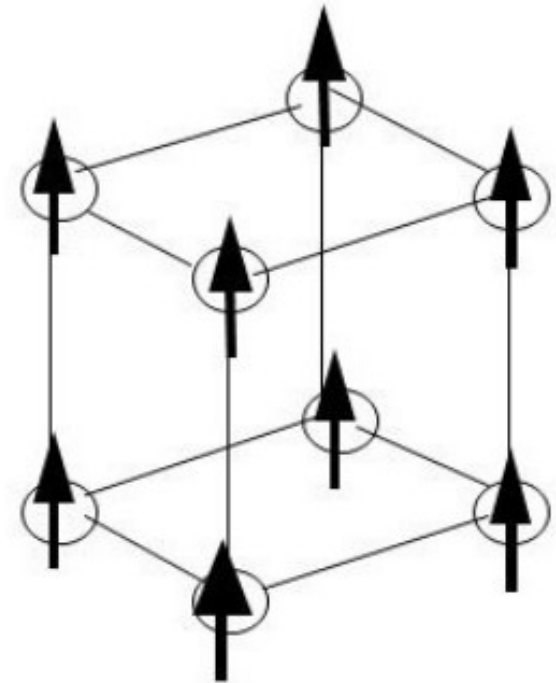
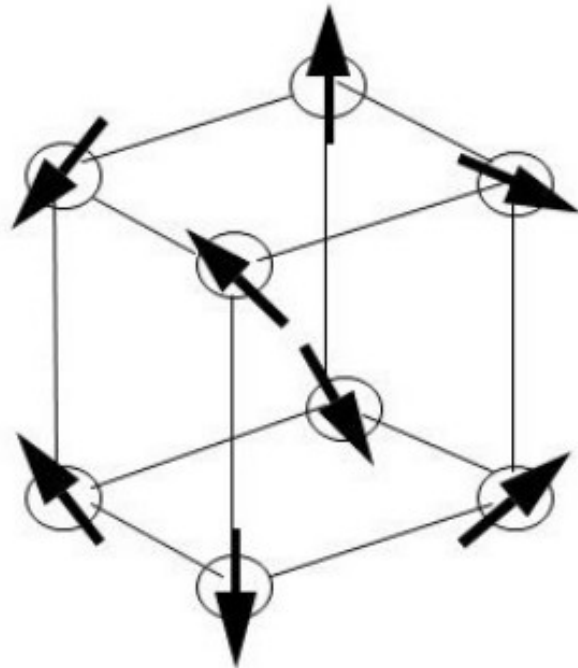
# Simple Materials

## Solid Liquid Gas



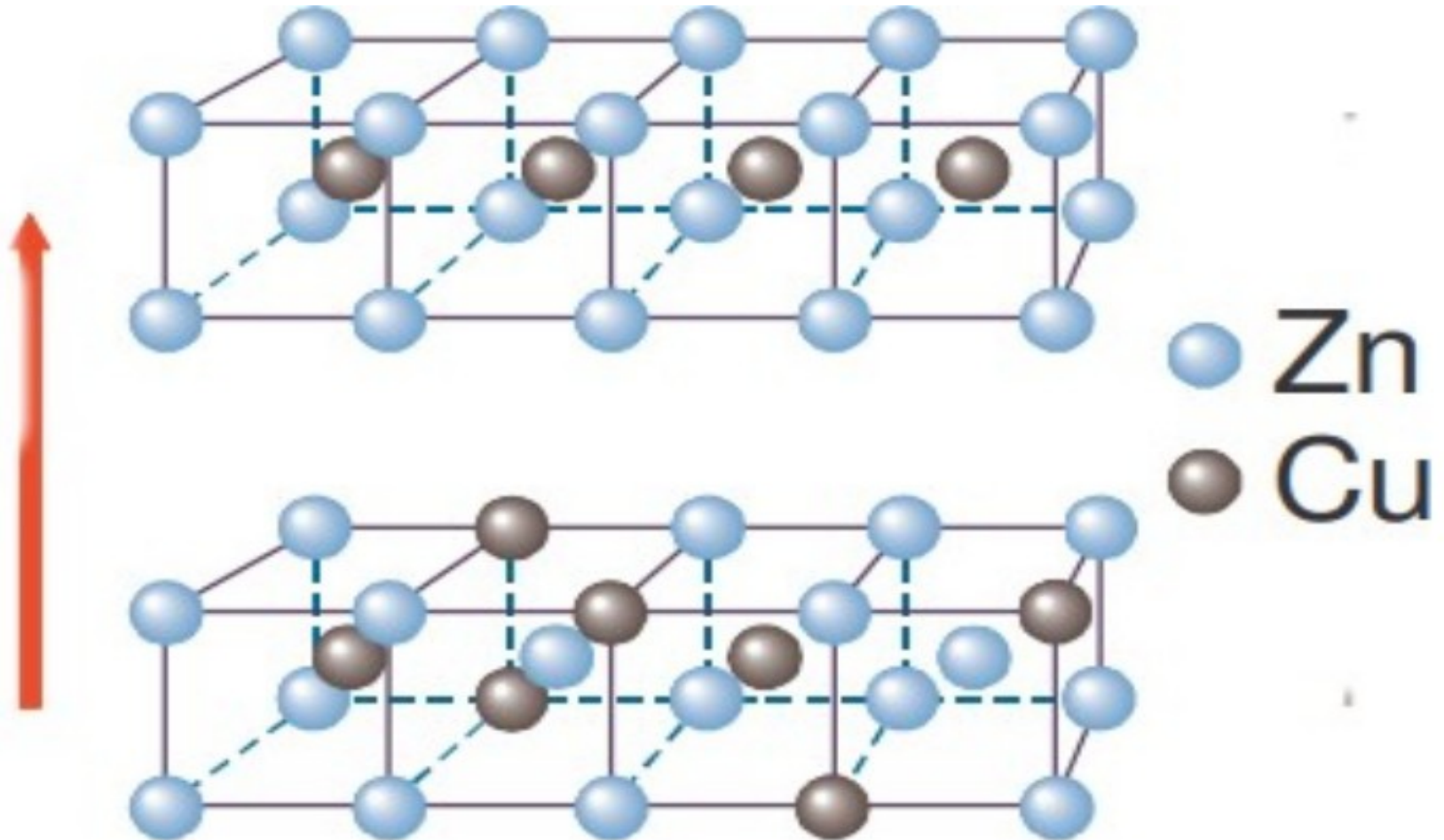
# Simple Magnetic Materials

## Paramagnetic e Ferromagnetic

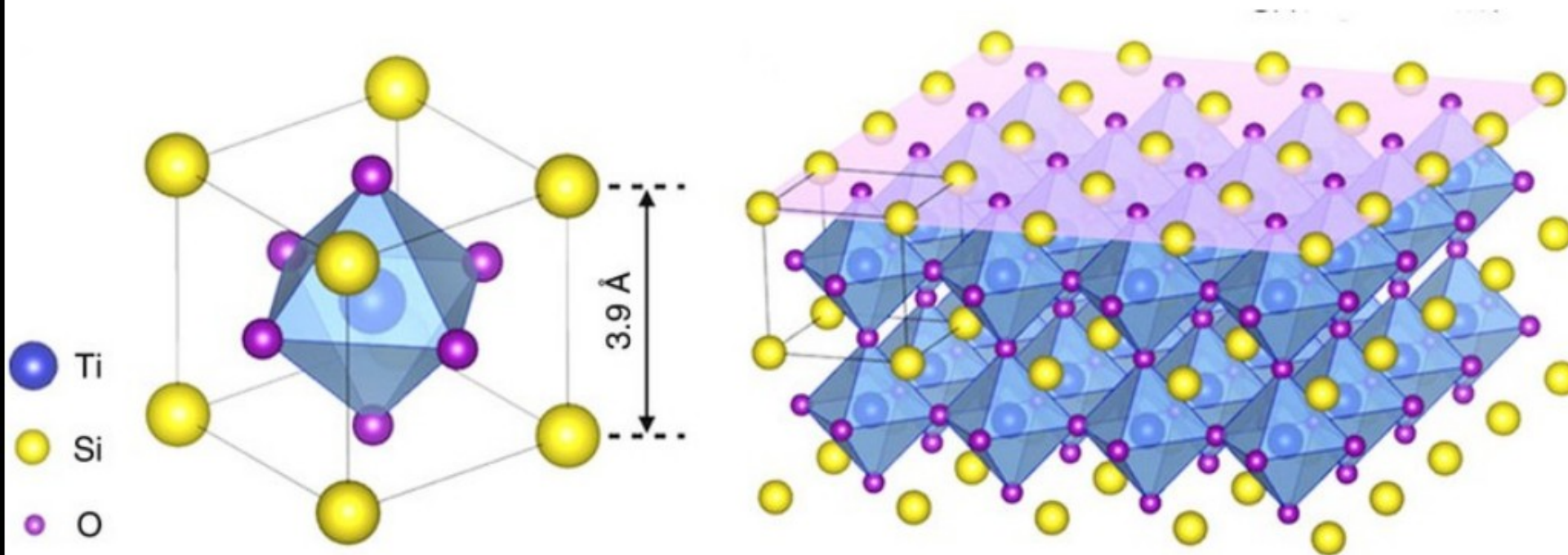




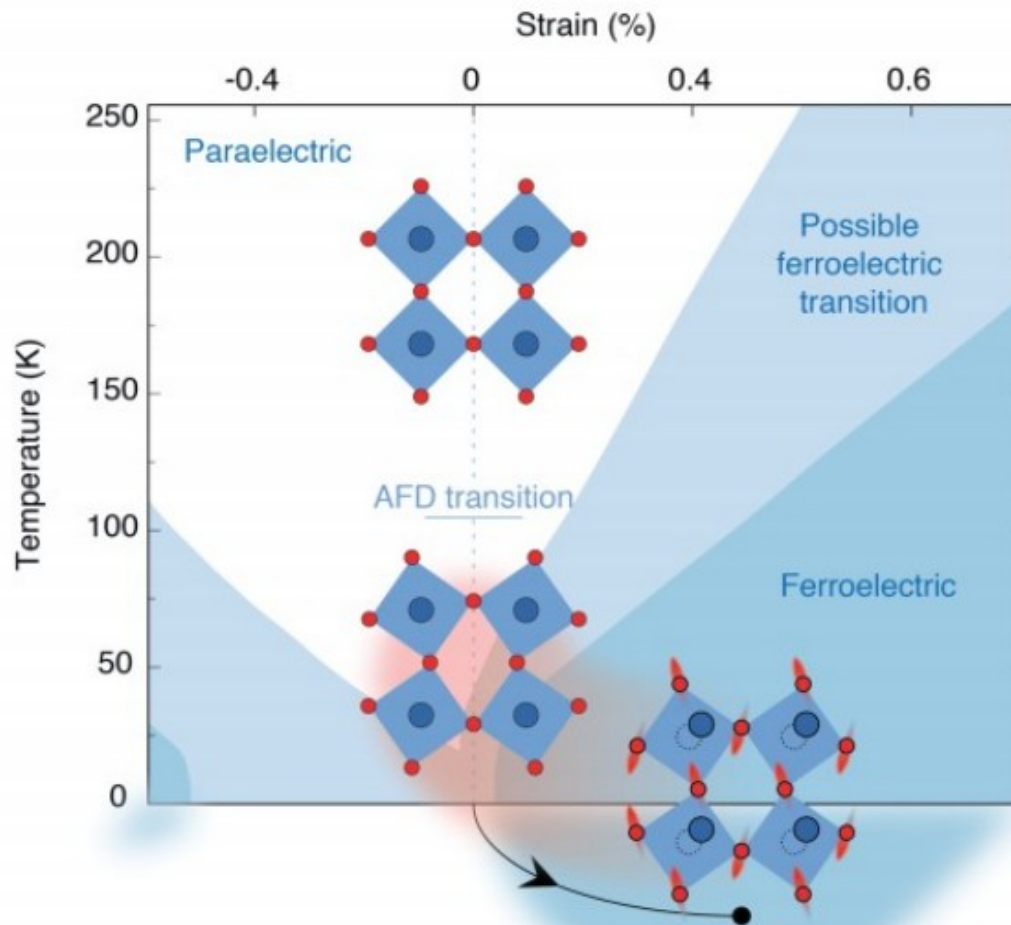
# Phases - ZnCu



# SrTiO<sub>3</sub>

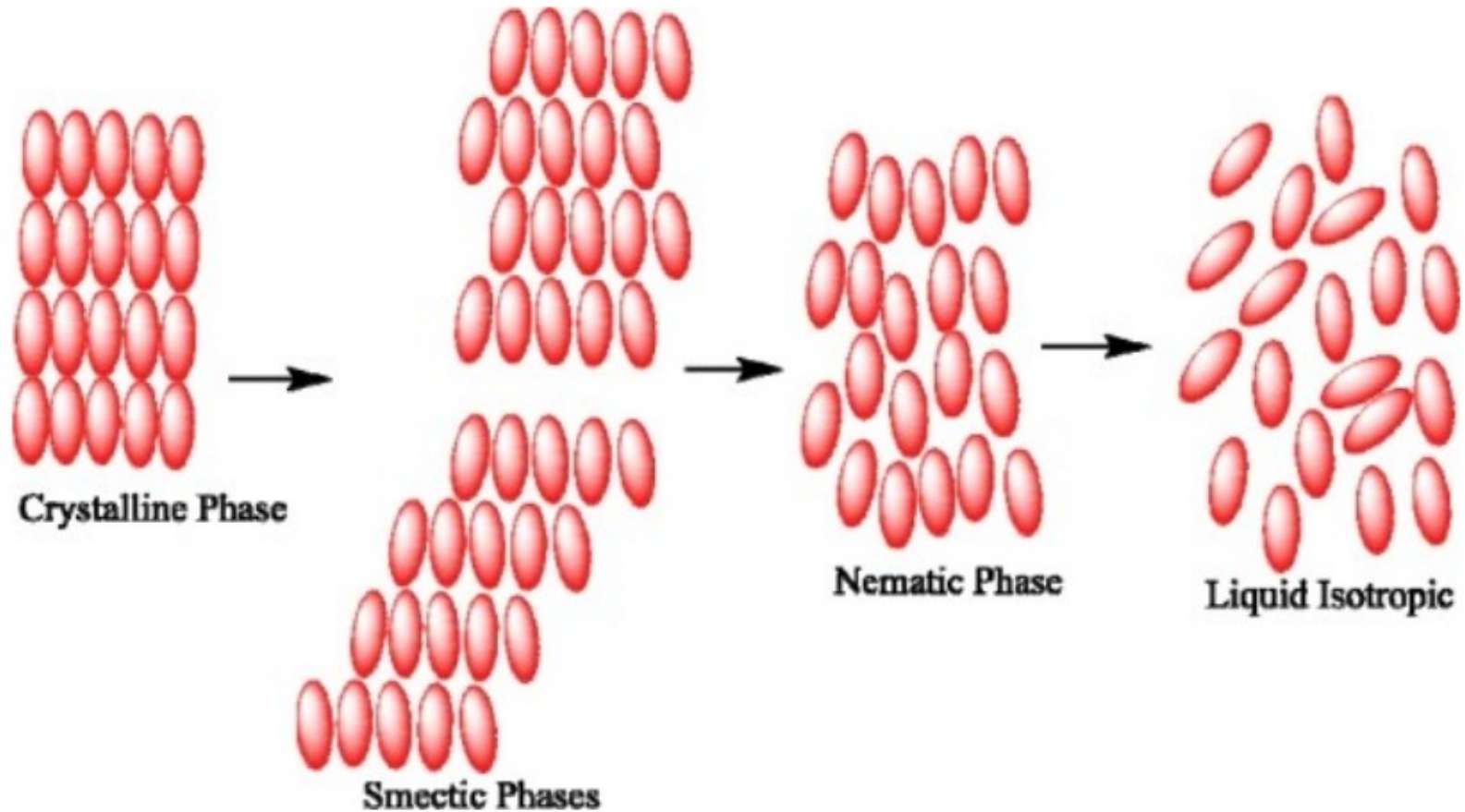


# SrTiO<sub>3</sub>

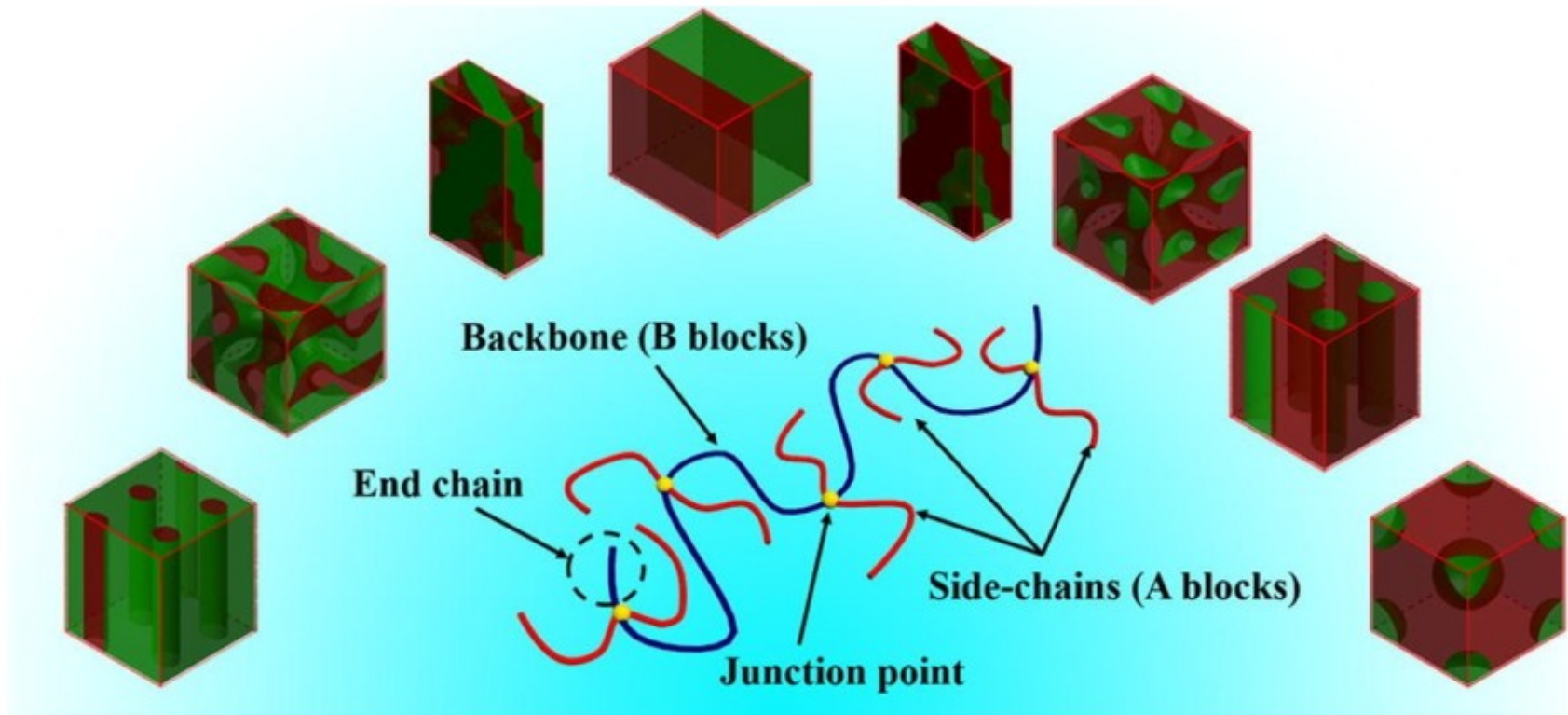


<https://arxiv.org/pdf/1812.10560.pdf>

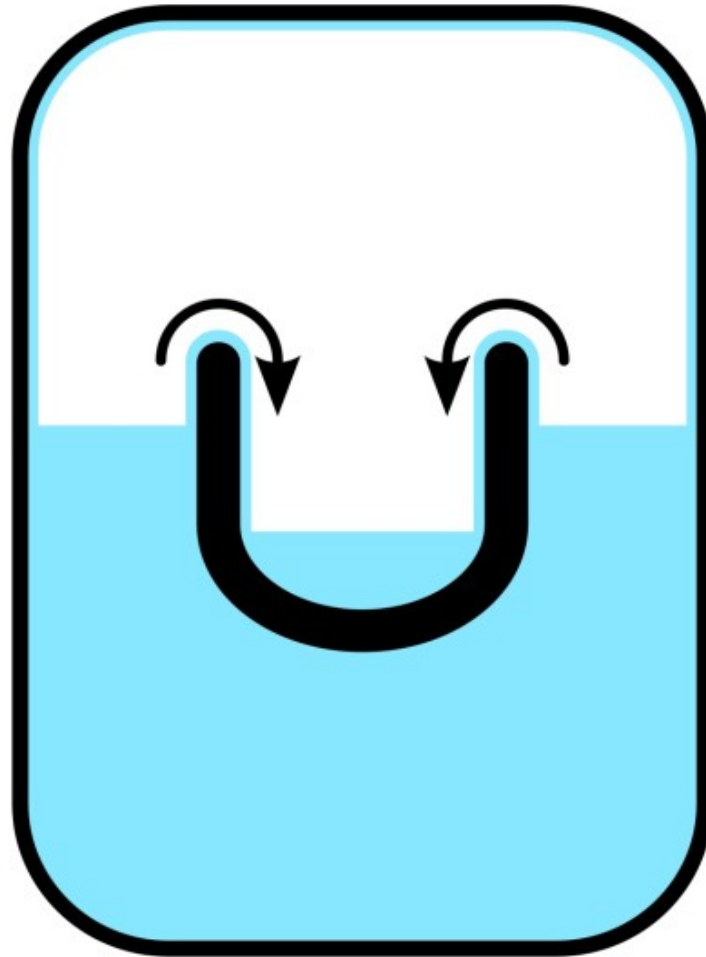
# Liquid Crystals



# Block Copolymers

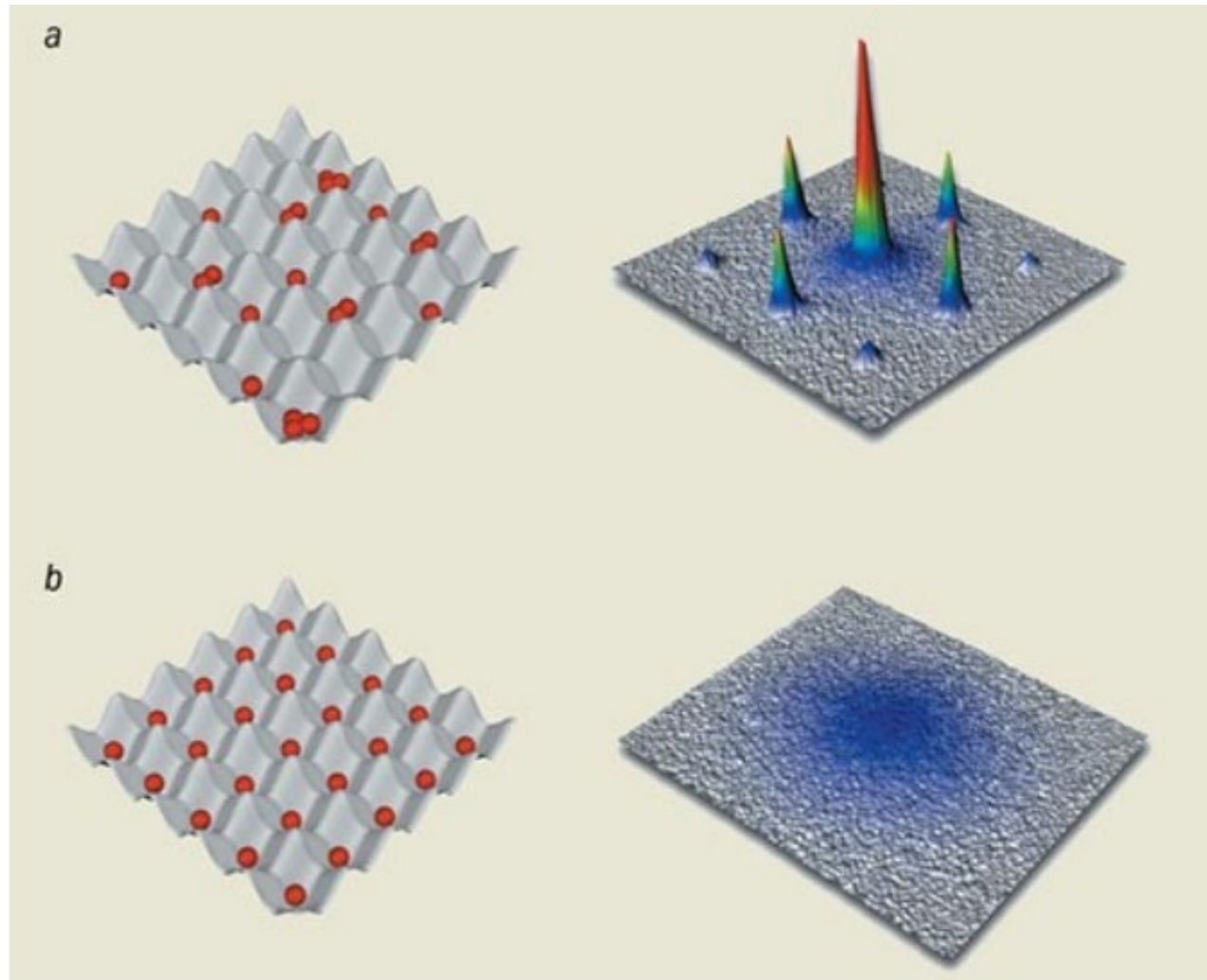


# Superfluid Helium



<https://en.wikipedia.org/wiki/Helium>

# Cold Atoms in Lattice



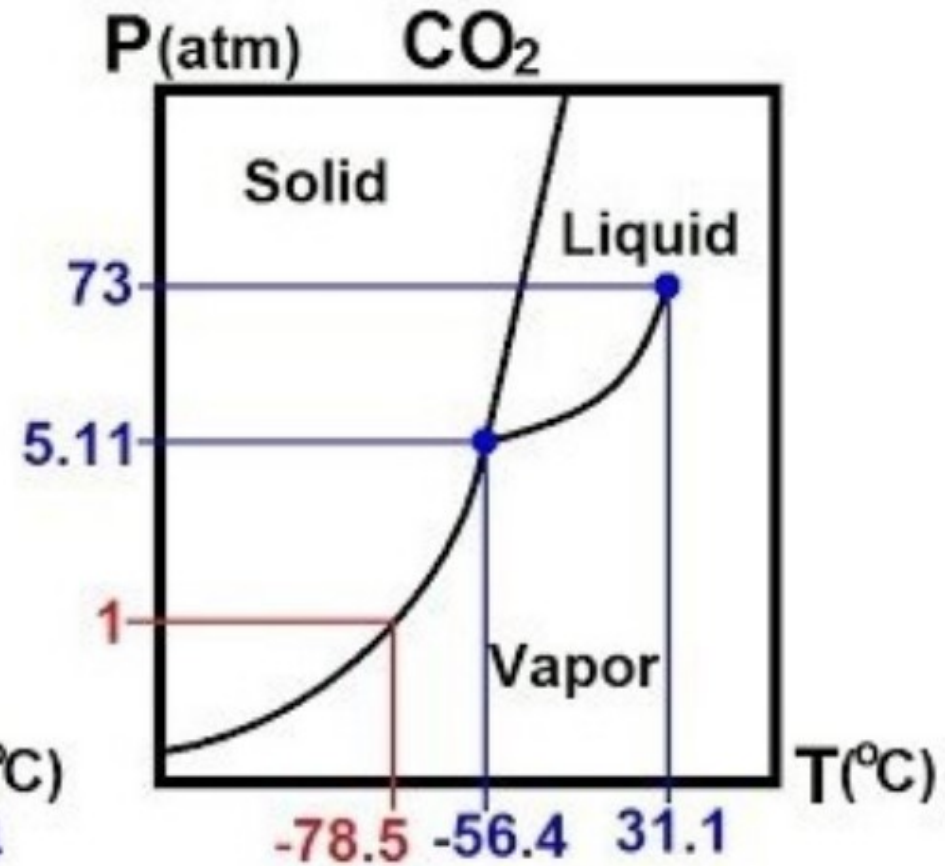
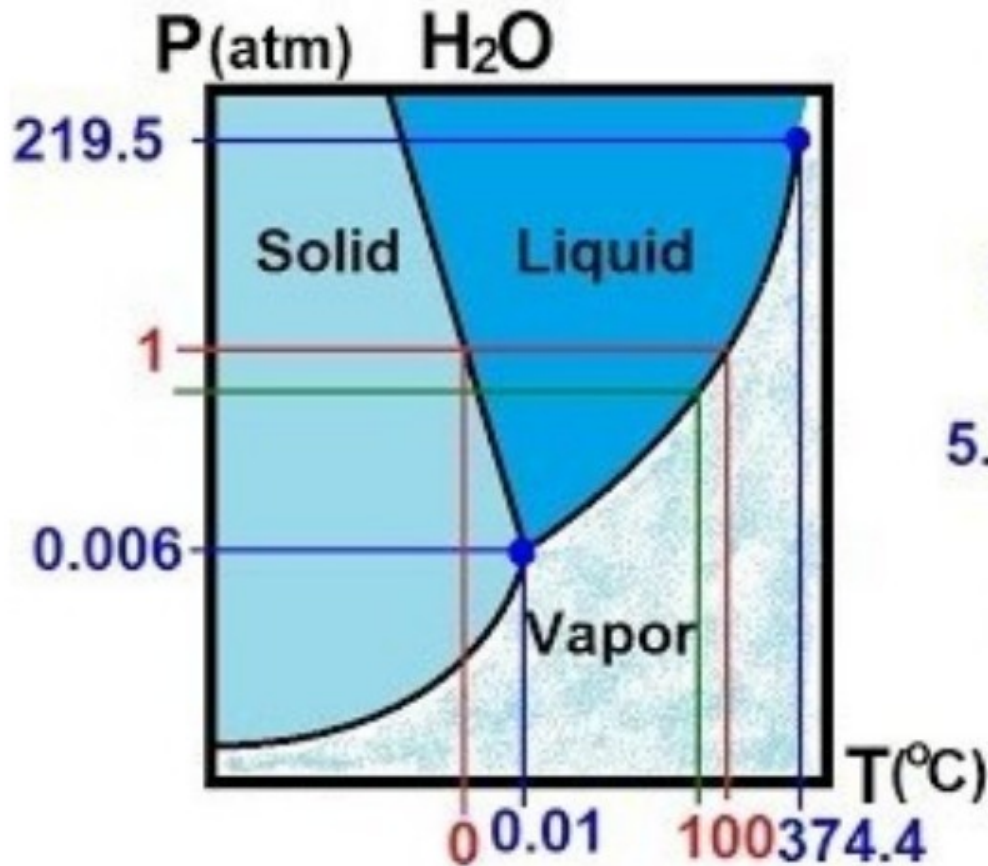
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# **PHASE DIAGRAMS**

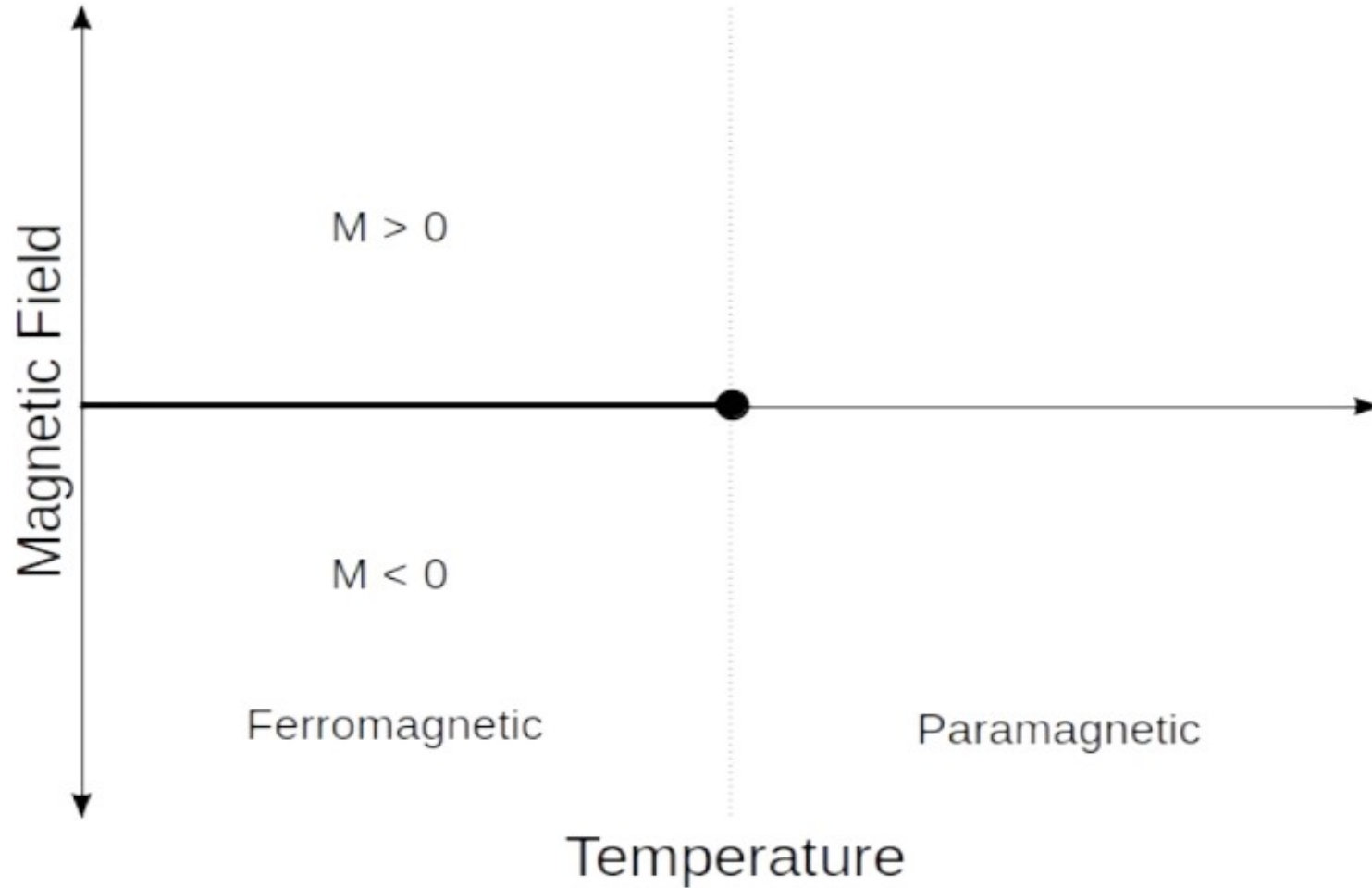
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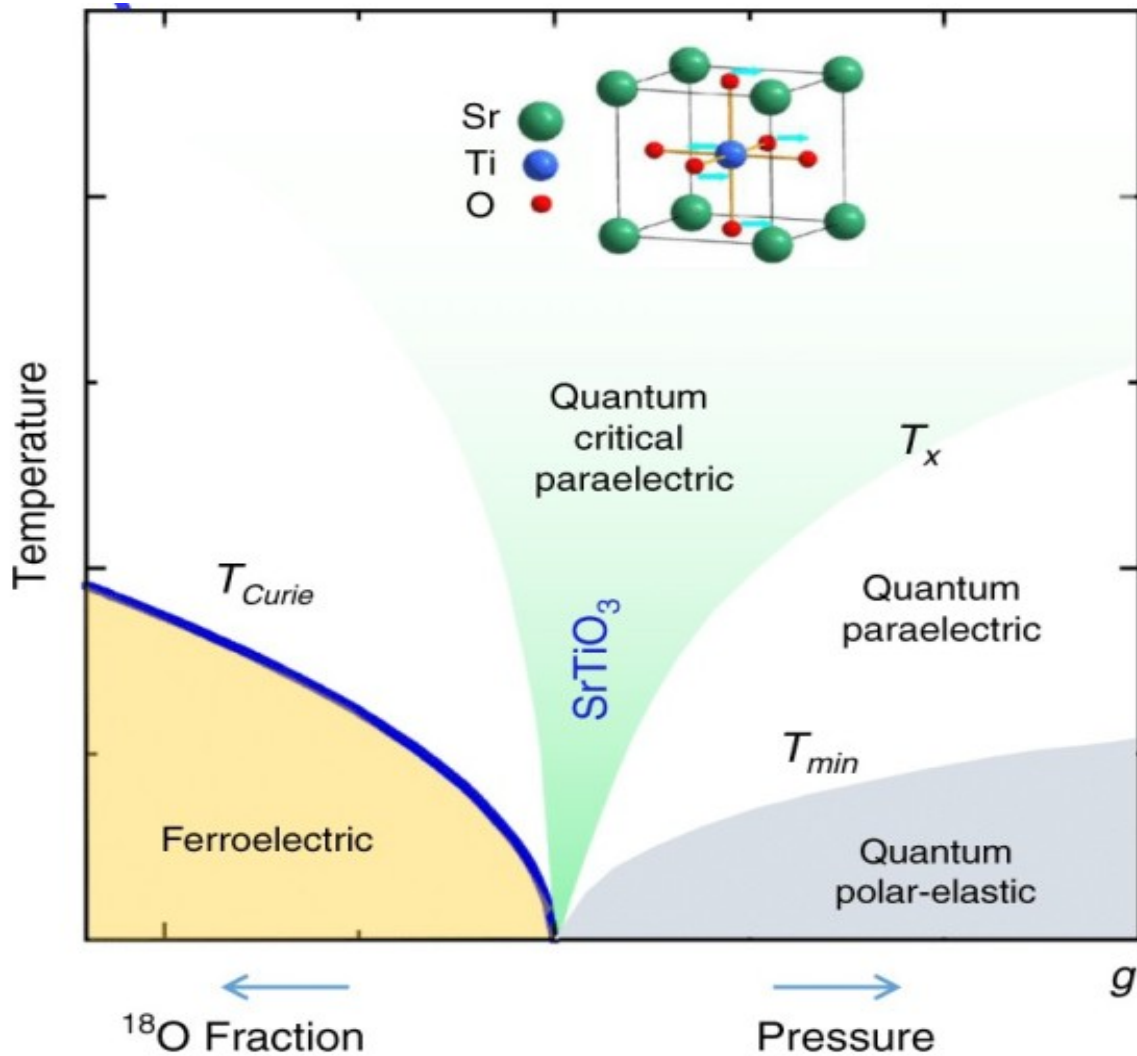
# Phase Diagram



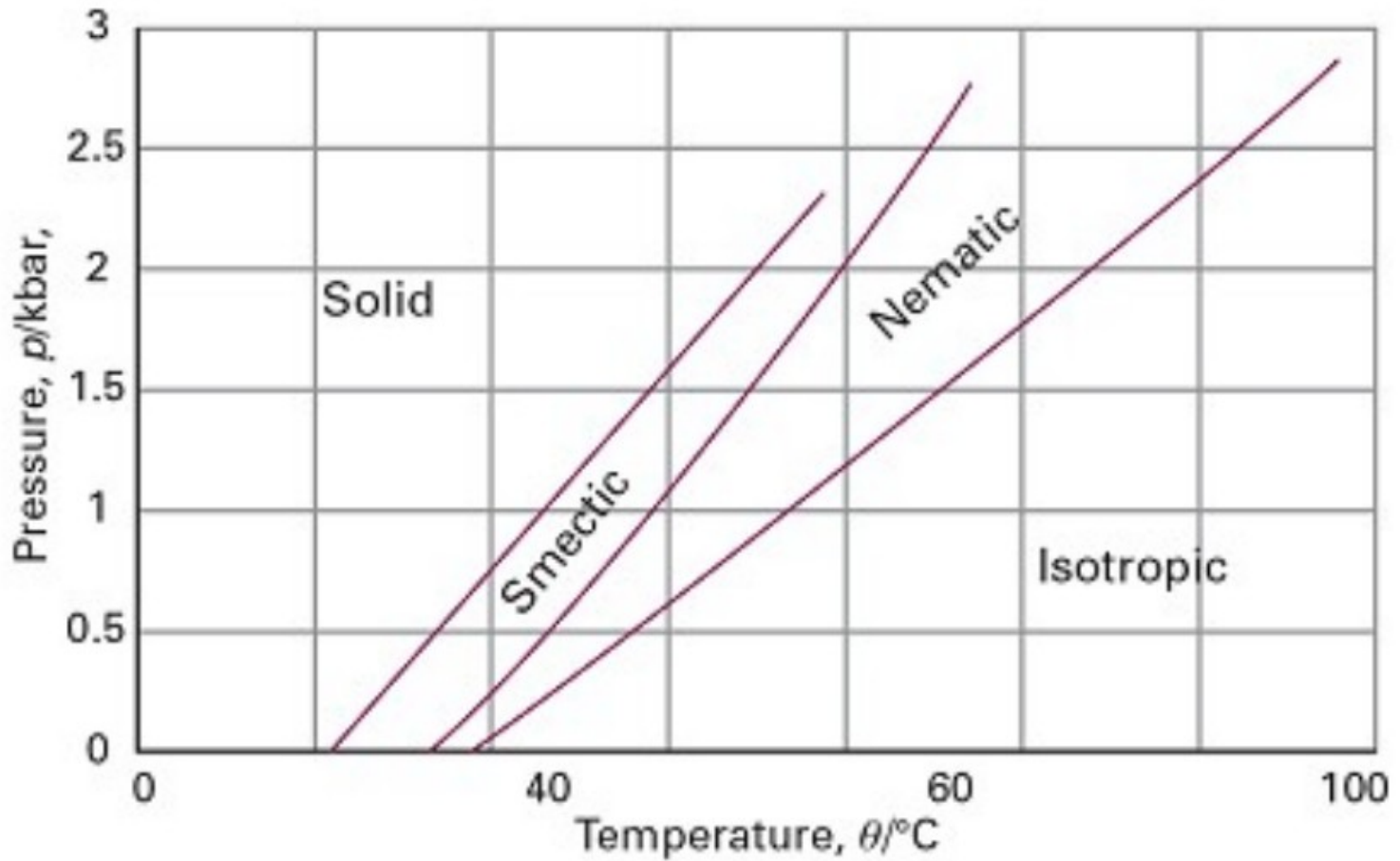
# Magnetic Phase Transition



# SrTiO<sub>3</sub>



# Liquid Crystal



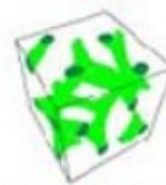
# Block Copolymers



Spheres (BCC)



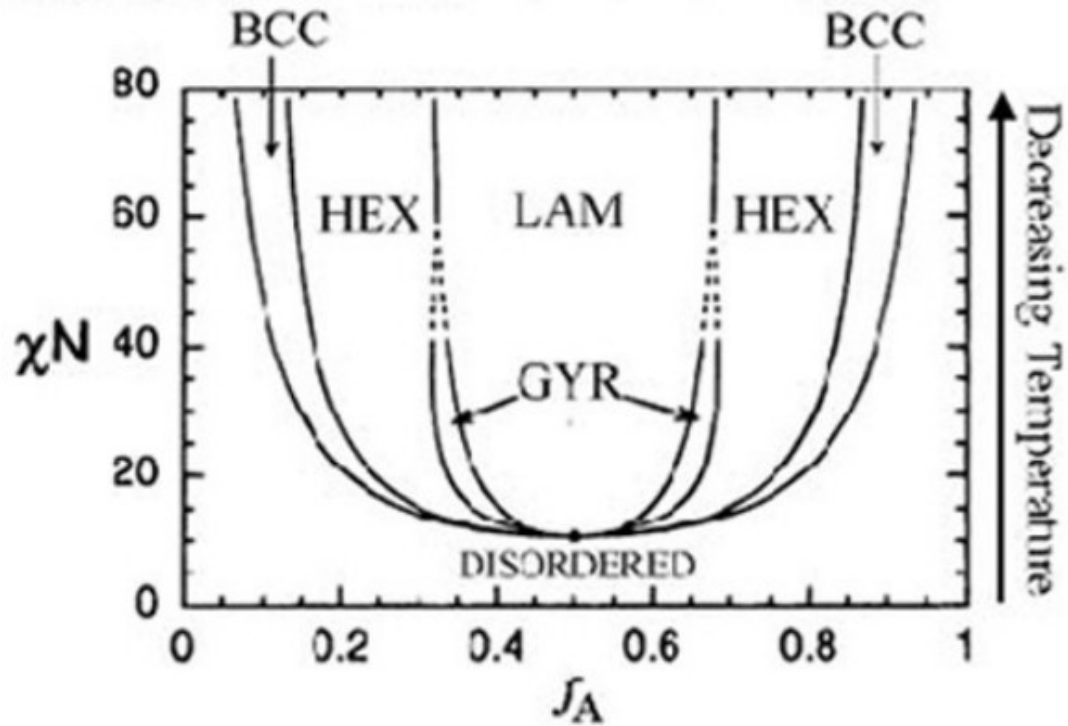
Cylinders (HEX)



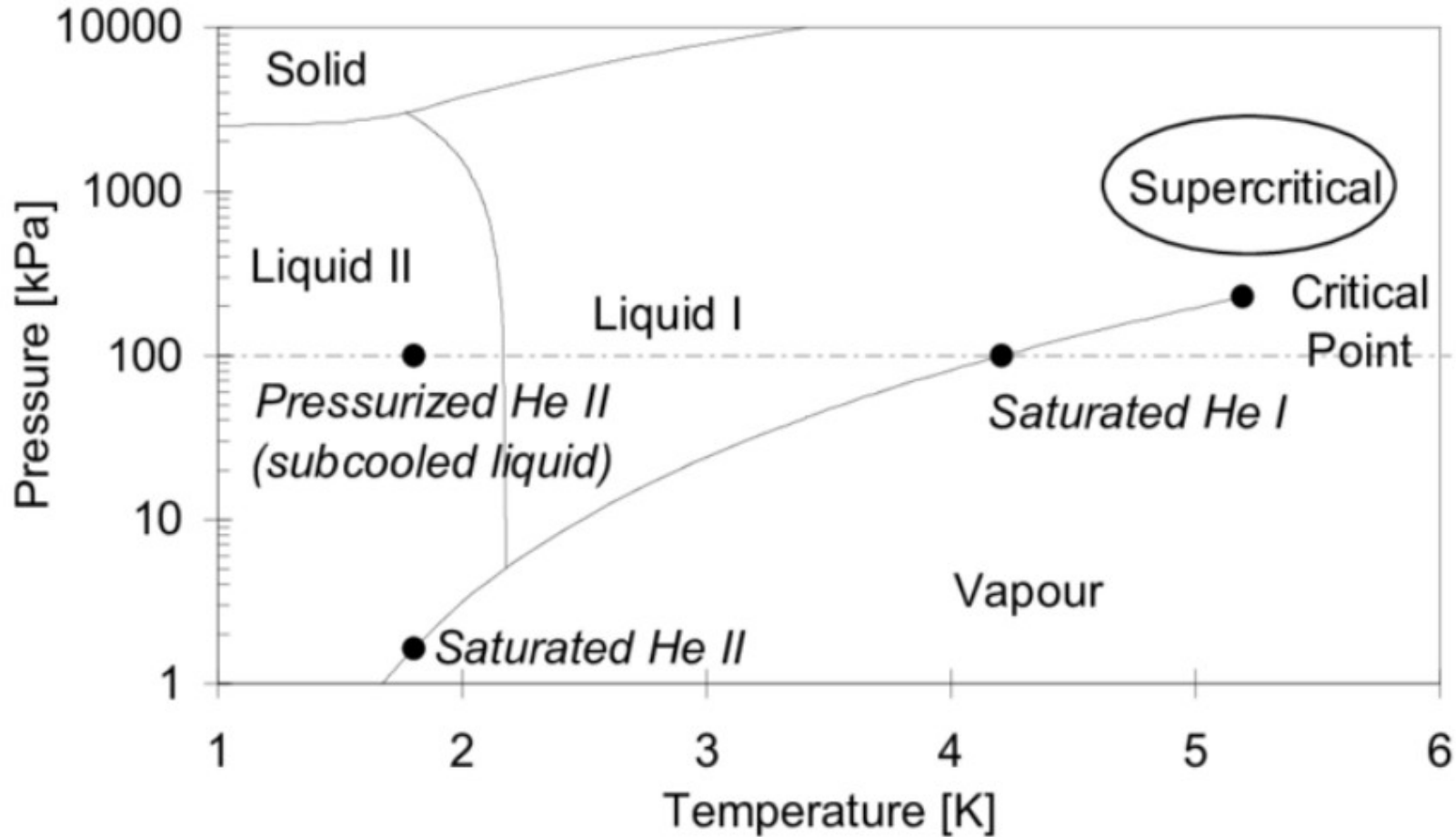
Gyroid (GYR)



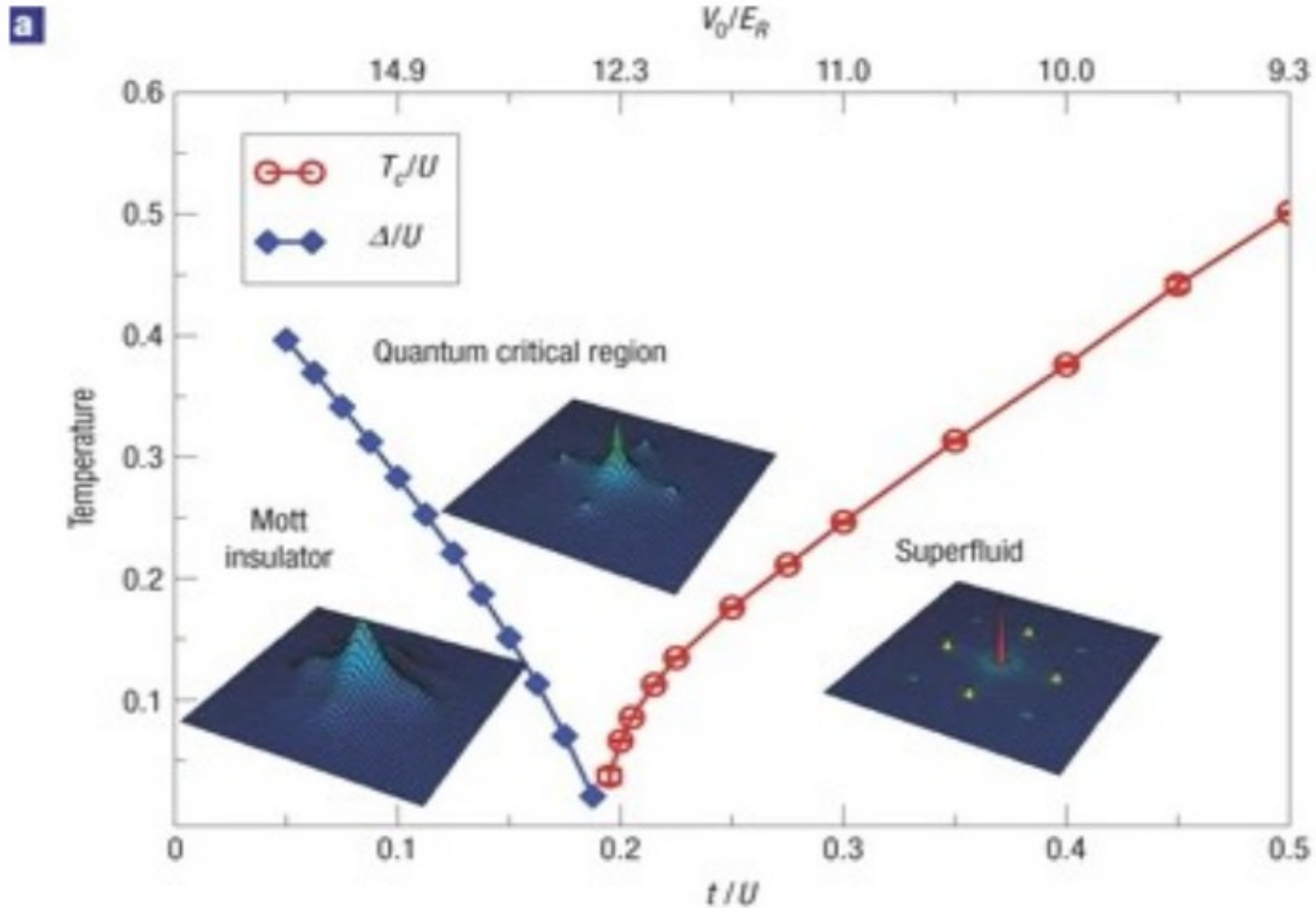
Lamellar (LAM)



# Superfluid Helium



# Quantum Systems



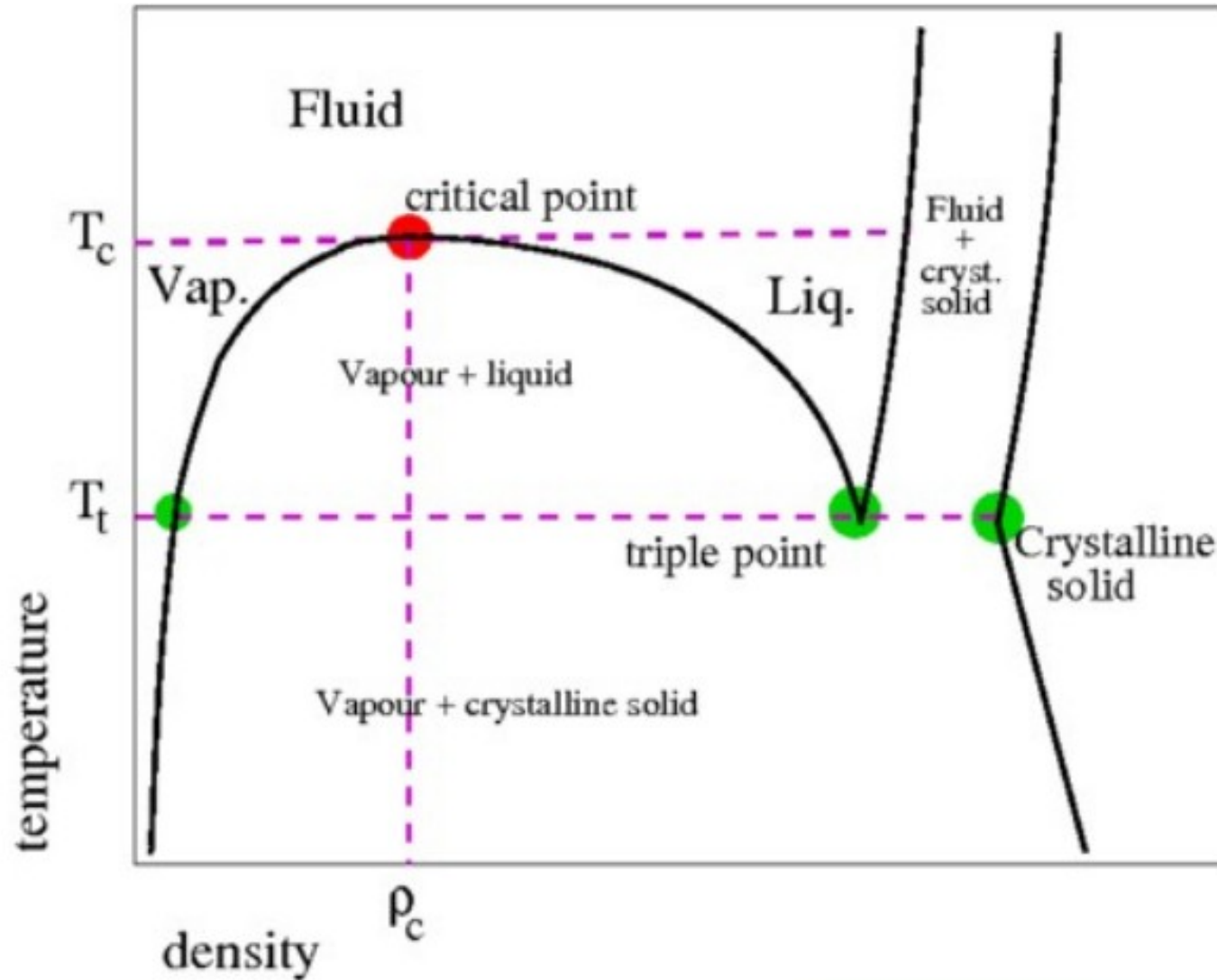
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# **PHASE TRANSITION**

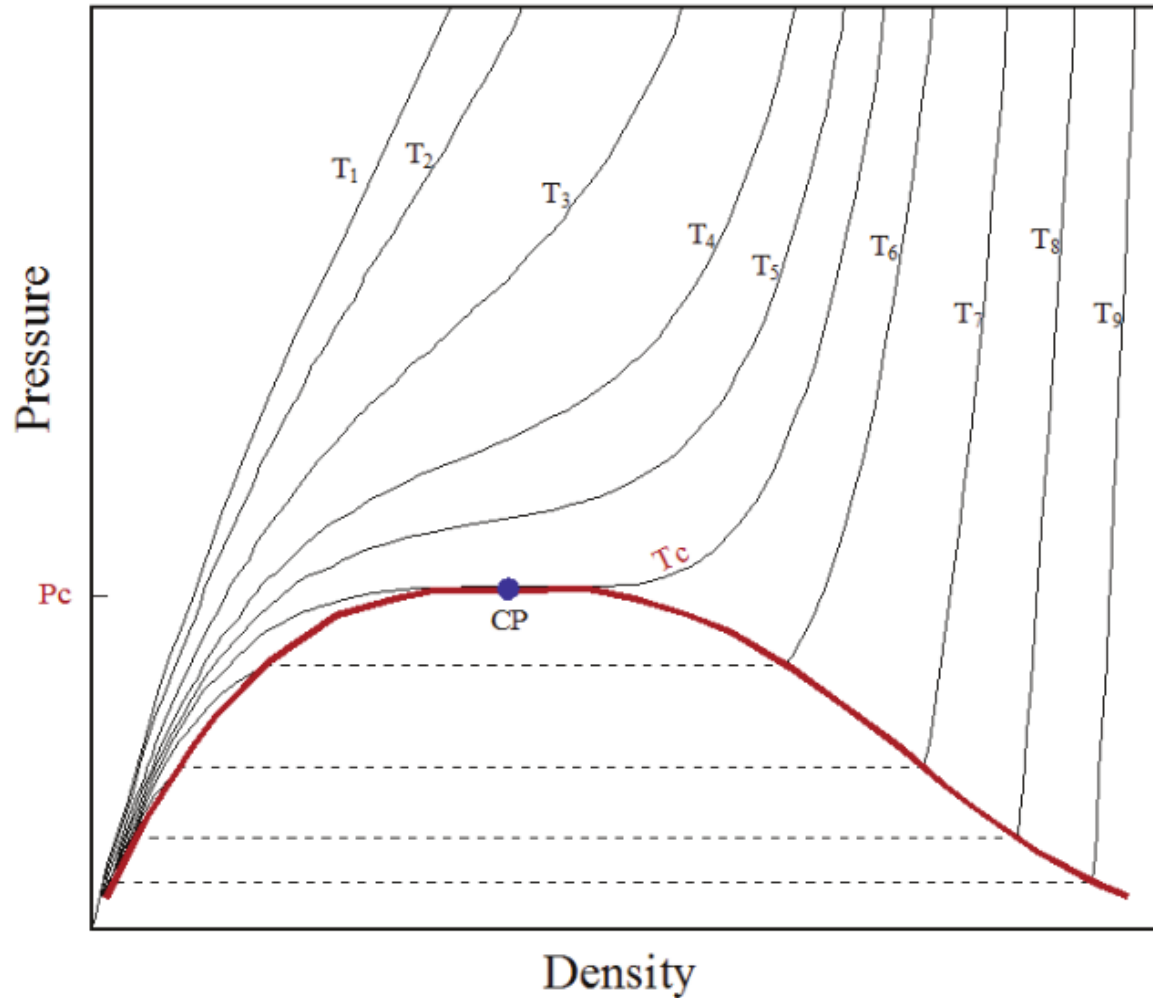
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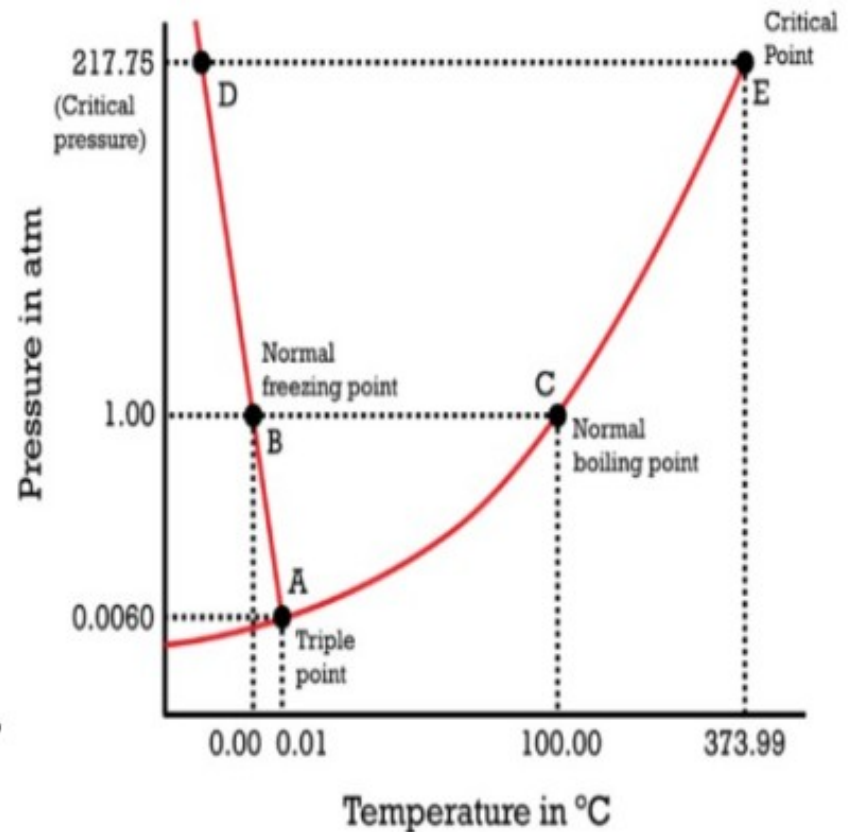
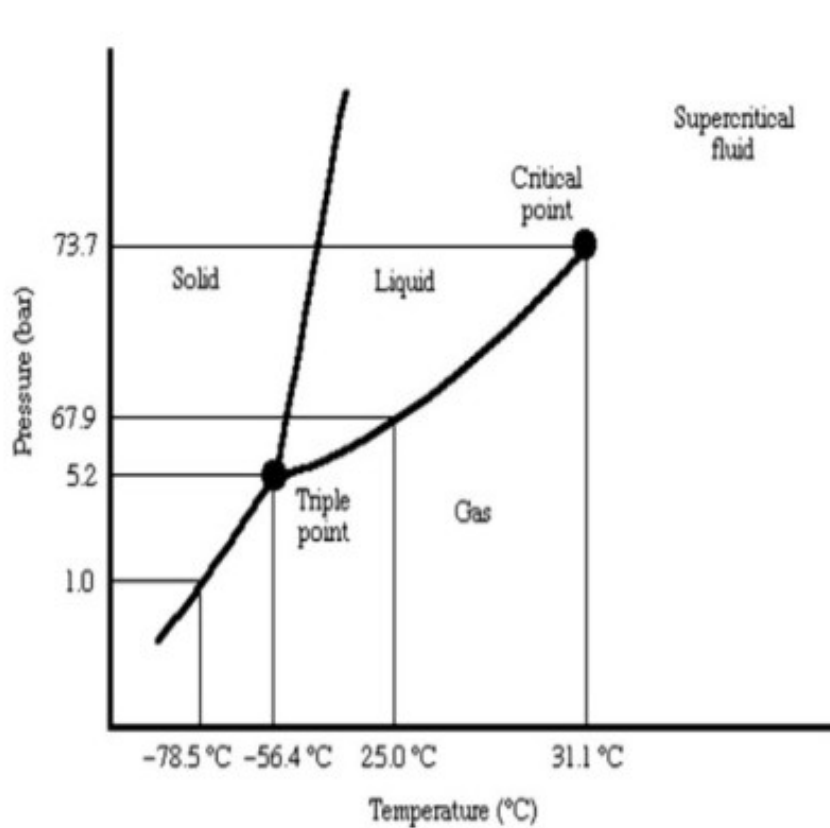
# Simple Fluids



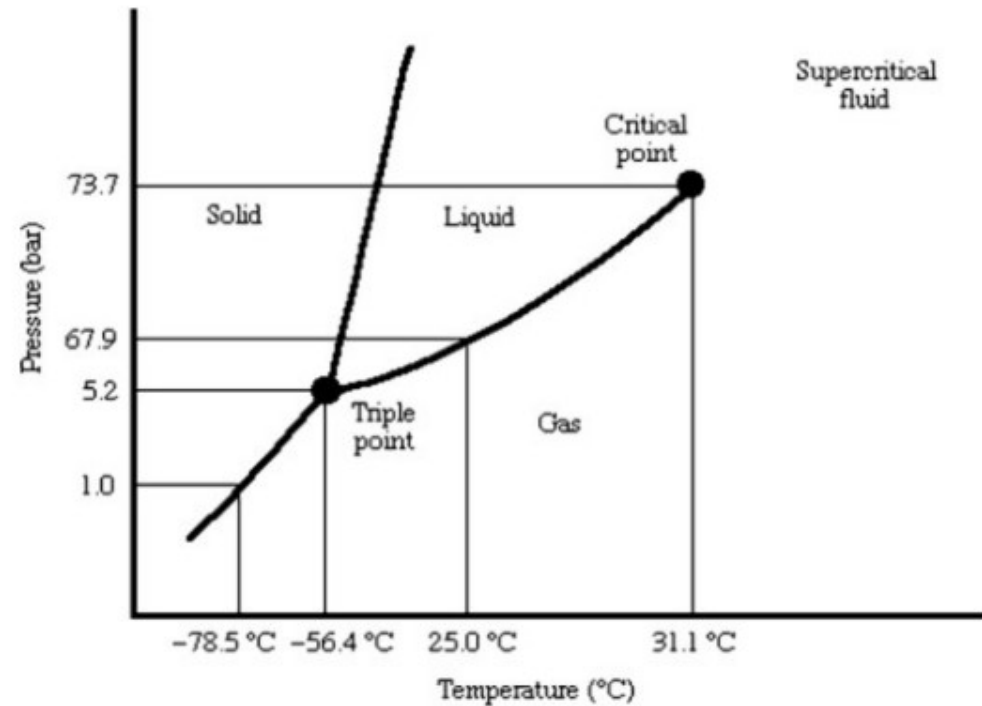
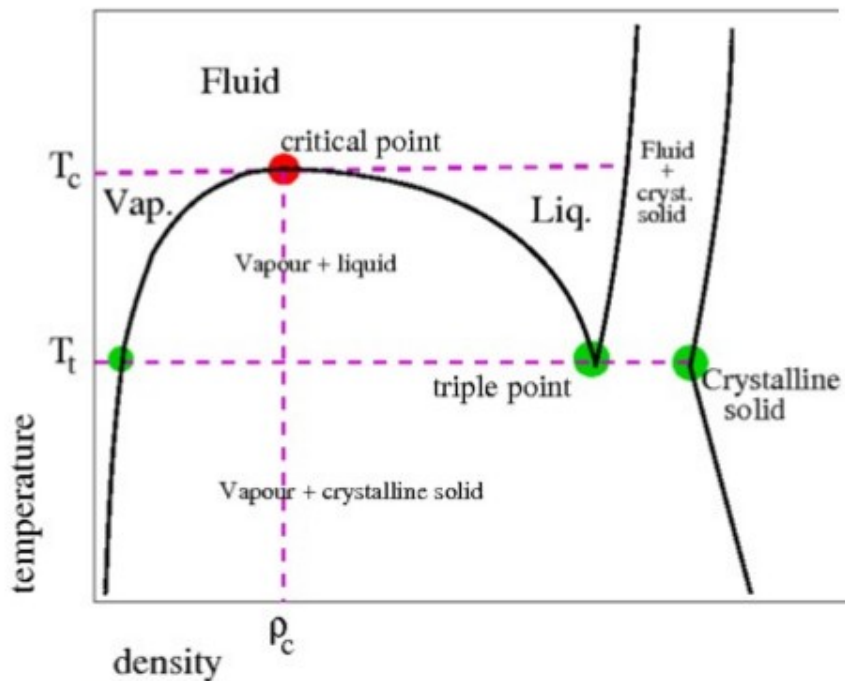
# First Order Transition



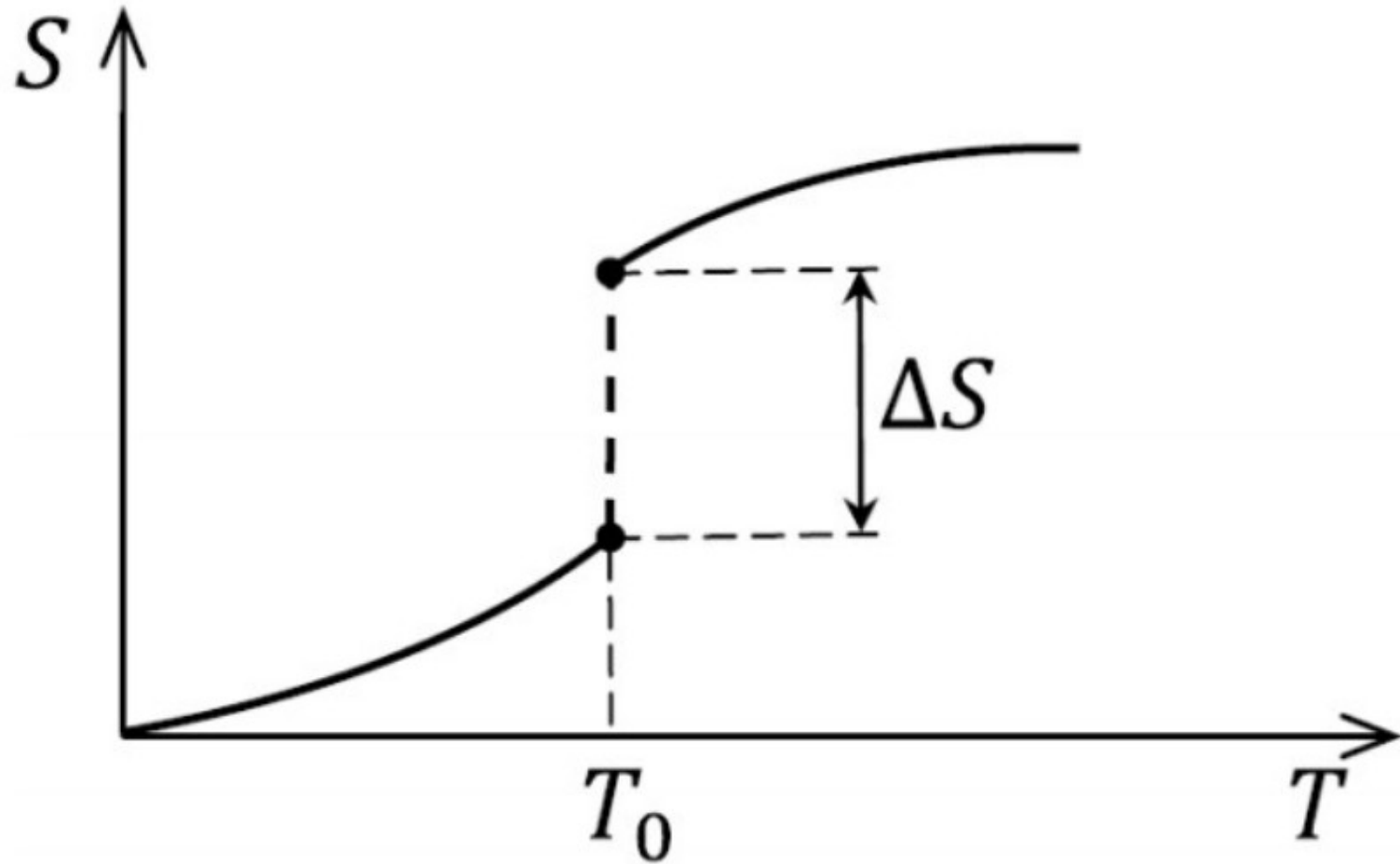
# First Order Transition



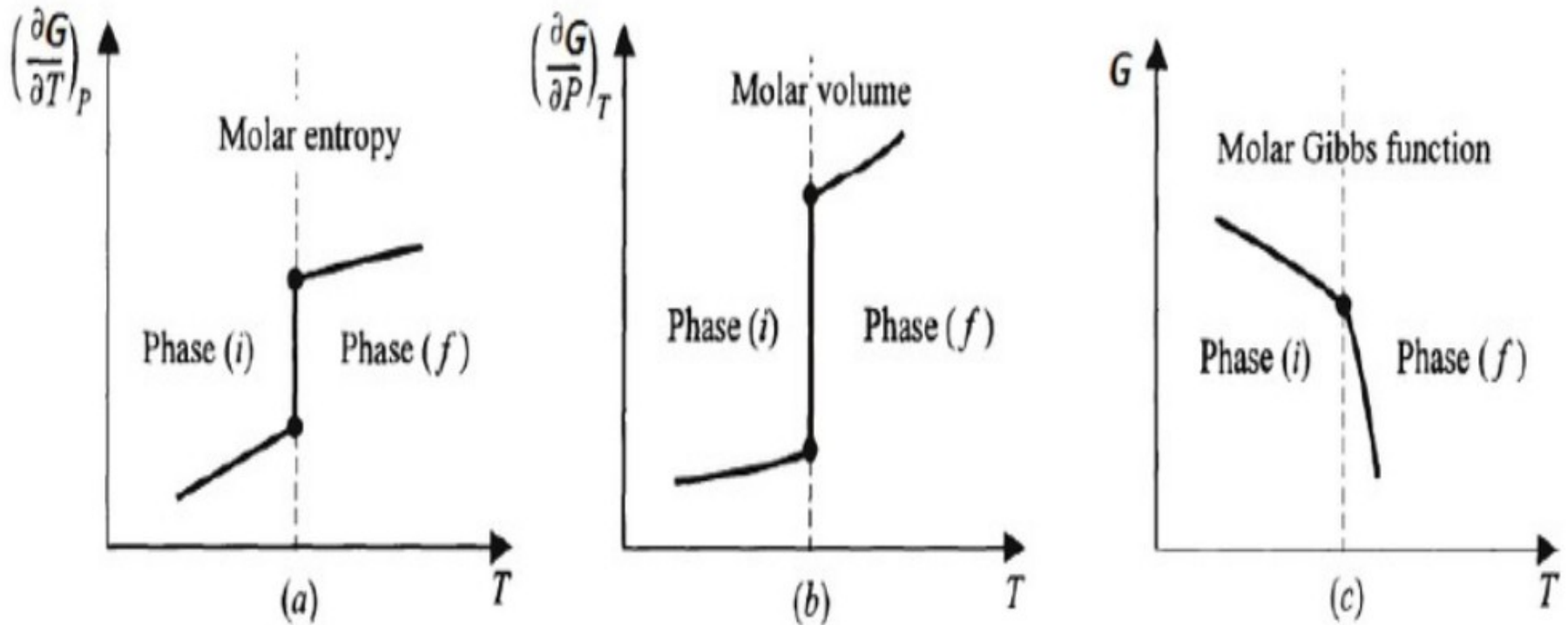
# Simple Fluids



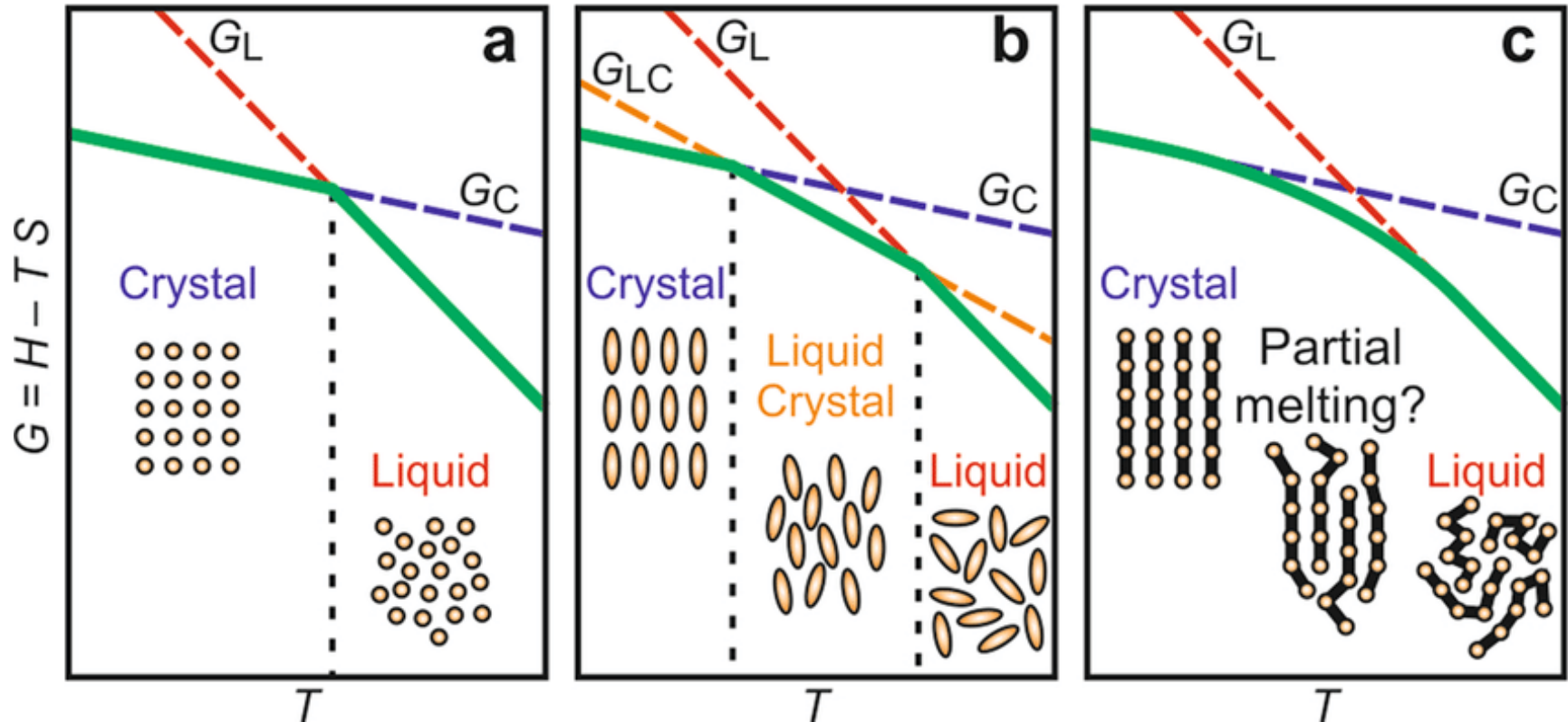
# First Order Transition



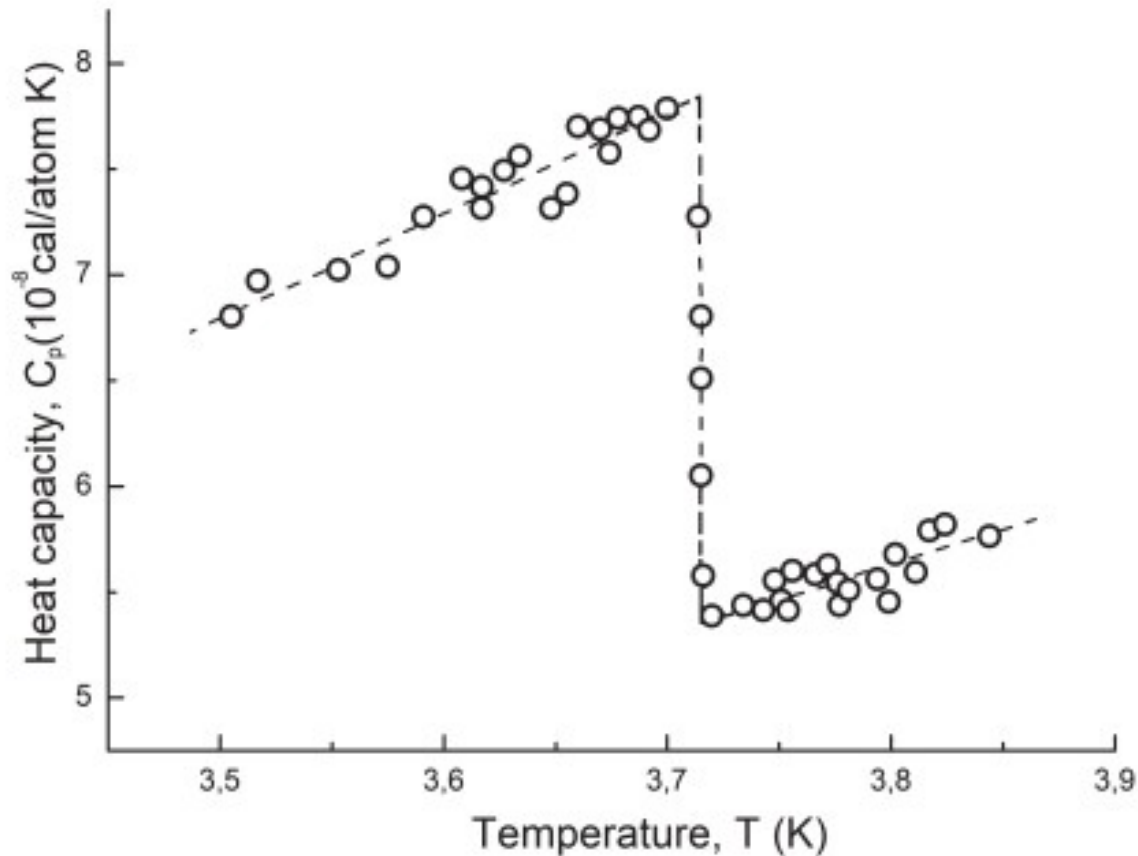
# First Order Transition



# First Order Transition



# First Order Heat Capacity





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# **First Order Phase Transition**

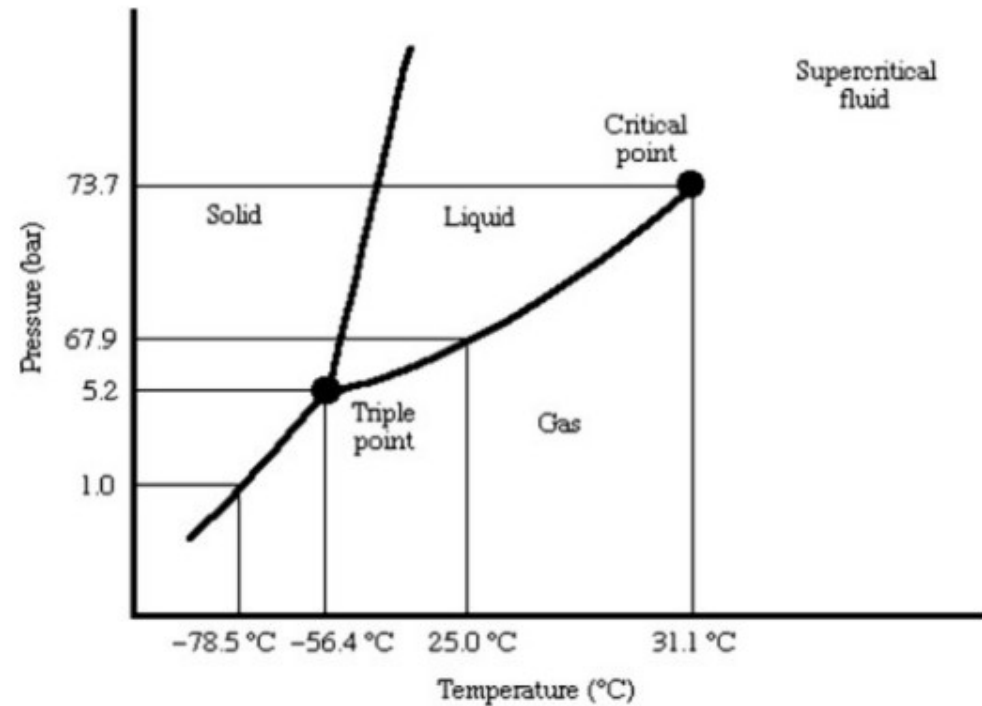
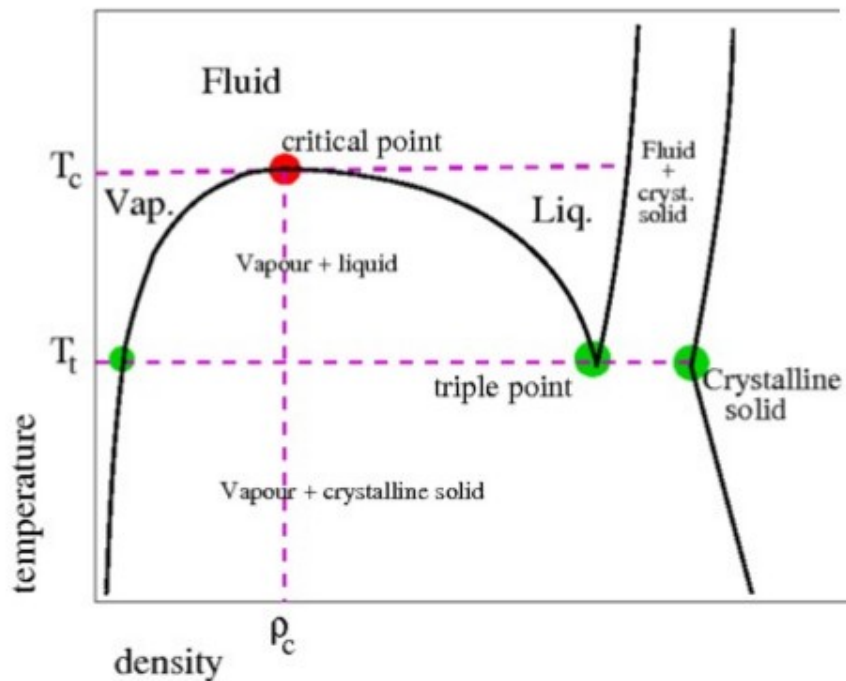
**Discontinuity of the derivative of the  
Gibbs Free energy with respect to the  
intensive parameter**

**Non zero Latent Heat**

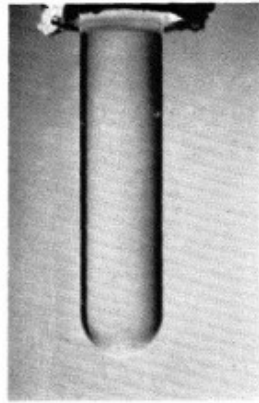
**Discontinuous Heat Capacity at  
Constant Pressure**

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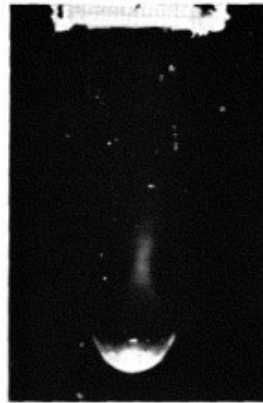
# Second Order - Continuous Phase Transition



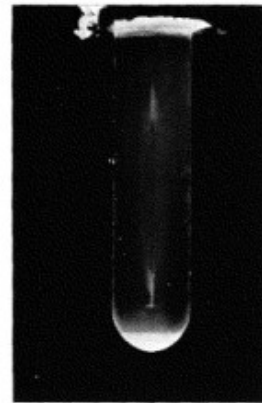
# Second Order Phase Transition



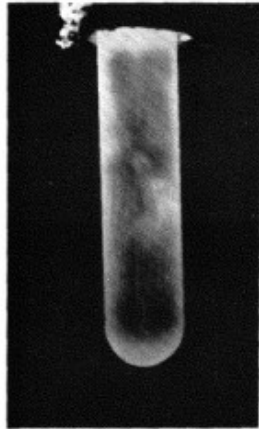
*a*



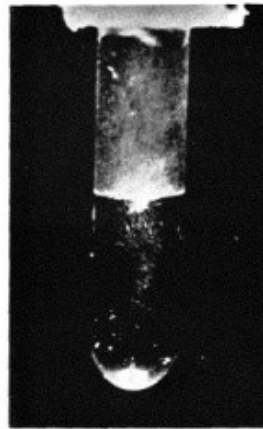
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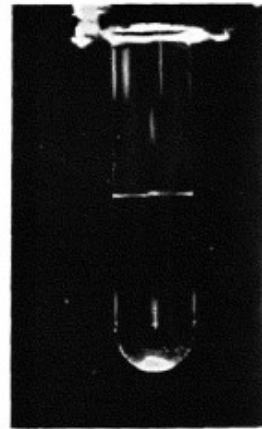
*c*



*d*



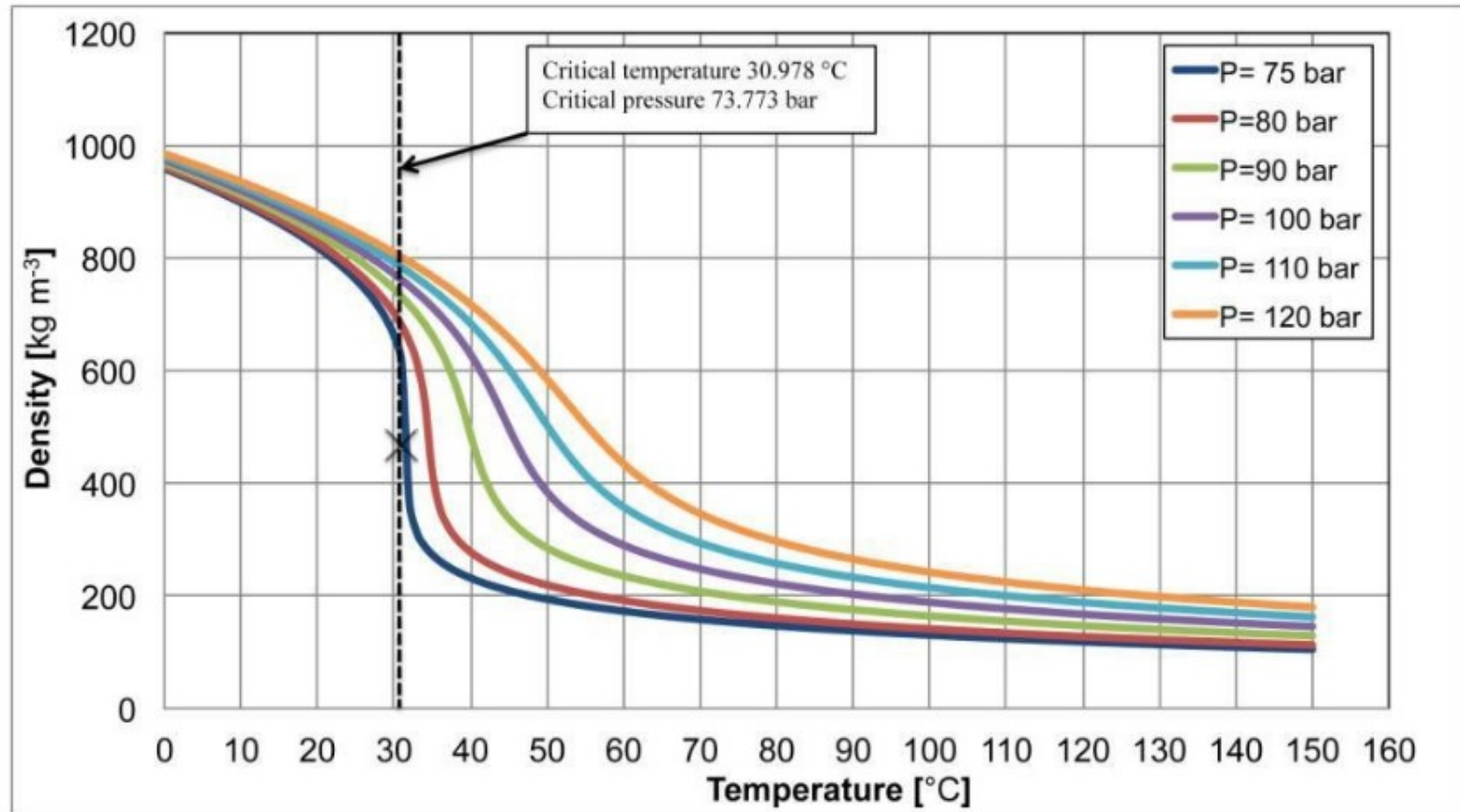
*e*



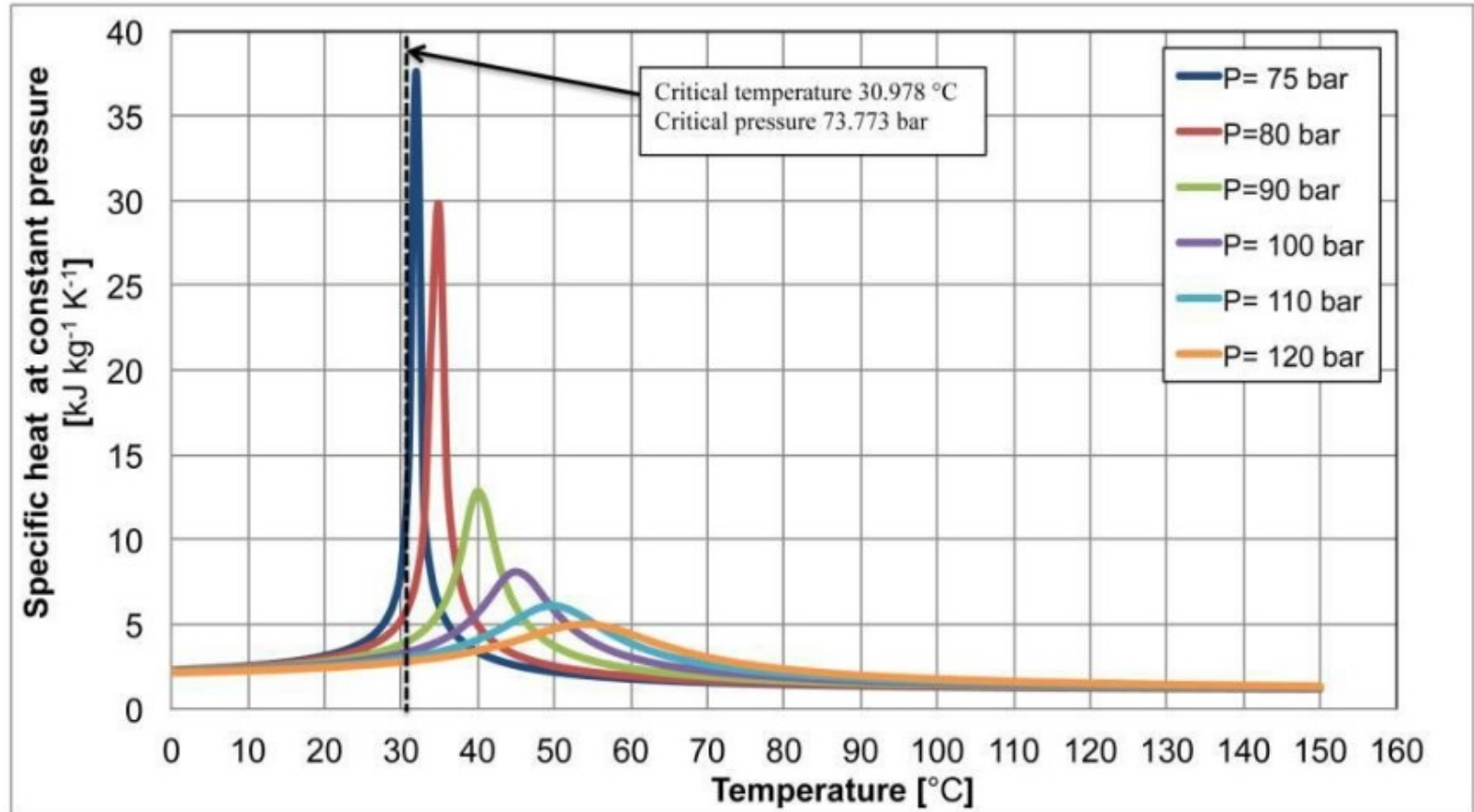
*f*

Mistura de ciclohexano e anilina Ferrel 1968

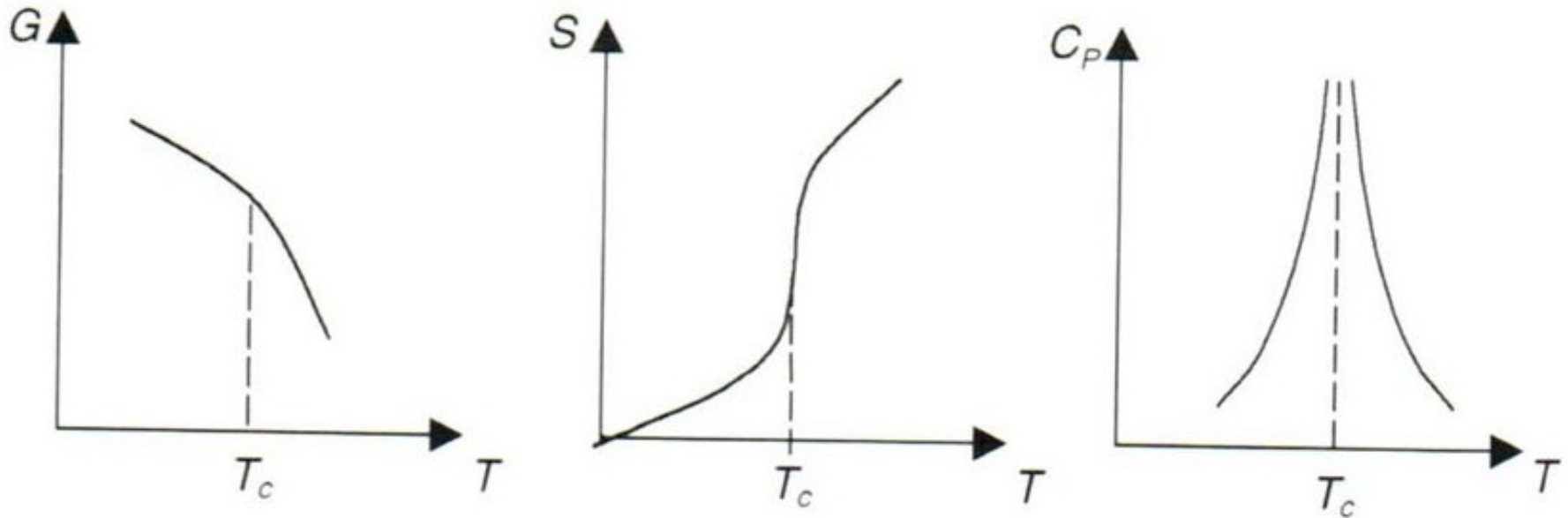
# Second Order Phase Transition



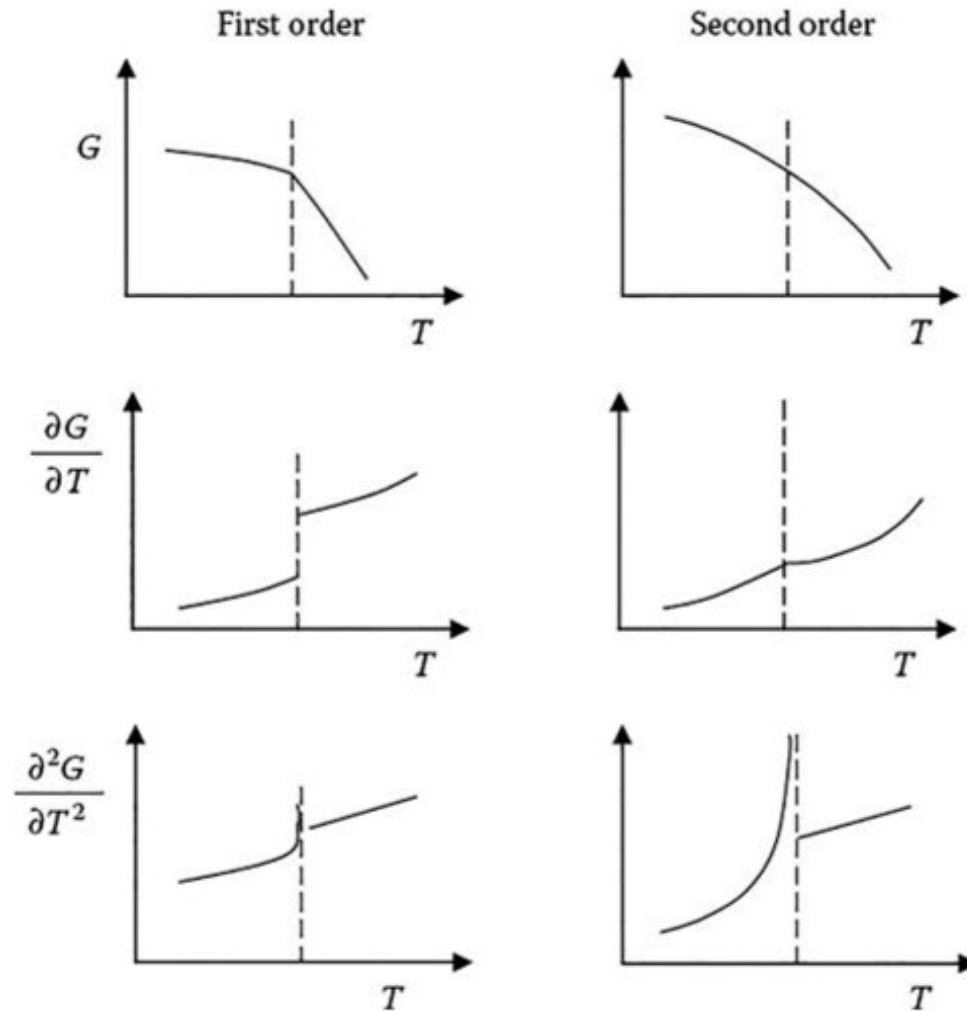
# Second Order Phase Transition



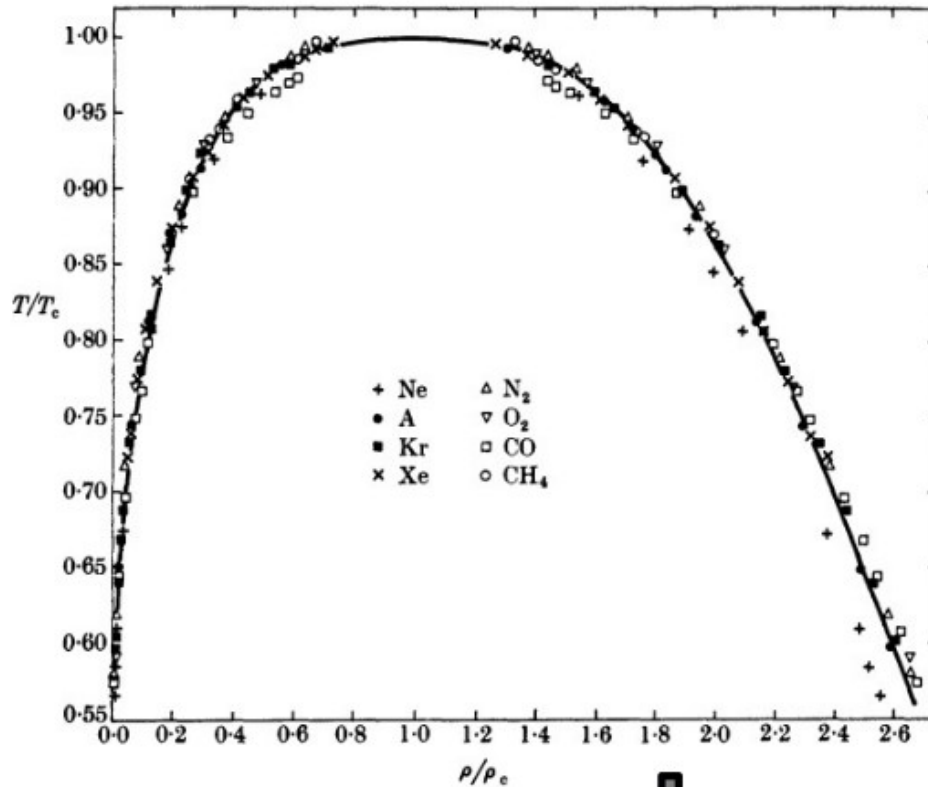
# Continuous Phase Transition



# Phase Transitions



# Density

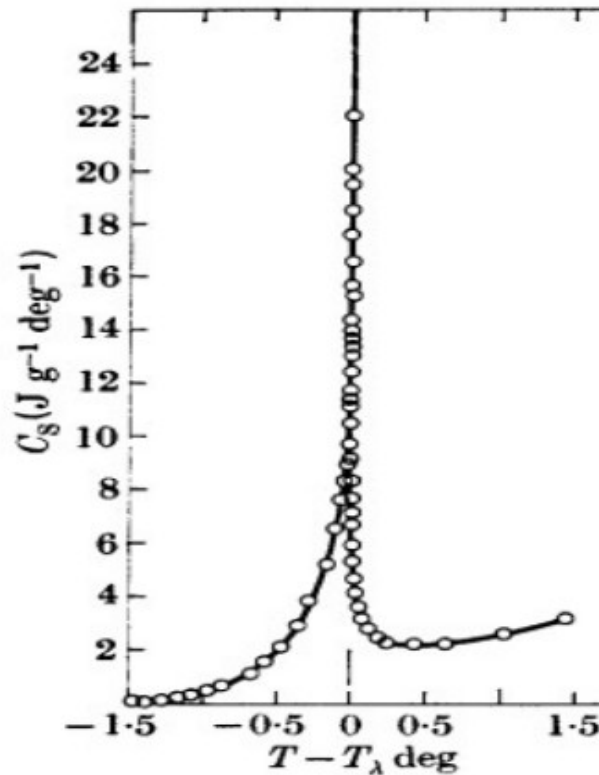


$$C_{V=v_c} \sim (-\epsilon)^{-\alpha'} \quad \rho_L - \rho_G \sim (-\epsilon)^\beta \quad K_T \sim (-\epsilon)^{-\gamma'}$$

E. A. Guggenheim, Journal Chem. Phys. 13M 253 (1945)



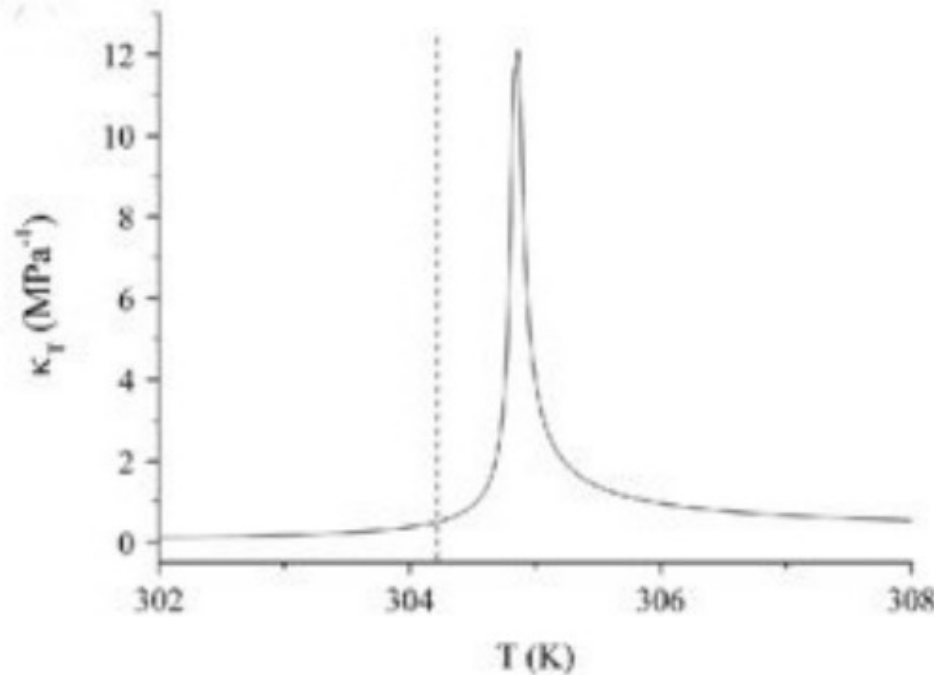
# Specific Heat



$$C_{V=V_c} \sim (-\epsilon)^{-\alpha'} \quad \rho_L - \rho_G \sim (-\epsilon)^\beta \quad K_T \sim (-\epsilon)^{-\gamma'}$$

H. E. Stanley, Phase Transition and Critical Phenomena.

# Compressibility



$$C_{V=v_c} \sim (-\epsilon)^{-\alpha'} \quad \rho_L - \rho_G \sim (-\epsilon)^\beta \quad K_T \sim (-\epsilon)^{-\gamma'}$$

<https://link.springer.com/article/10.1007/s12665-014-3716-5>

# Scaling

$$\alpha' + 2\beta + \gamma' = 2$$

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# Scattering - Correlation

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# **WATER ANOMALIES**

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# Water Anomalies



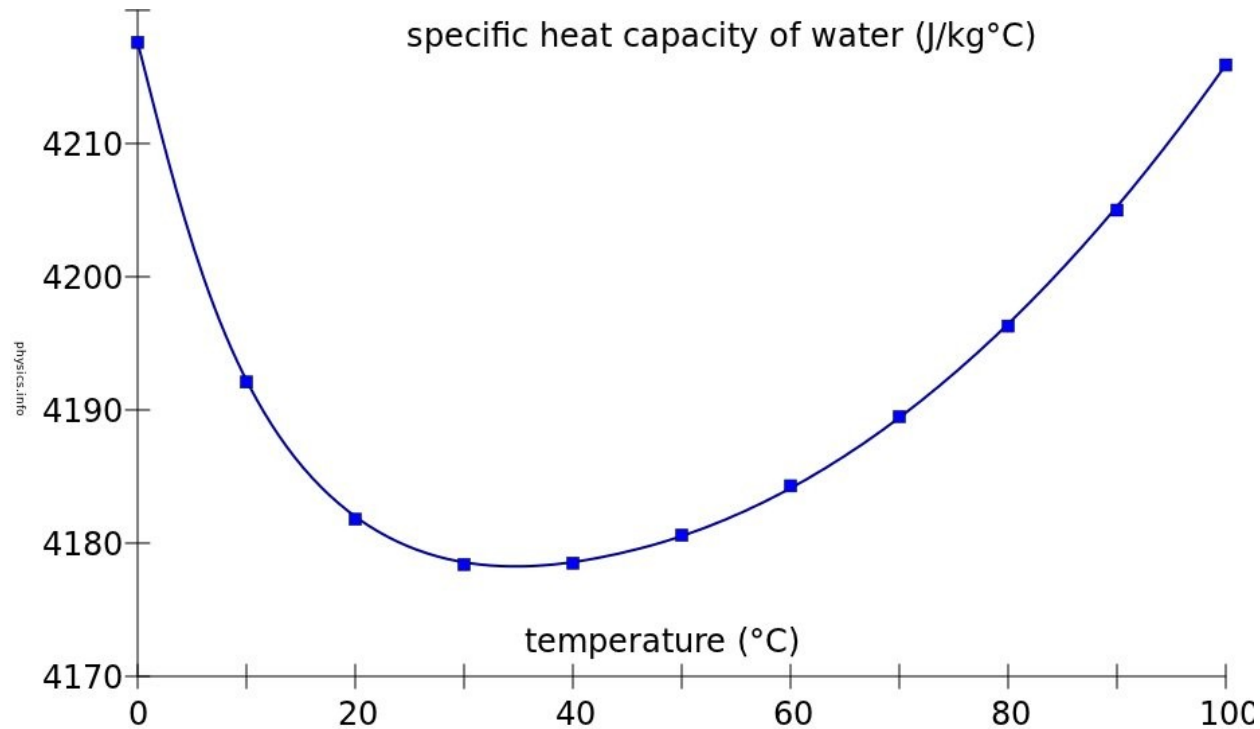
**photo by Clóvis Jardim**

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# Specific Heat

Methanol: Lombari, Ferrari, Salvetti, CPL 300 (99)

Water: G. S. Kell, J. Chem. Eng. Data 20, 97 (75)

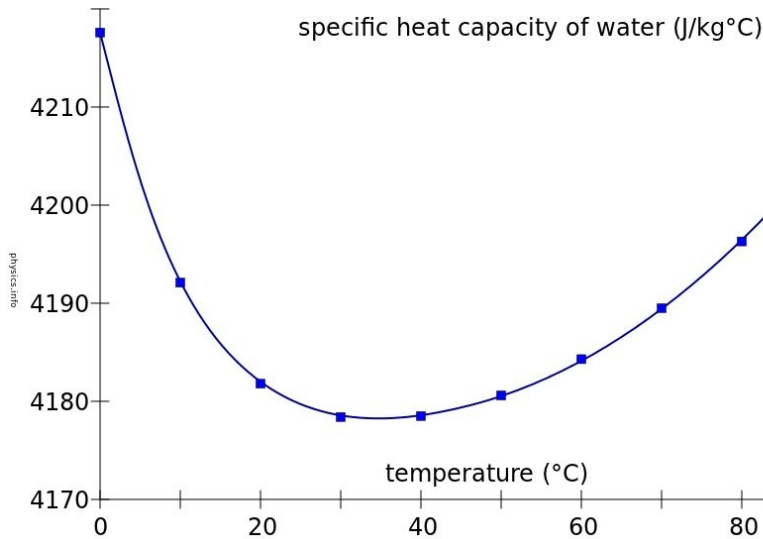


$$C_p = dQ_p/dT$$

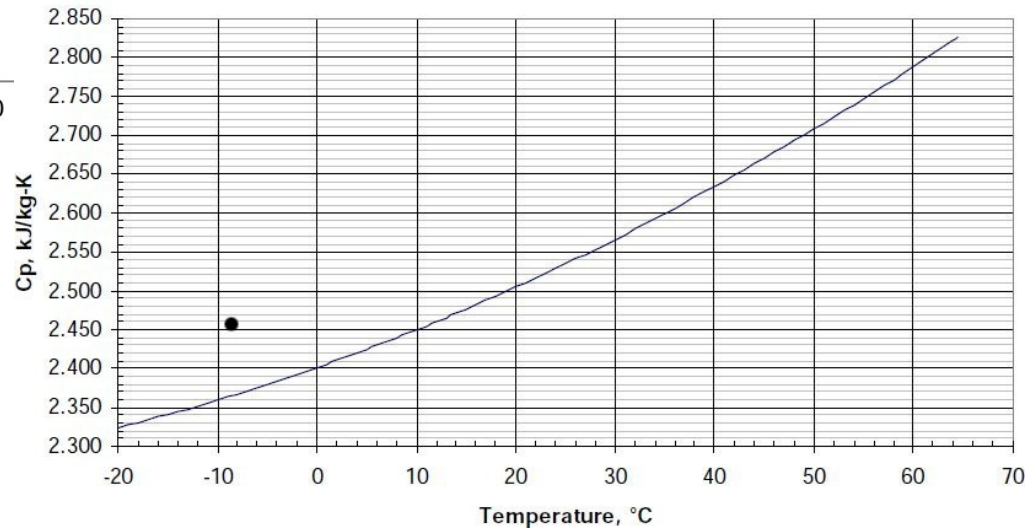
# Specific Heat

Methanol: Lombari, Ferrari, Salvetti, CPL 300 (99)

Water: G. S. Kell, J. Chem. Eng. Data 20, 97 (75)



Methanol Specific Heat, Cp



$$C_p = dQ_p/dT$$



# Specific Heat



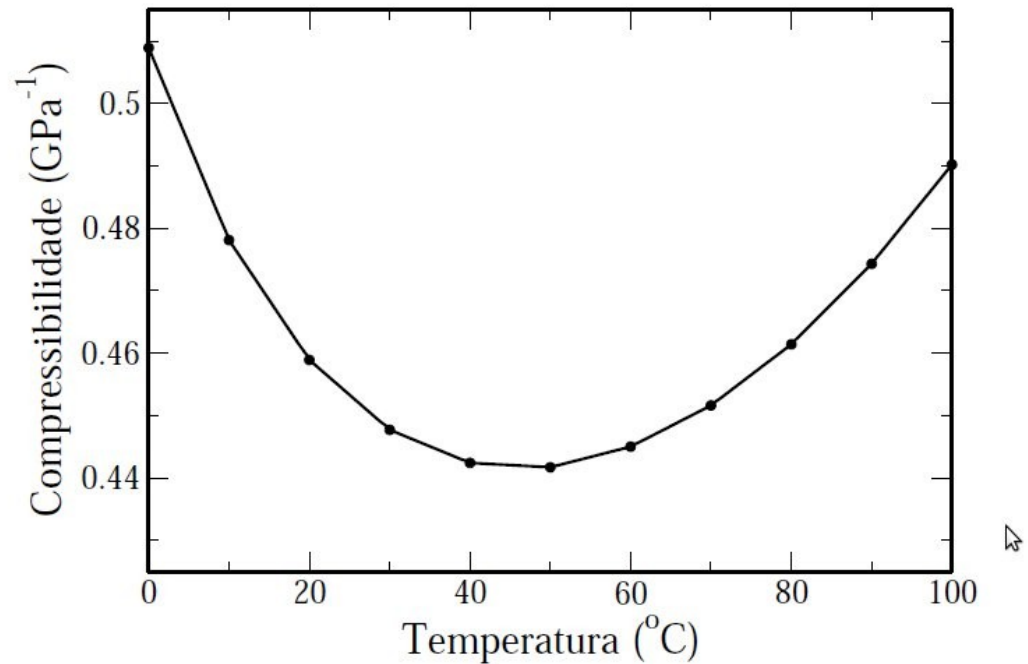
**Water → 4.18 kJ/kg°C**

**Silica → 0.68 kJ/kg°C**

# Compressibility

water: Speedy, Angell, JCP 65, 351 (76)

toluene: Minassian, Bouzar, Alba, JPC 92, 487 (88)

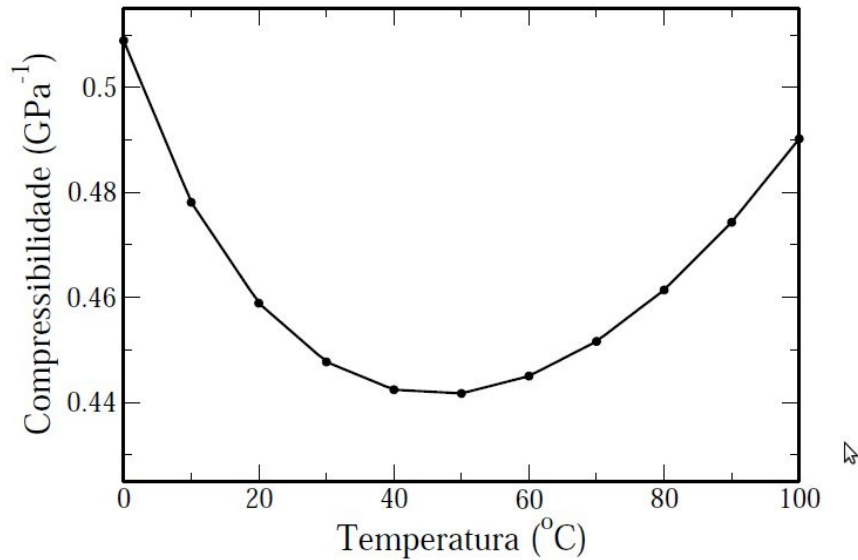


$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T$$

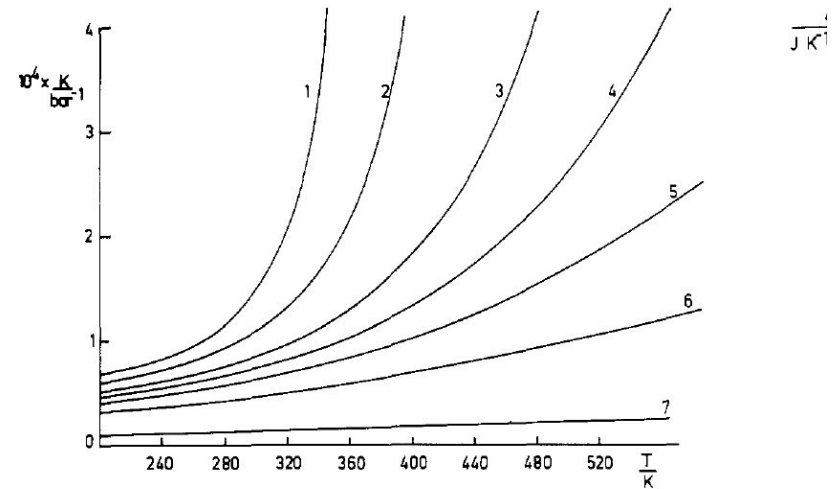
# Compressibility

water: Speedy, Angell, JCP 65, 351 (76)

toluene: Minassian, Bouzar, Alba, JPC 92, 487 (88)



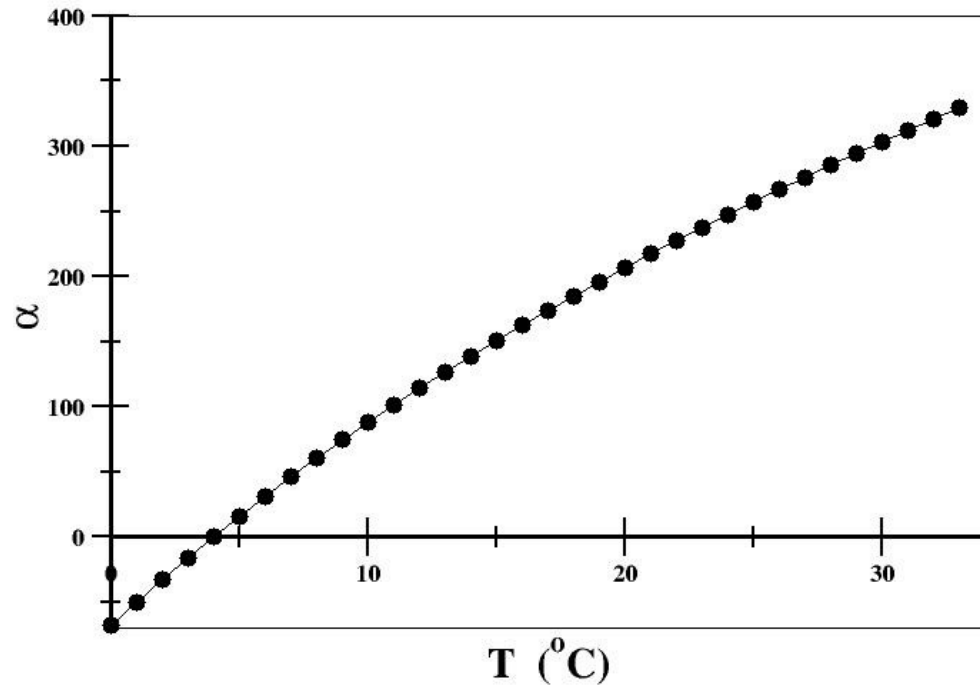
$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T$$



# Thermal Expansion Coefficient

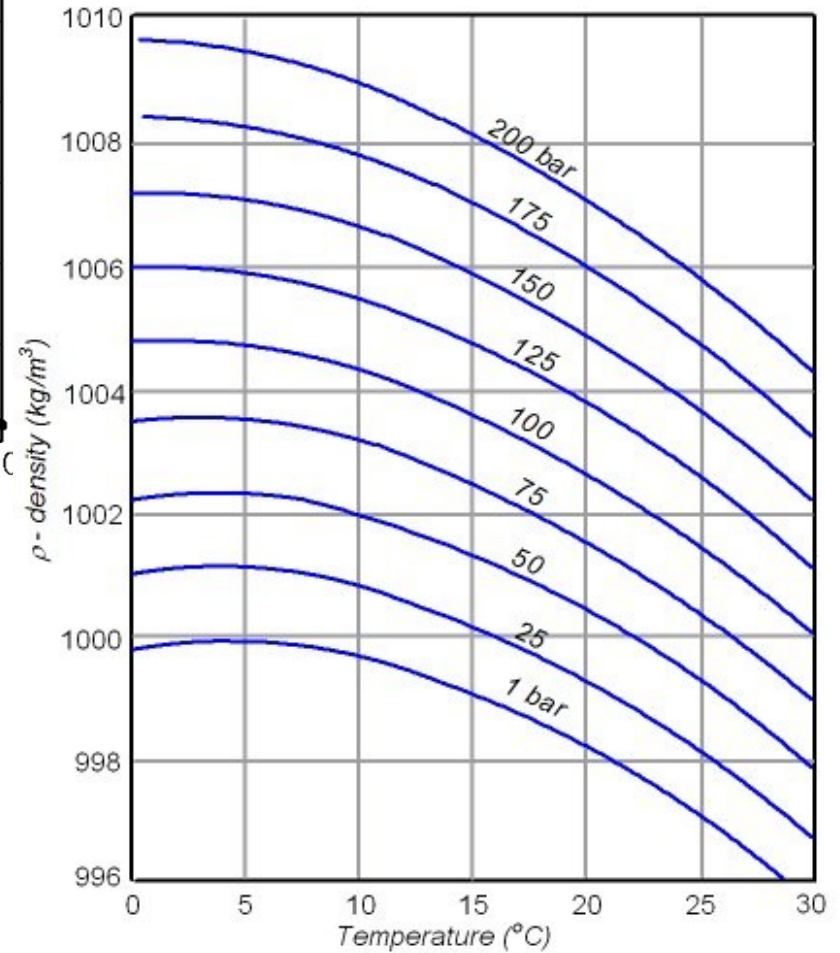
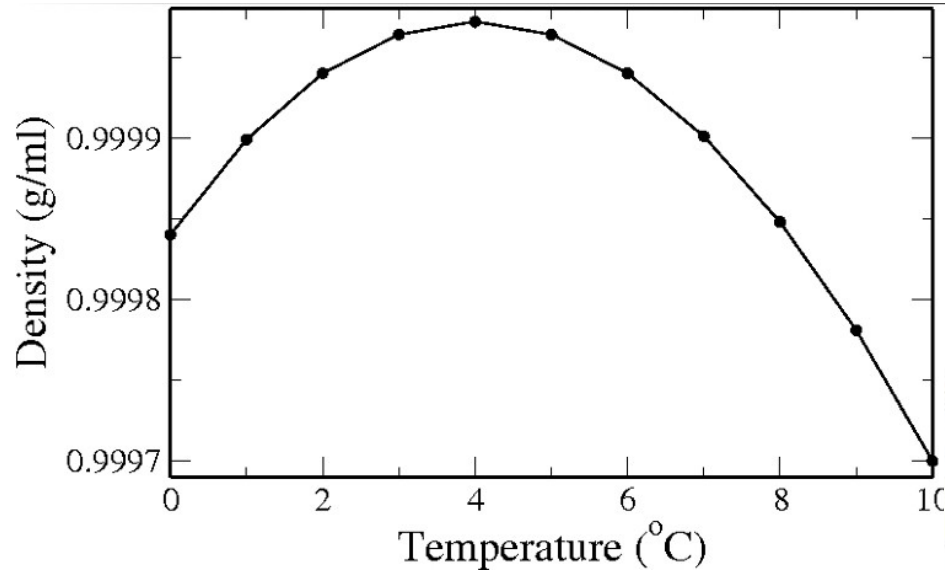
water: Kell, J. Chem. Eng. Data 20, 97 (75)

$$\alpha = \alpha_V = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_p$$



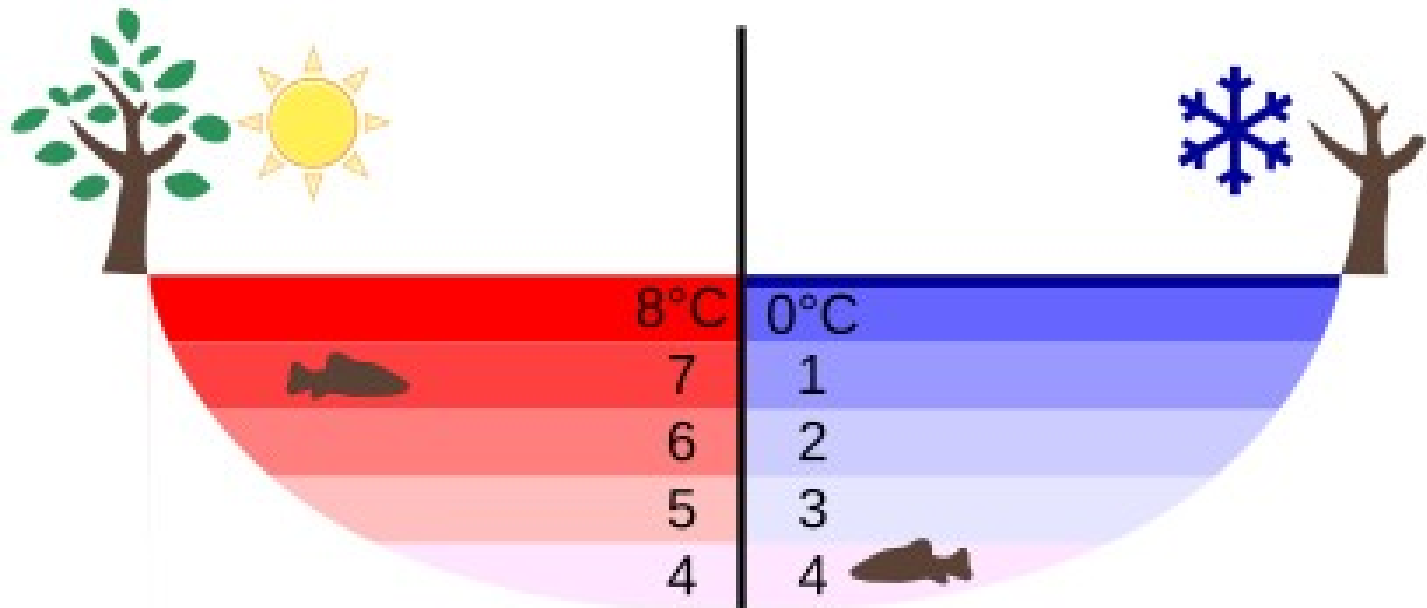
# Density

water: Kell, J. Chem. Eng. Data 20, 97 (75)



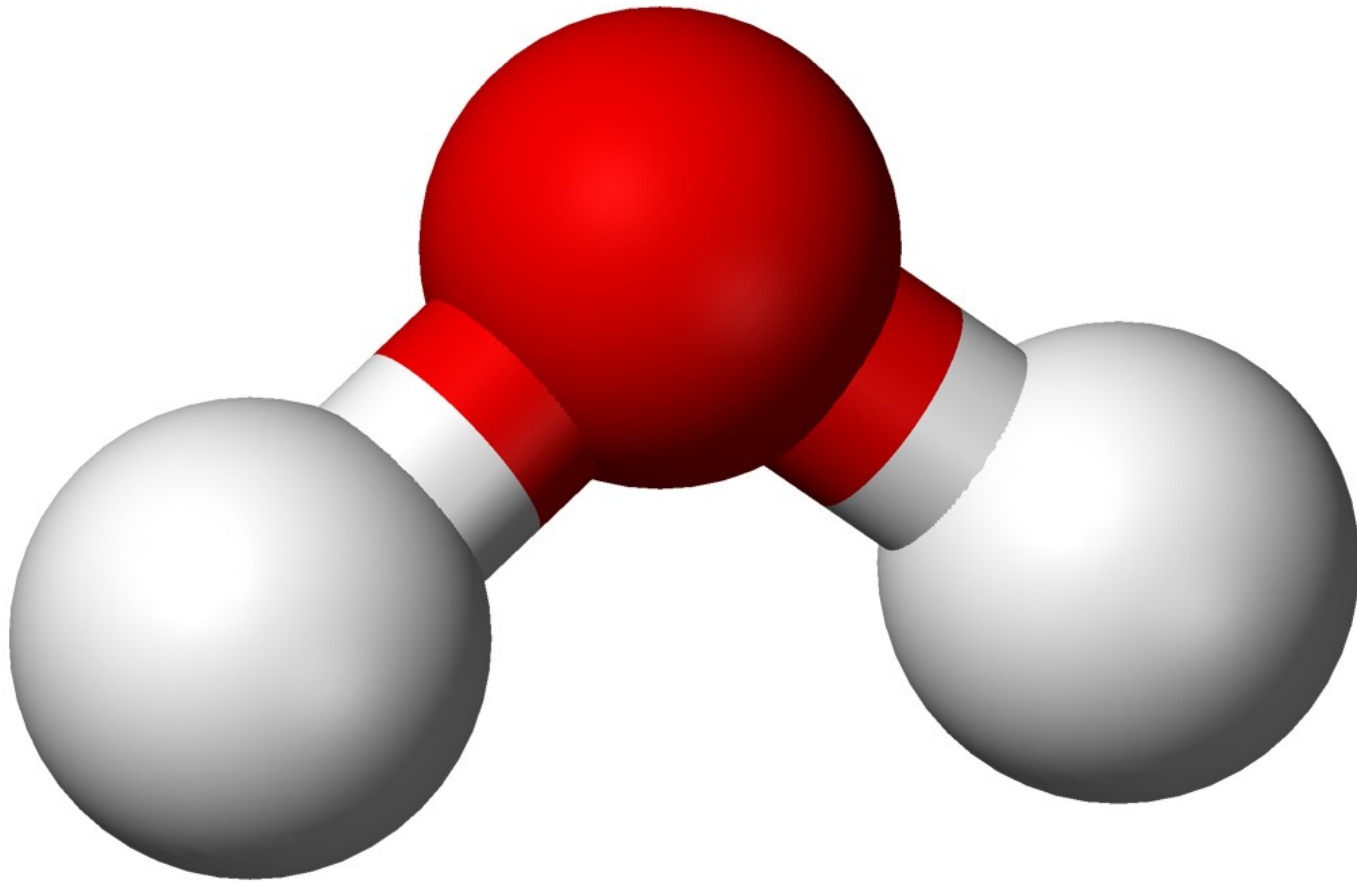
# Density

water: Kell, J. Chem. Eng. Data 20, 97 (75)

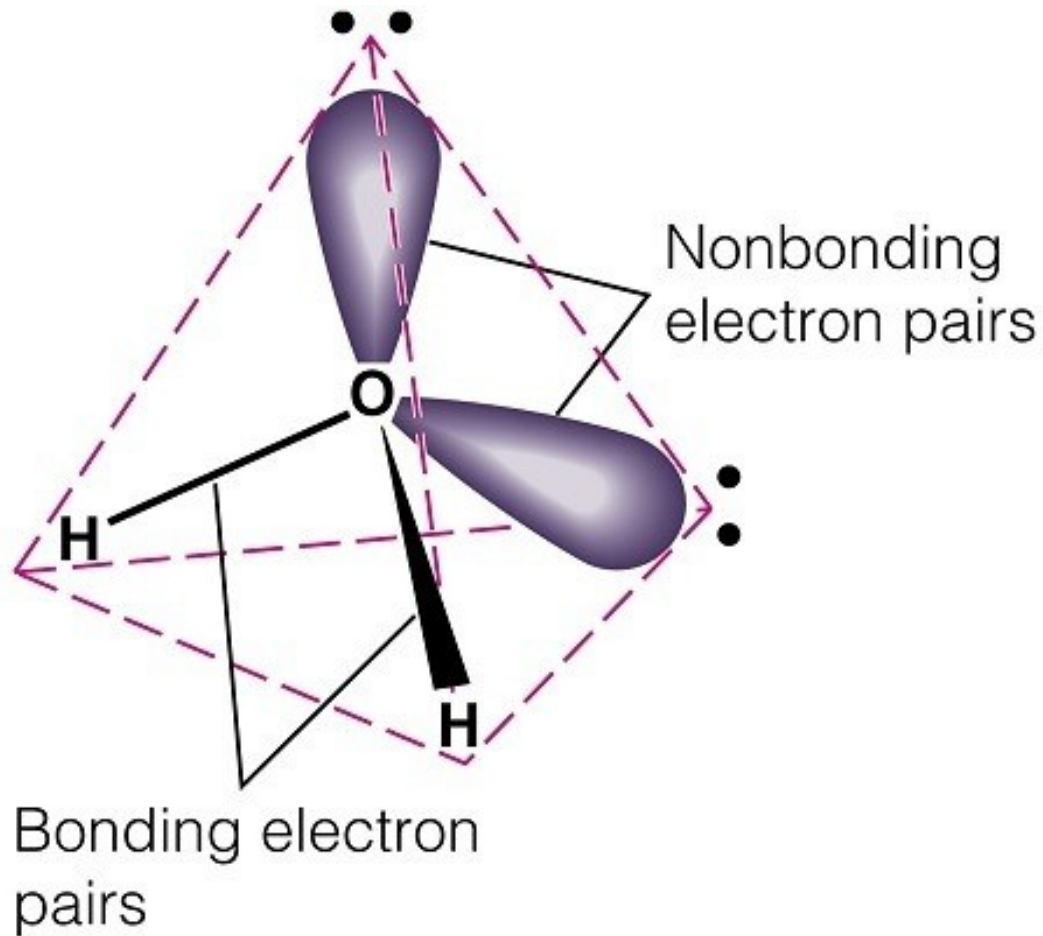


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# Water

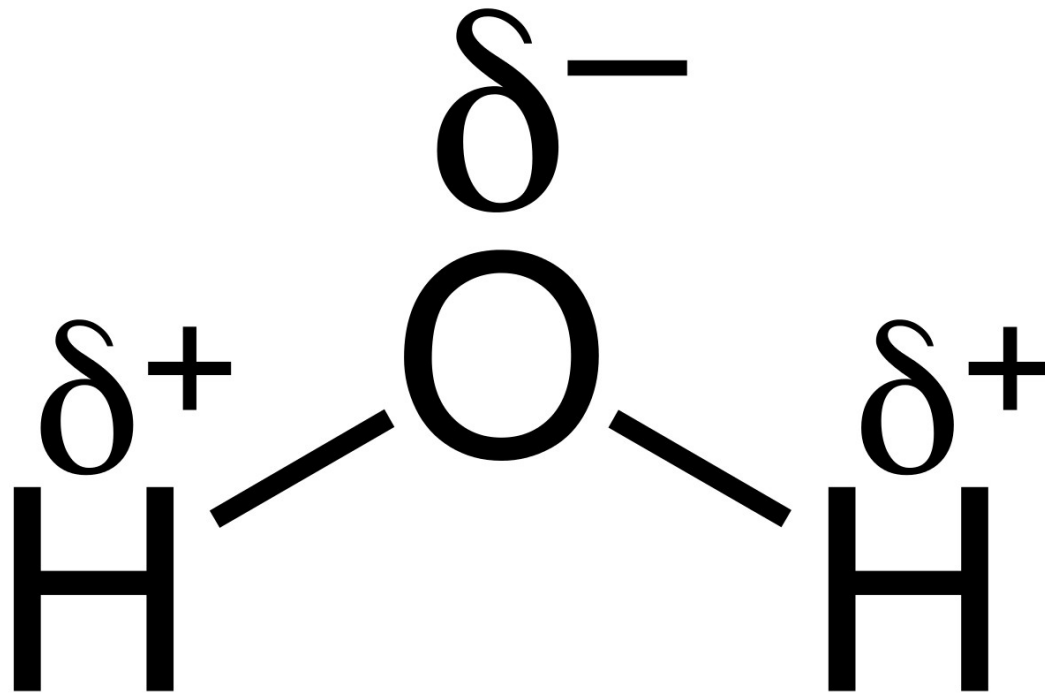


# Water

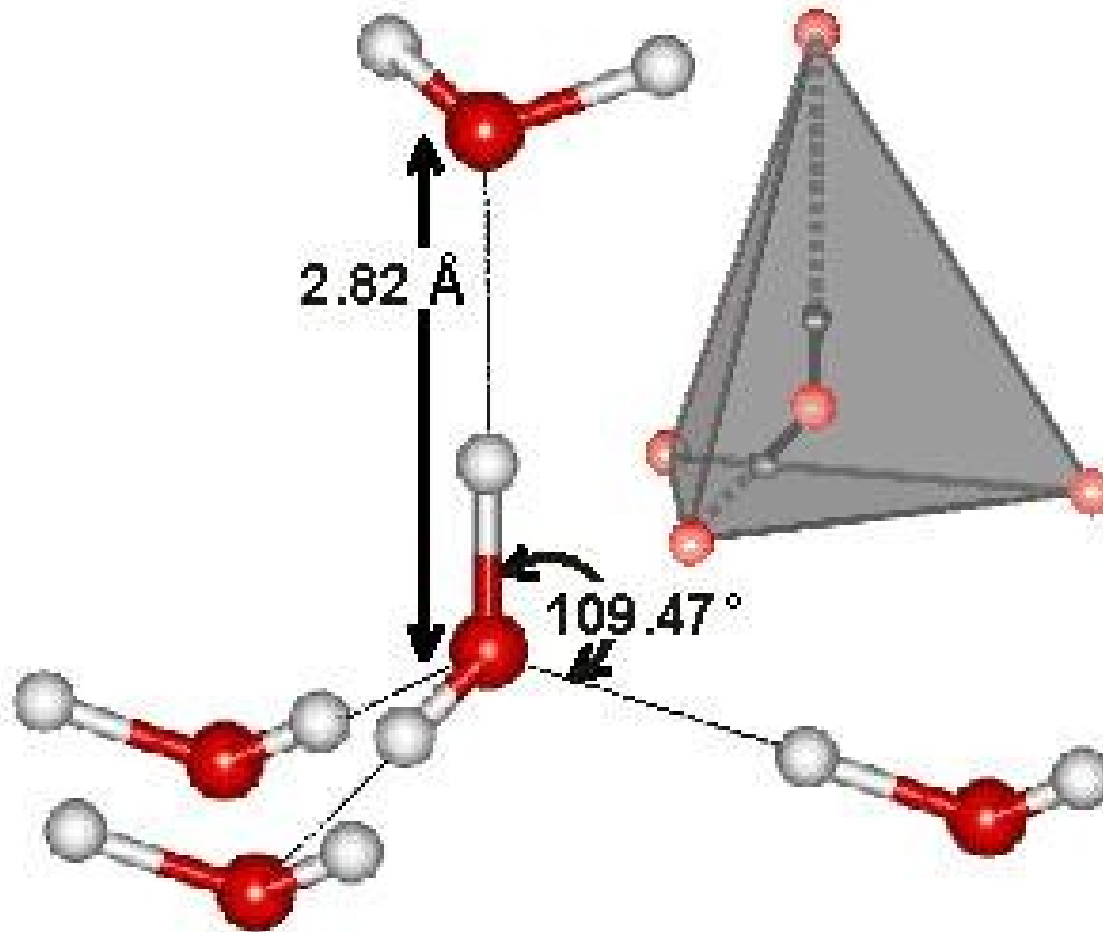




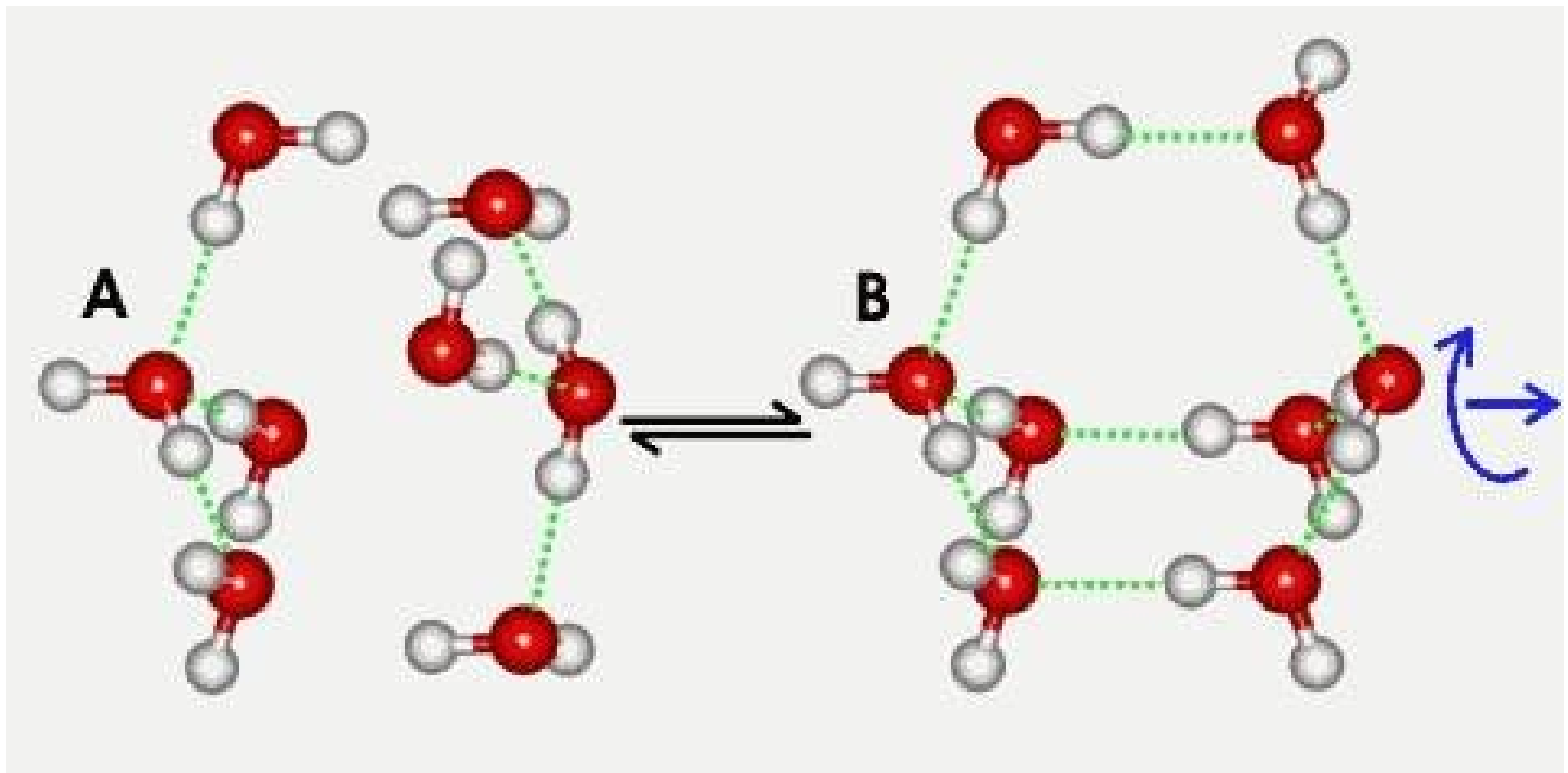
# Water



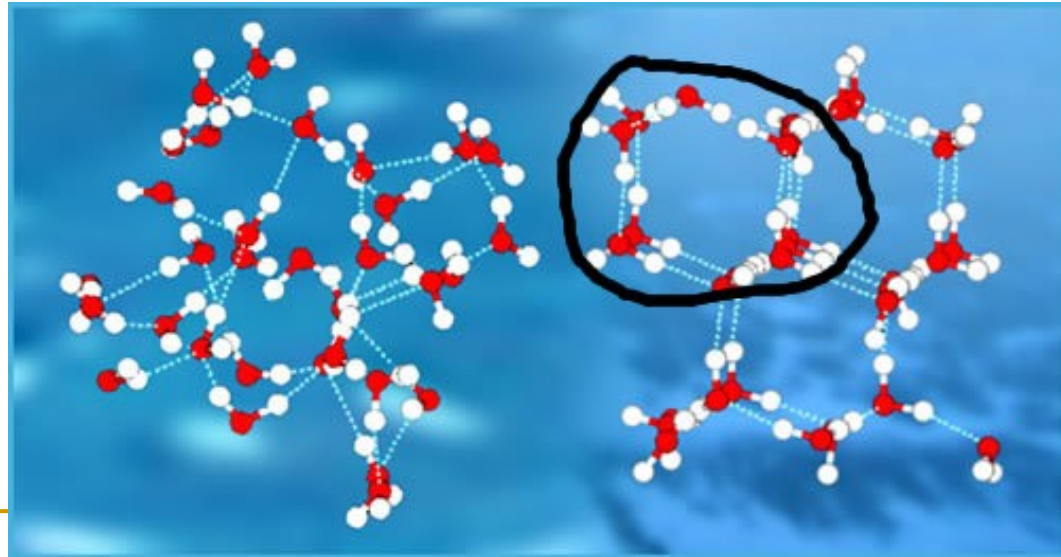
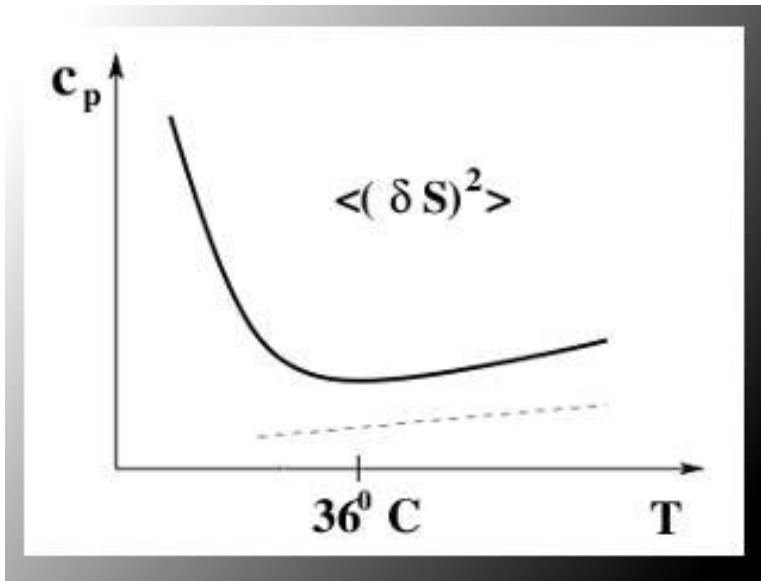
# Hydrogen Bonds



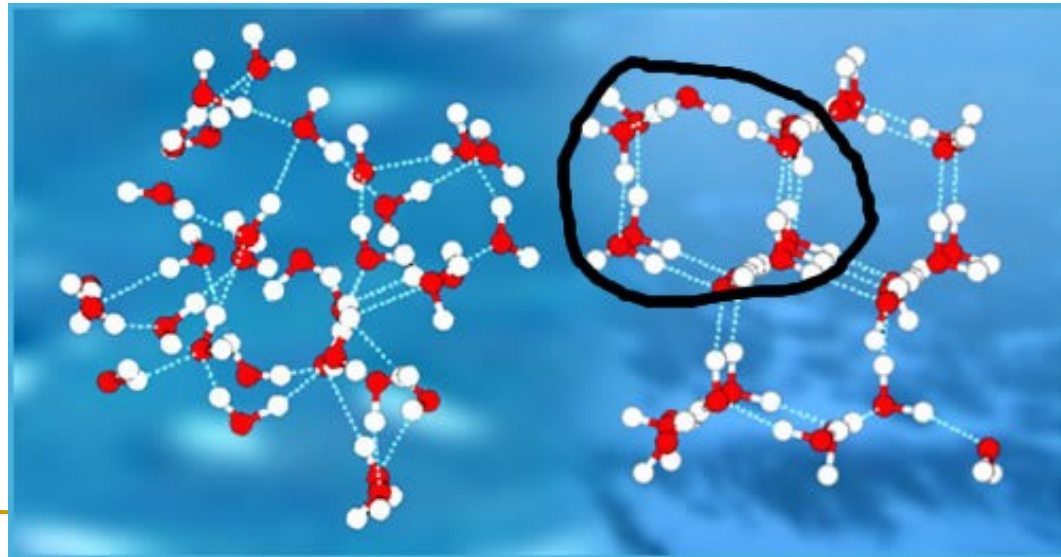
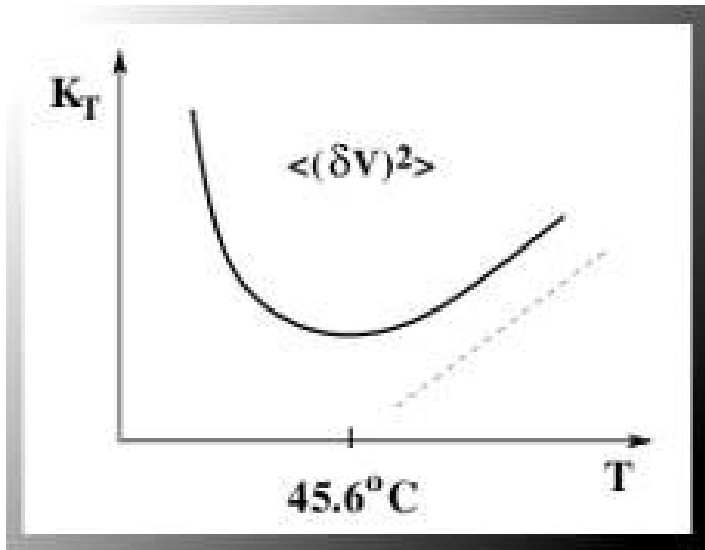
# Tetramers Open and Closed



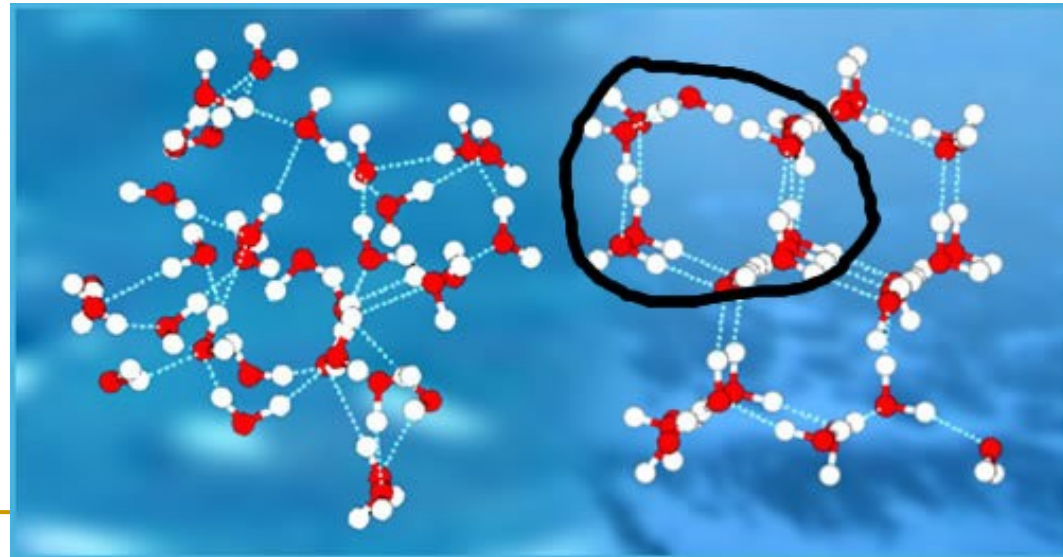
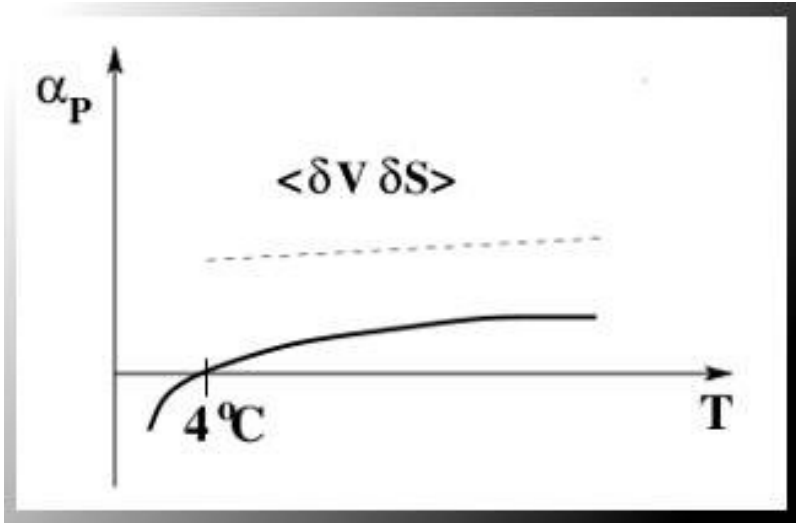
# Specific Heat



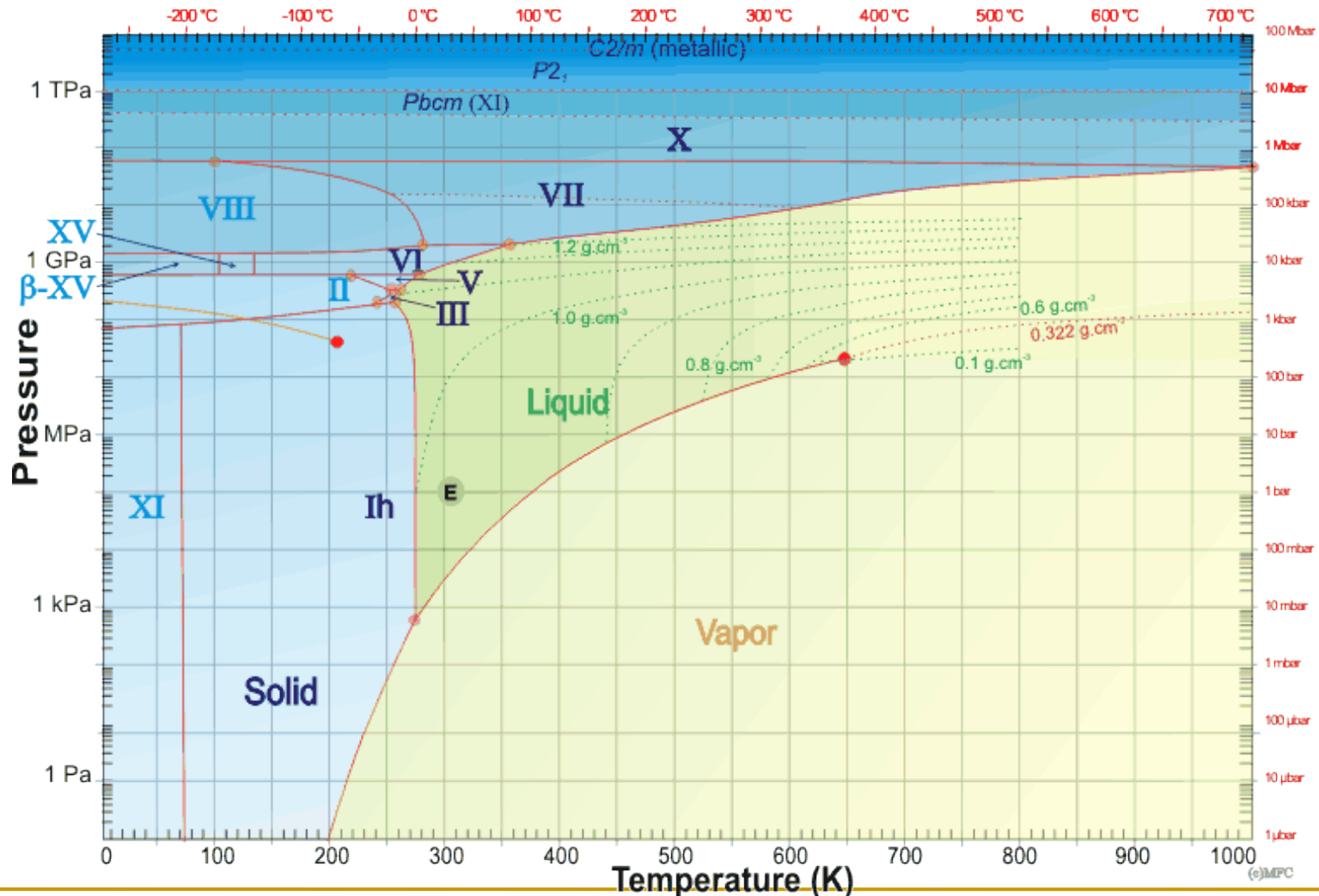
# Compressibility



# Thermal Expansion Coefficient

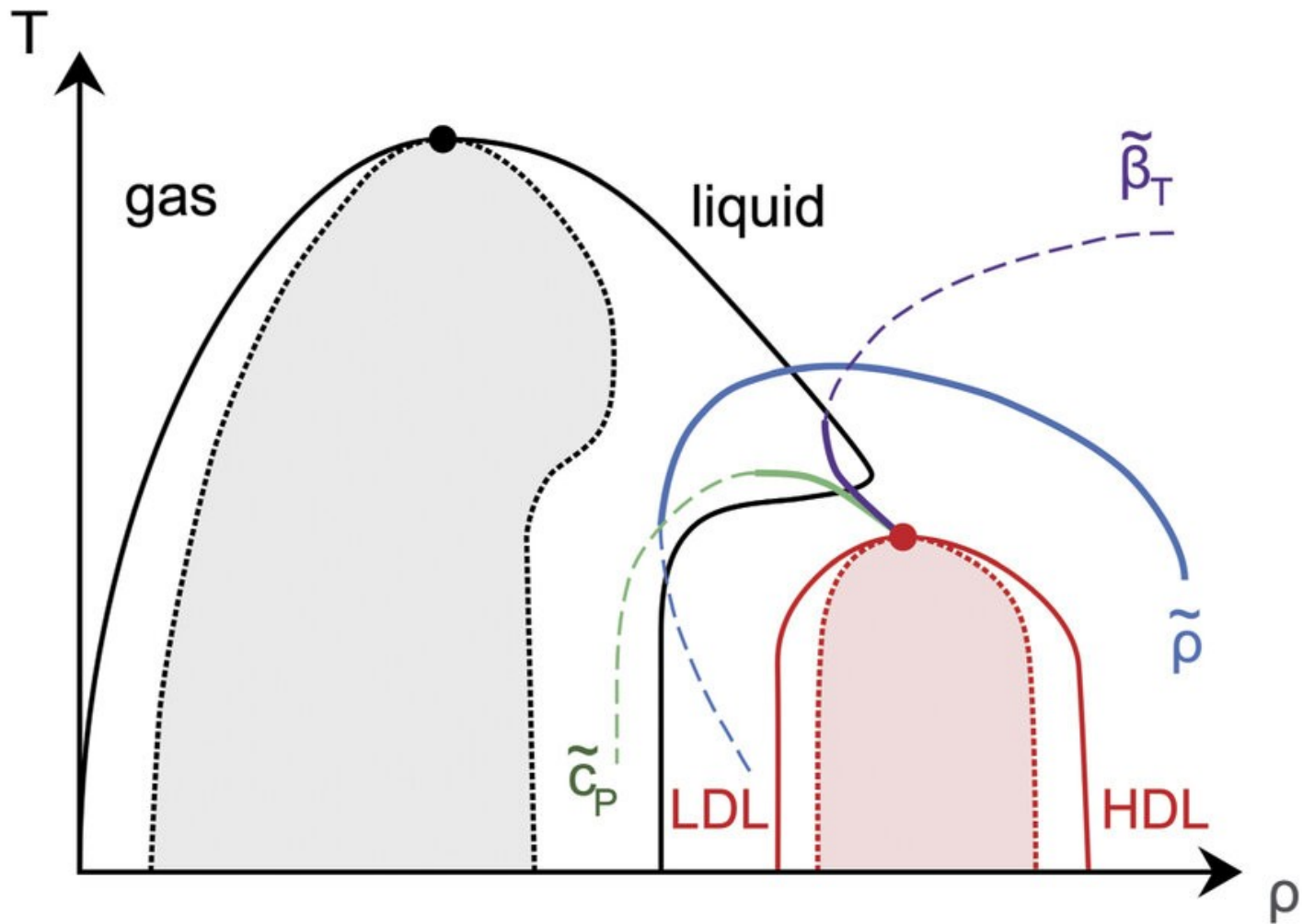


# Water Phase Diagram



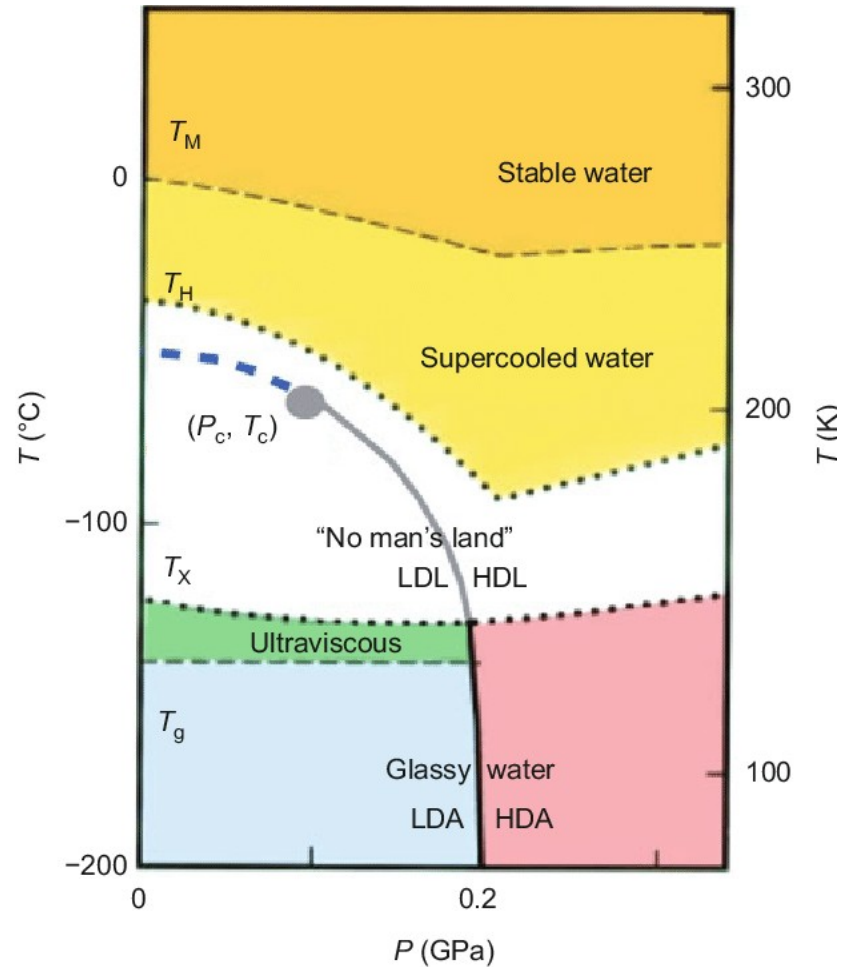
[https://water.lsbu.ac.uk/water/water\\_phase\\_diagram.html](https://water.lsbu.ac.uk/water/water_phase_diagram.html)

# Water Phase Diagram





# Water Phase Diagram



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**Next**

**Phase Transitions-  
Water Anomalies**

 **Nanoconfined Water in  
Solid State Materials**

**Nanoconfined Water in  
Biology**

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