# The Curious Case of… Water in Nanobottles

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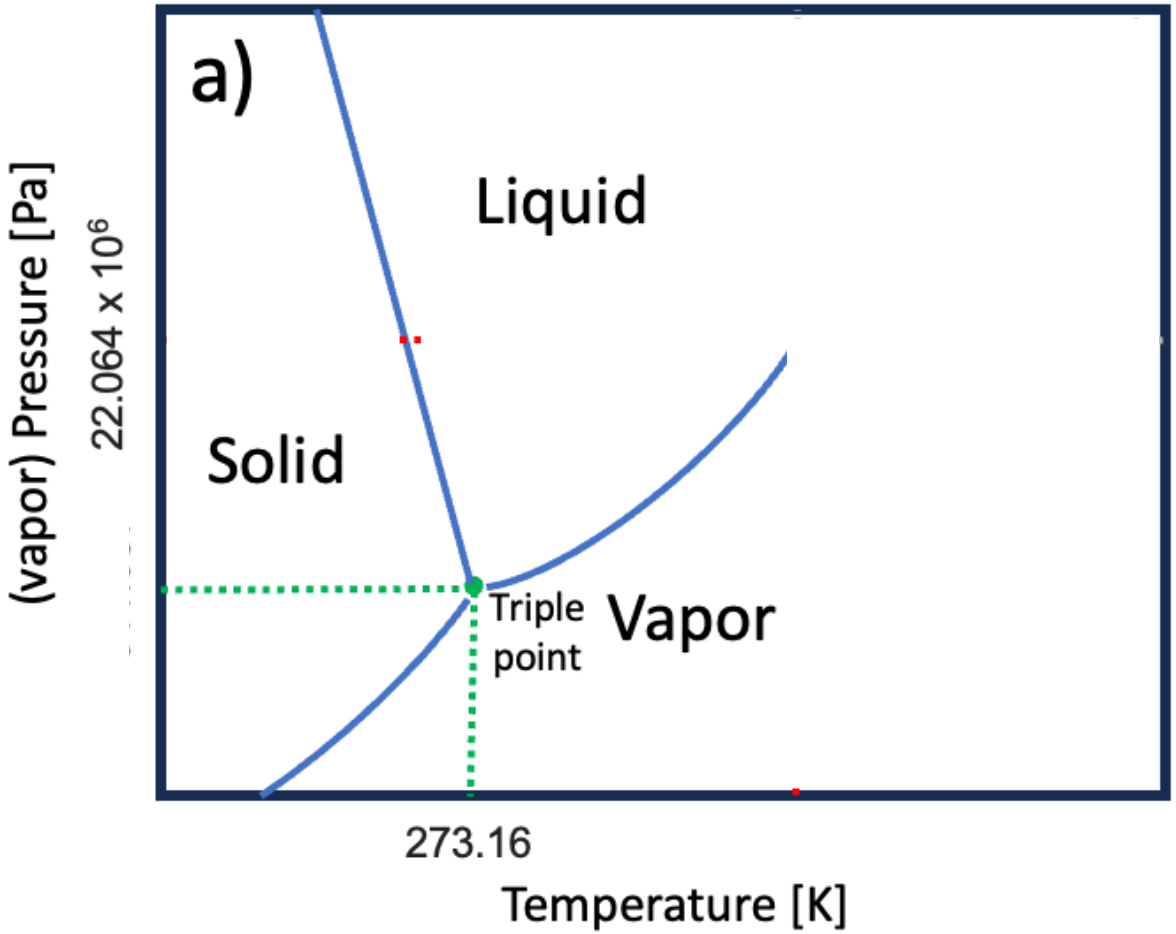
ELECTRO INTRUSION

**Workshop on Nanostructured Materials and Quantum Technologies**

European Innovation Council

Funded by the European Union

# Phase diagram of bulk water

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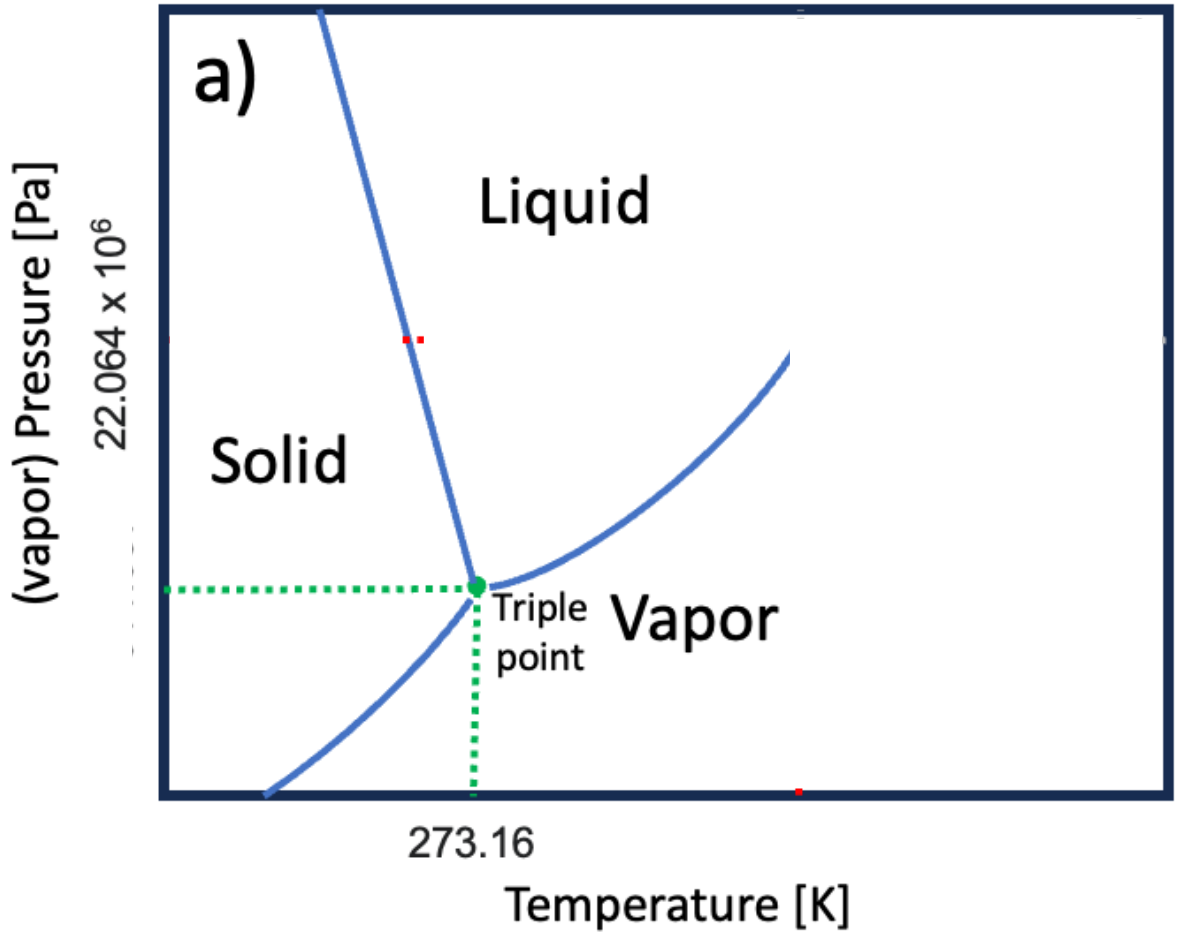
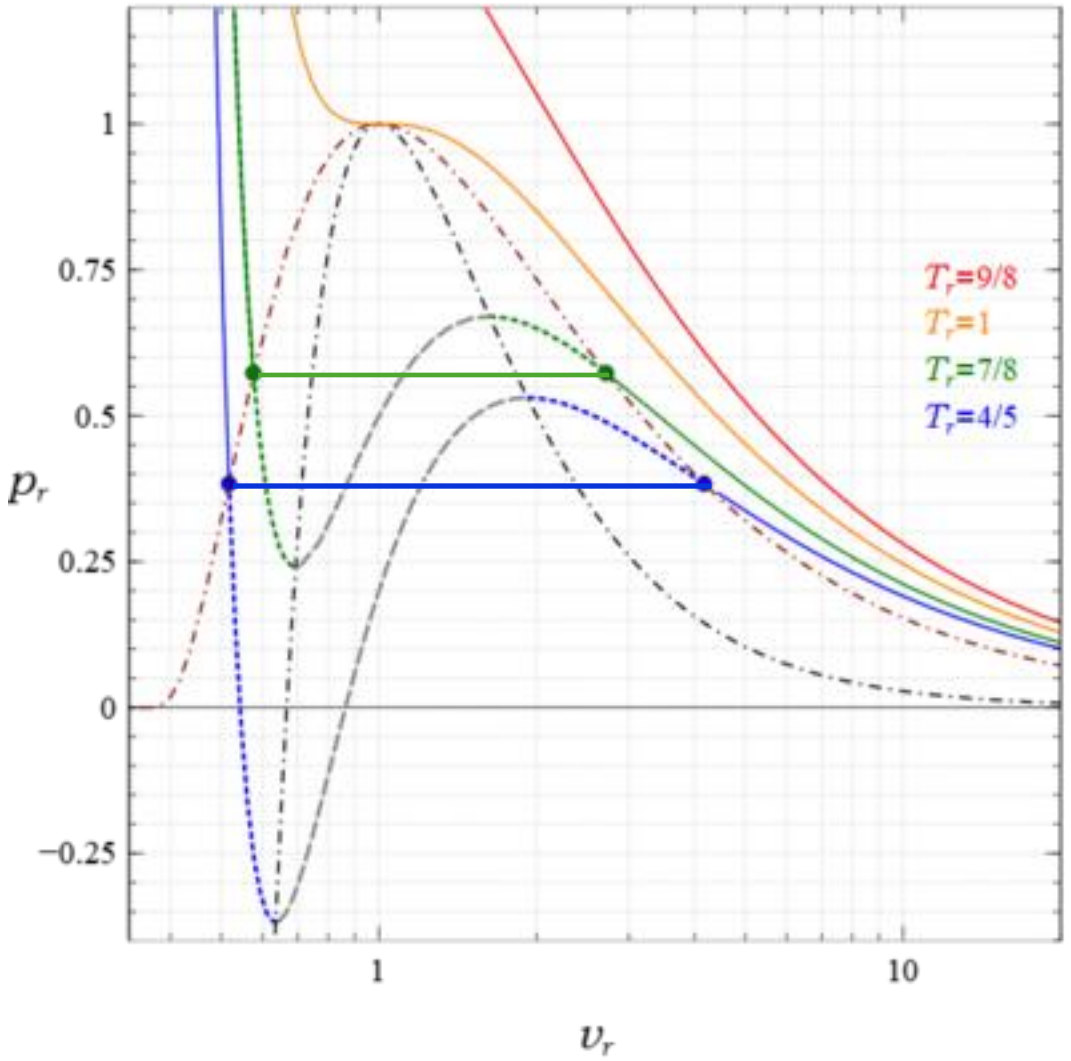
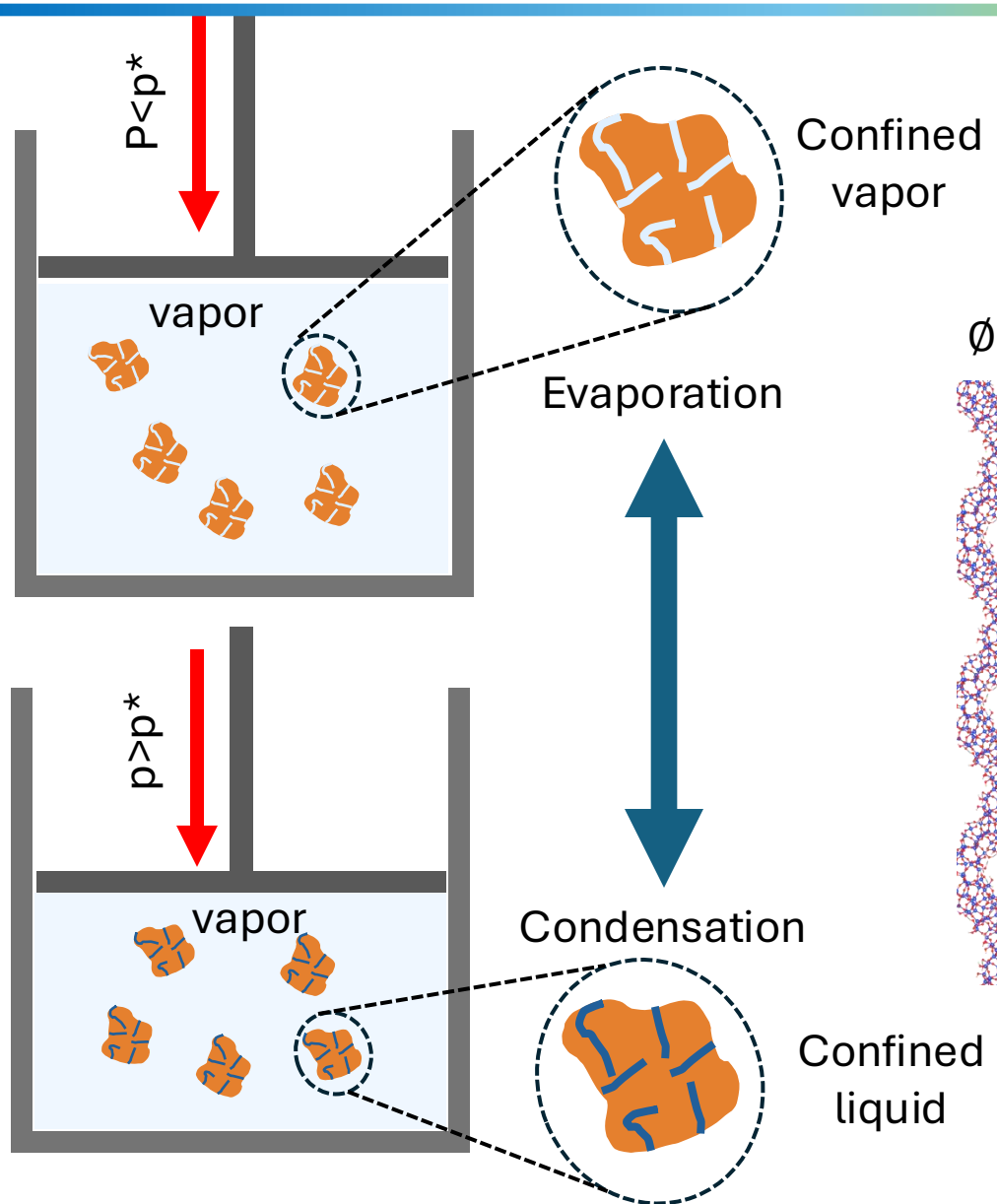



# Liquid/vapor Phase transition

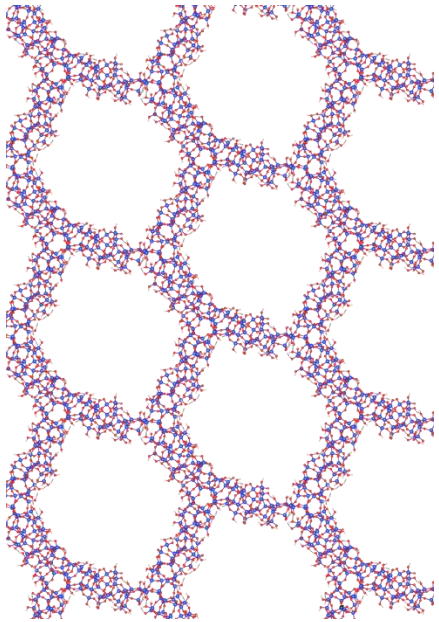


# Confined liquid-vapor phase transition: capillary condensation/evaporation

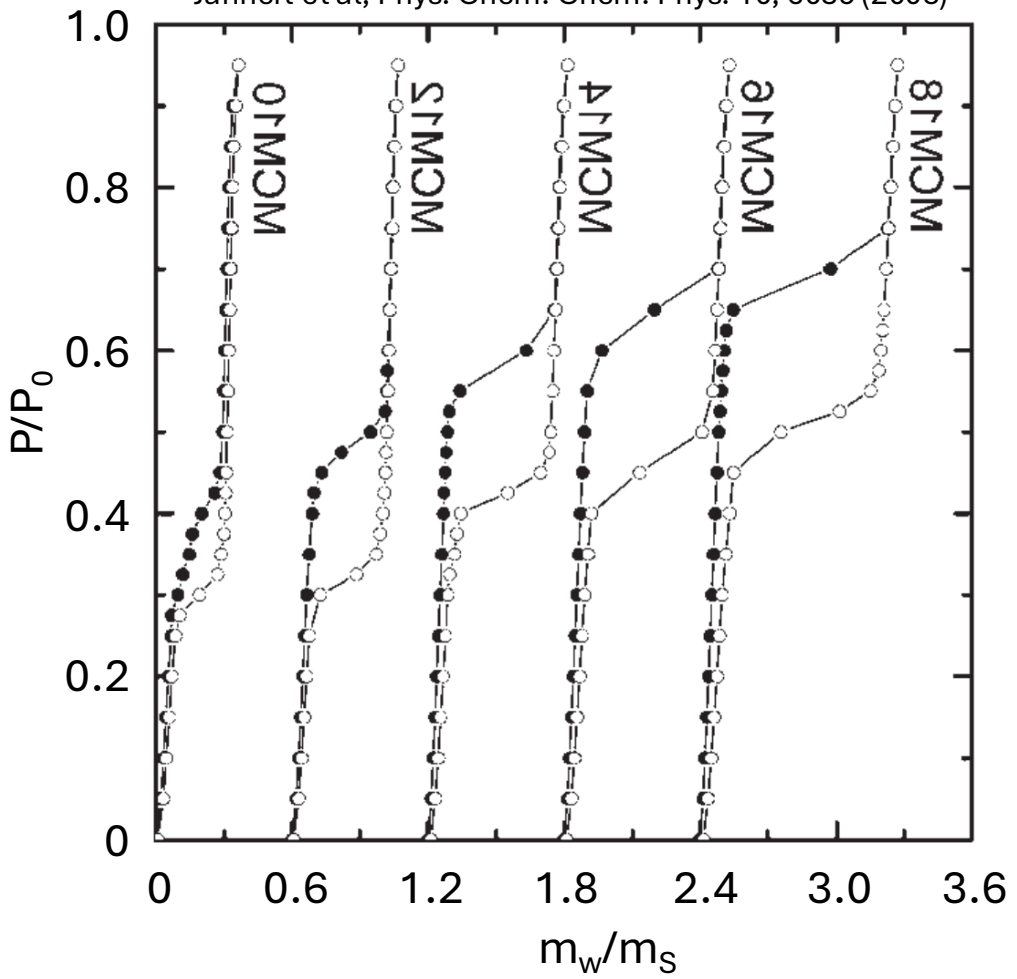



MCM

$\emptyset \in (2.5nm, 4.5nm)$



Jähnert et al, Phys. Chem. Chem. Phys. 10, 6039 (2008)



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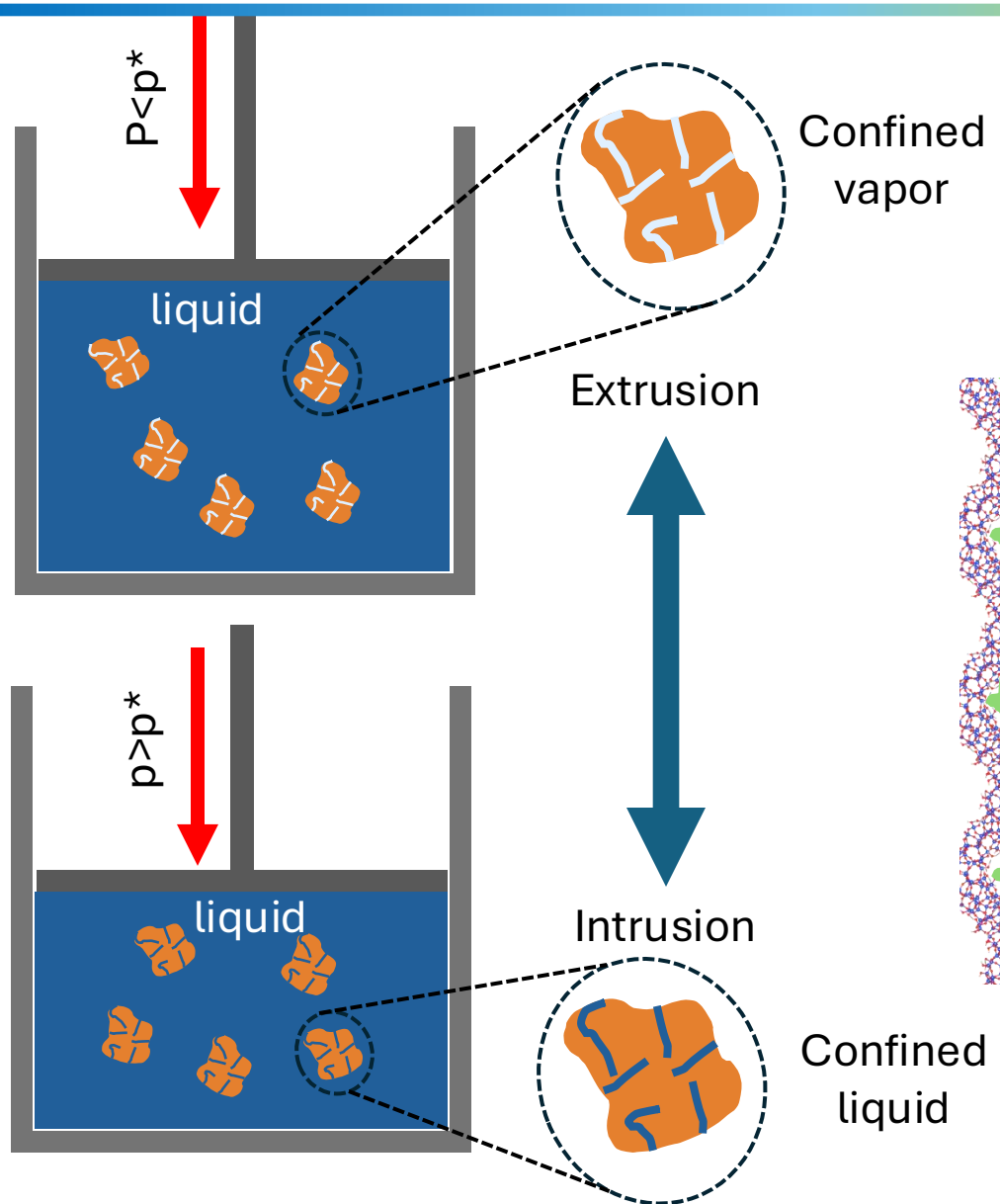
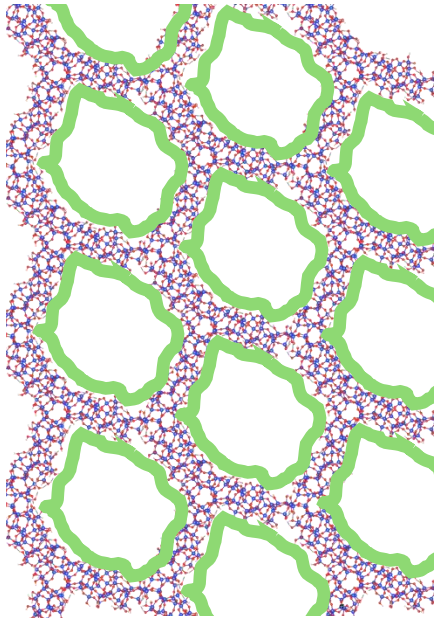
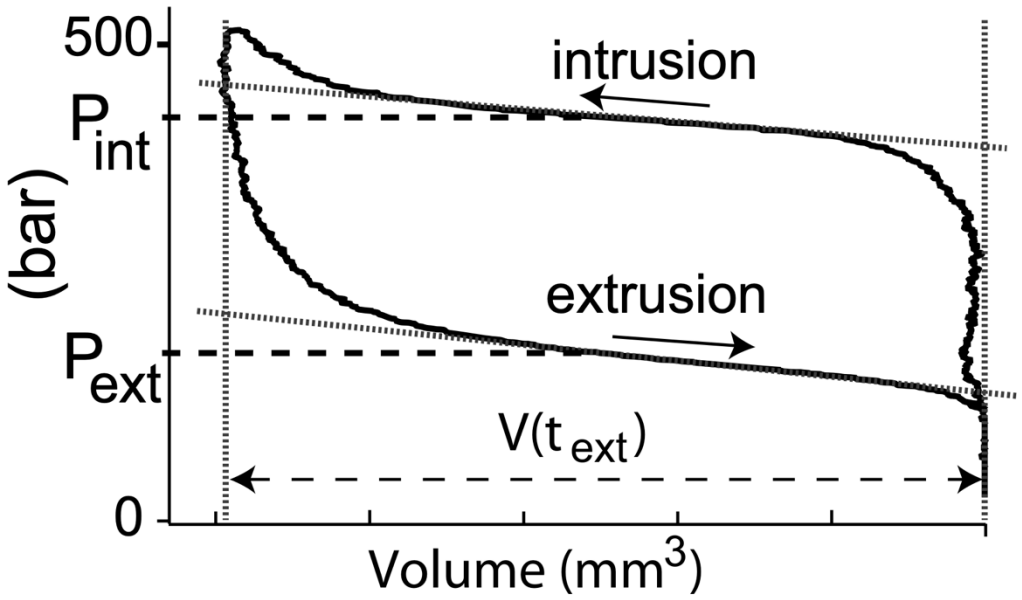



Grafted MCM-41
hydrophobic



Guillemot et al, PNAS 109,19557 (2012)



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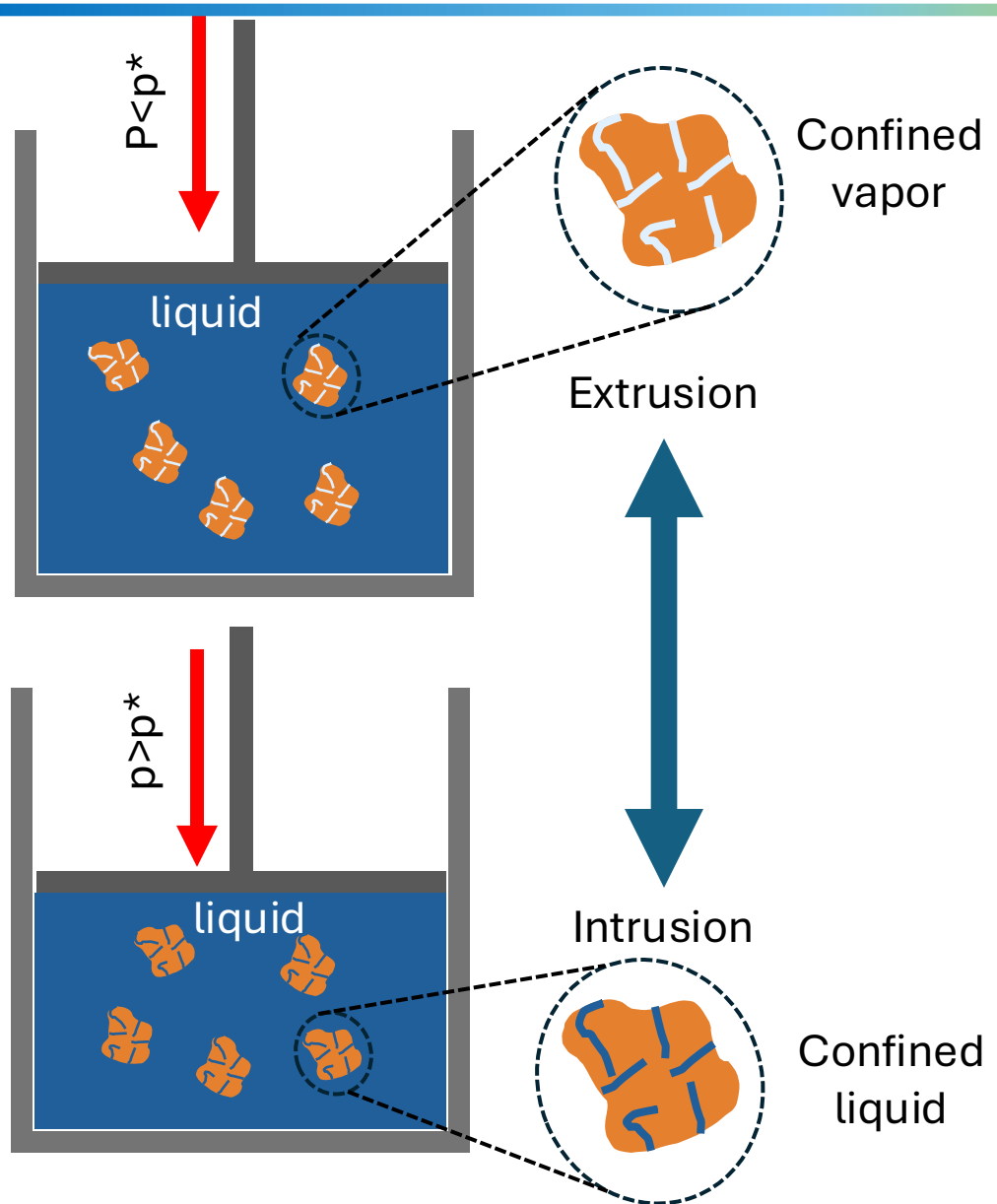
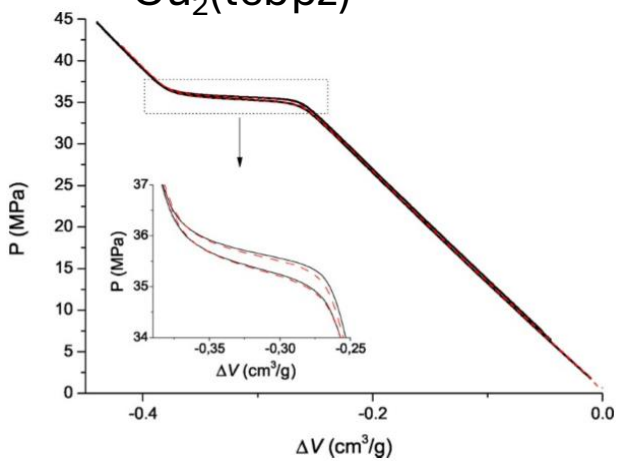
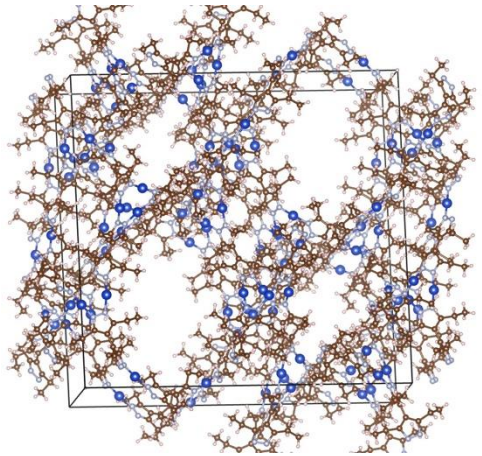
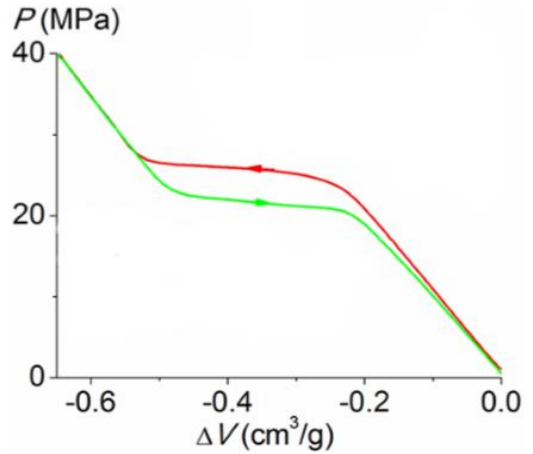


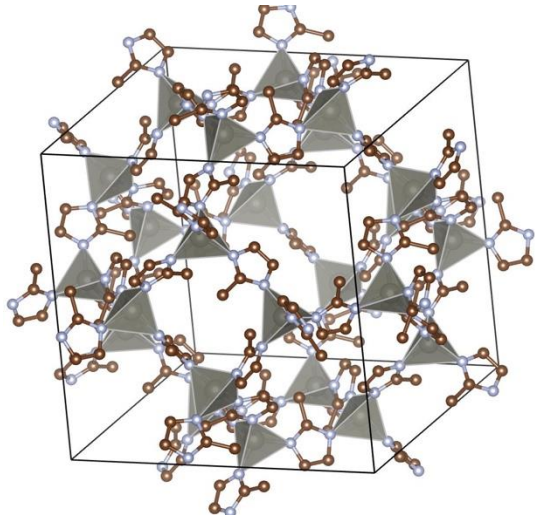

$Cu_2$(tebpz)



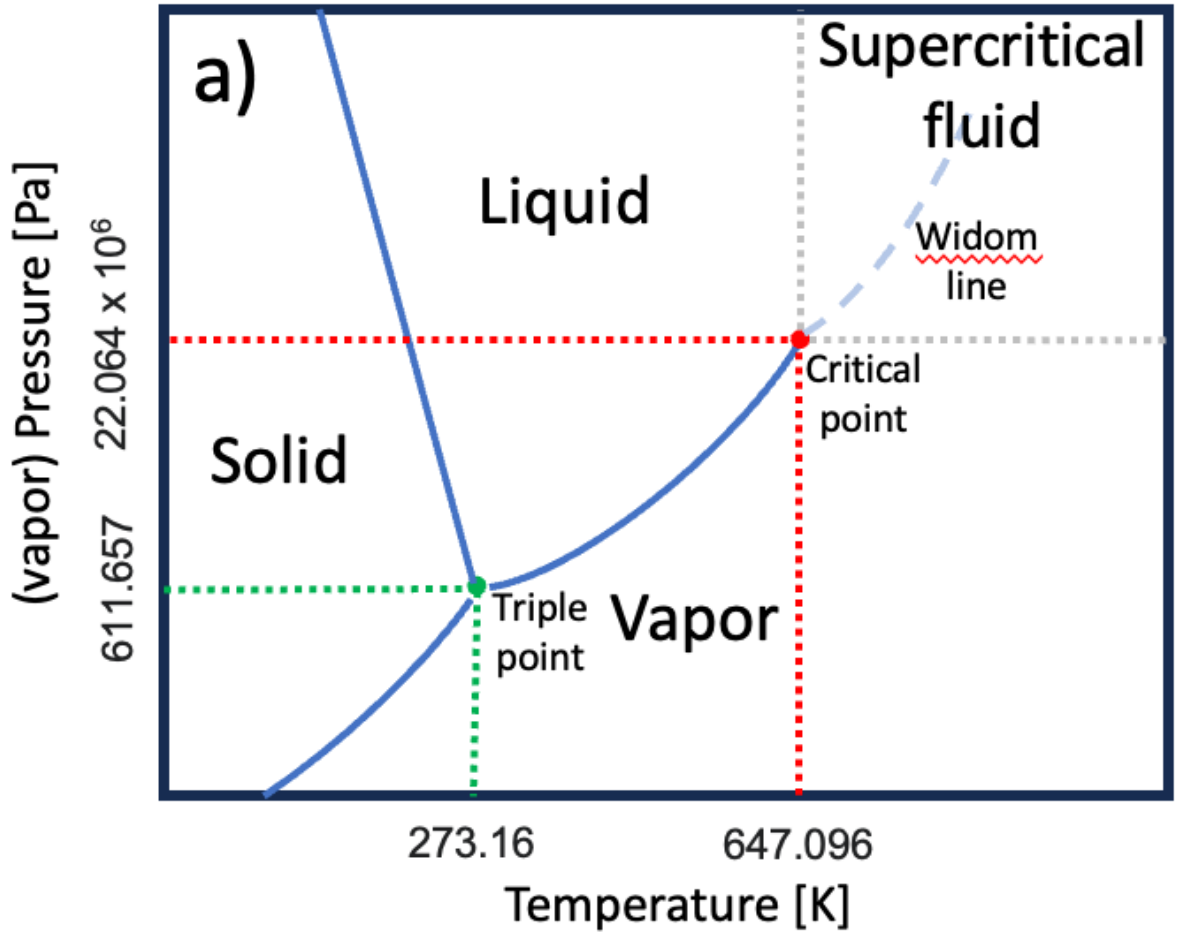



ZIF-8

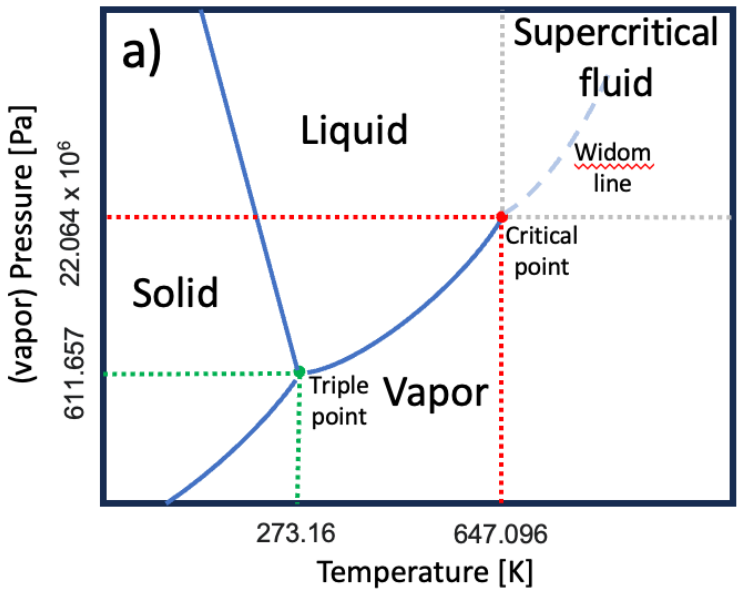


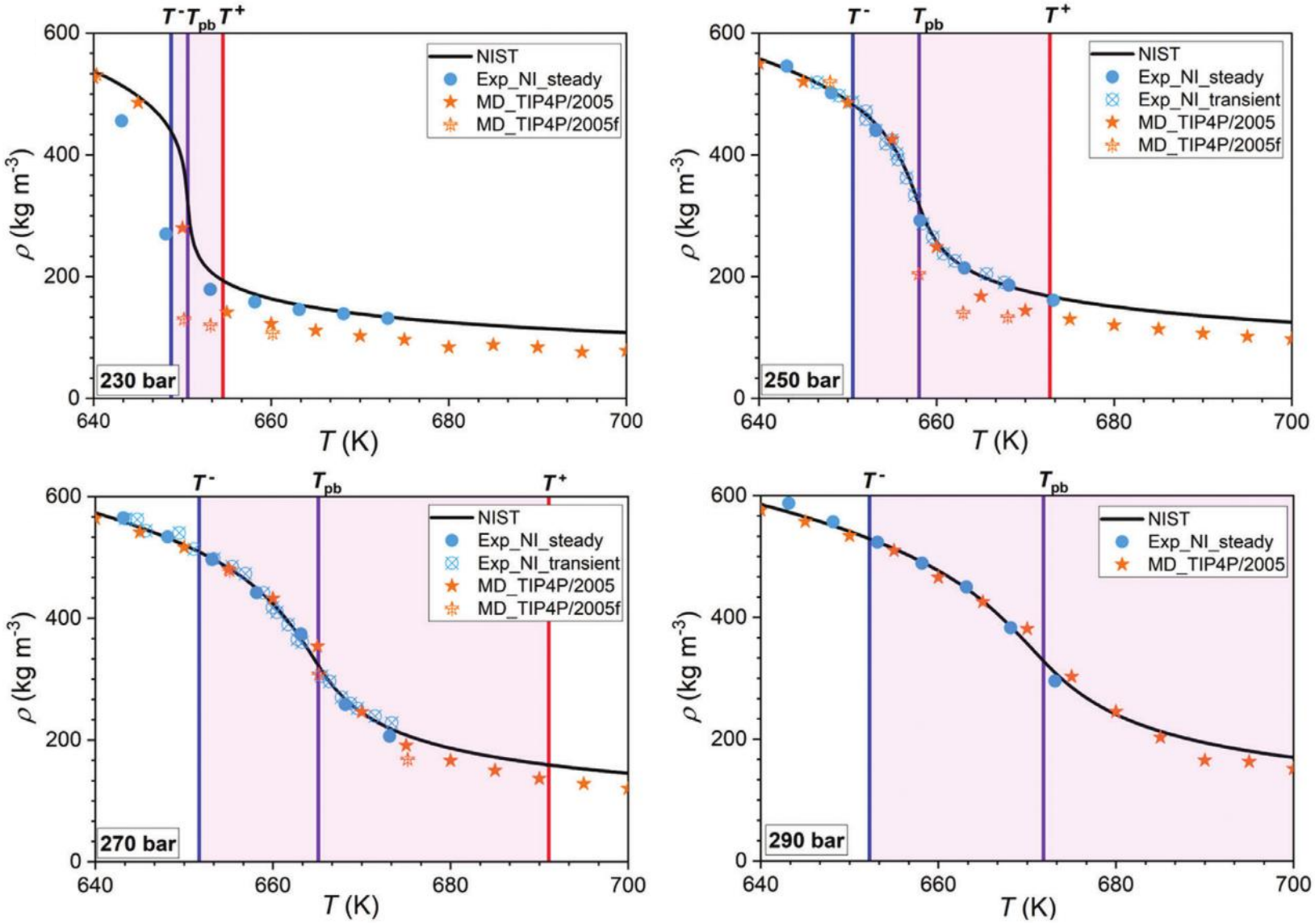



# Phase diagram of bulk water…including criticality




# Supercritical water and its kink/boundary lines




Adv. Sci. 2021, 8, 2002312

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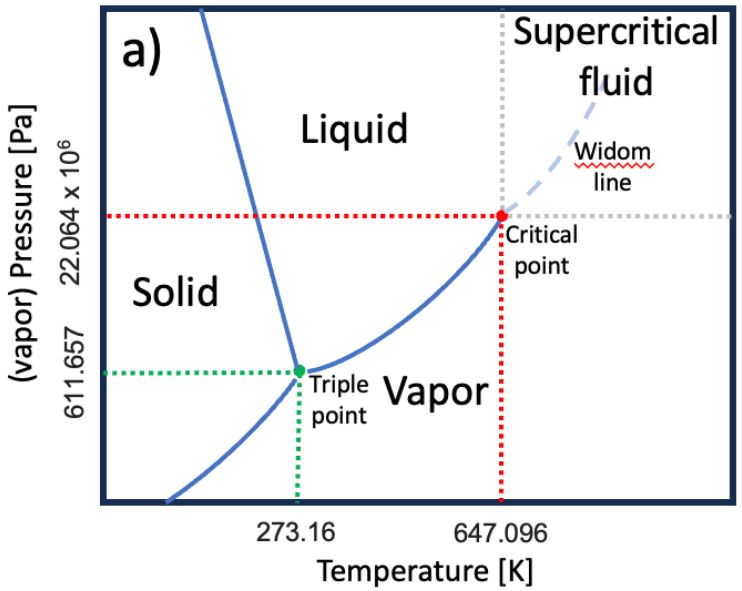


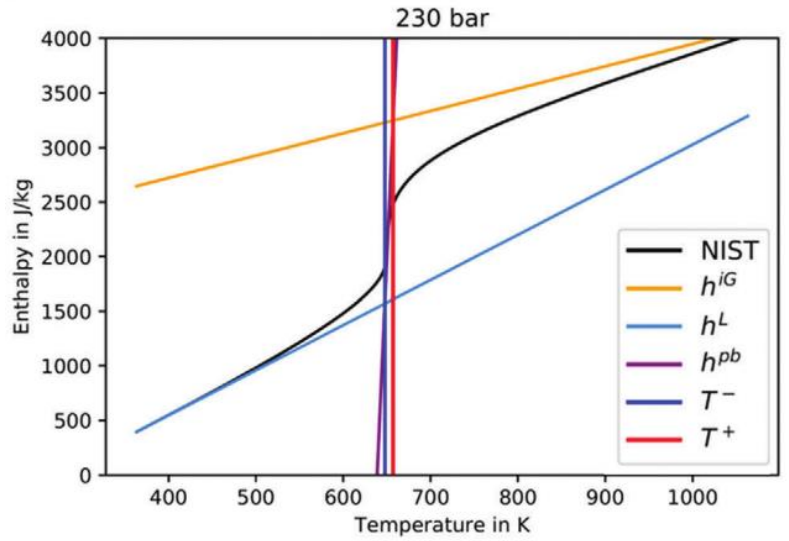


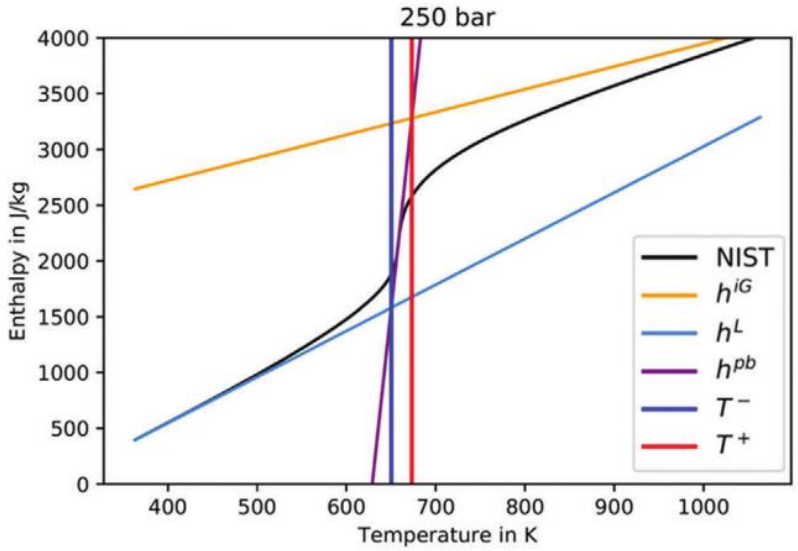


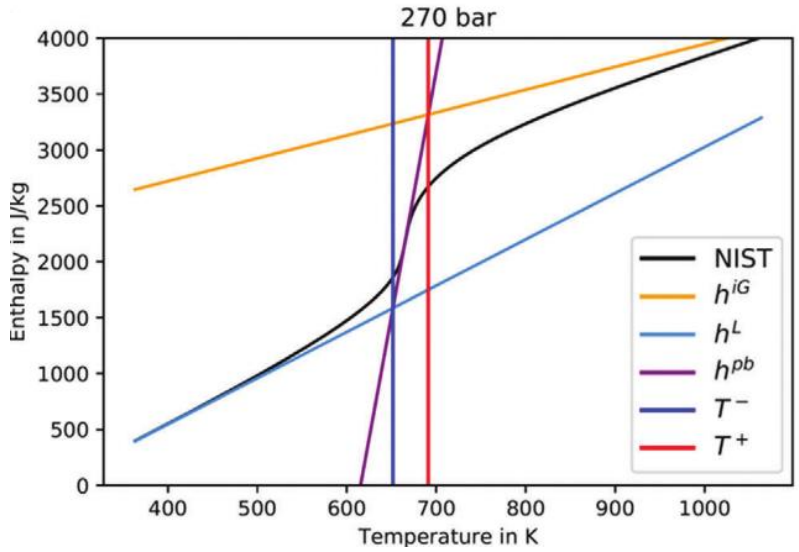


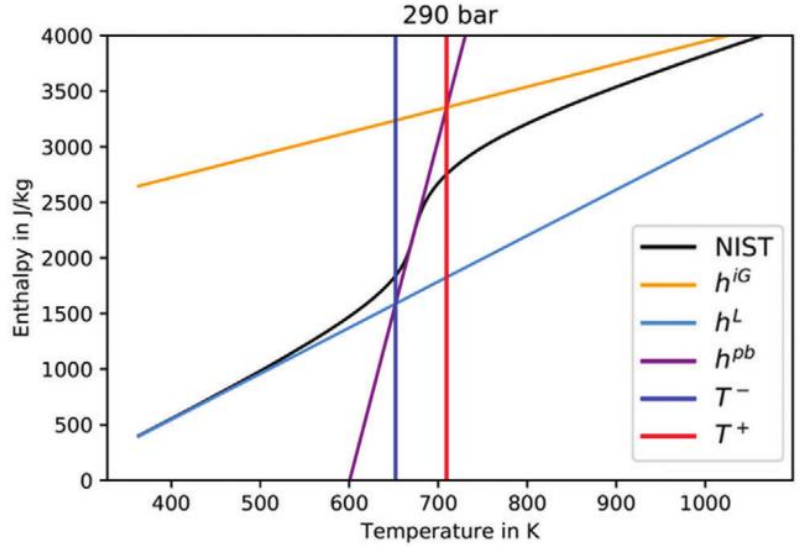


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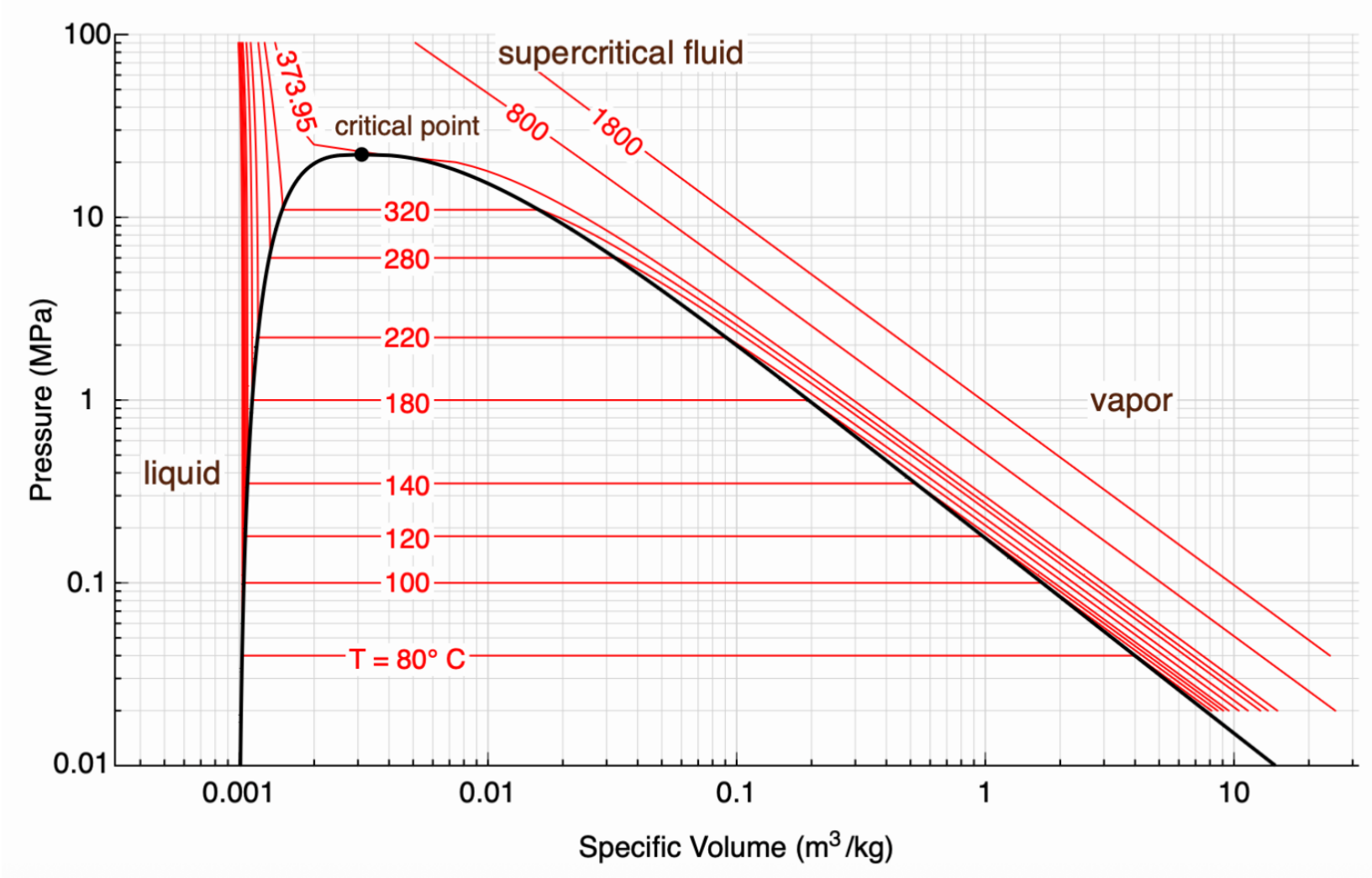
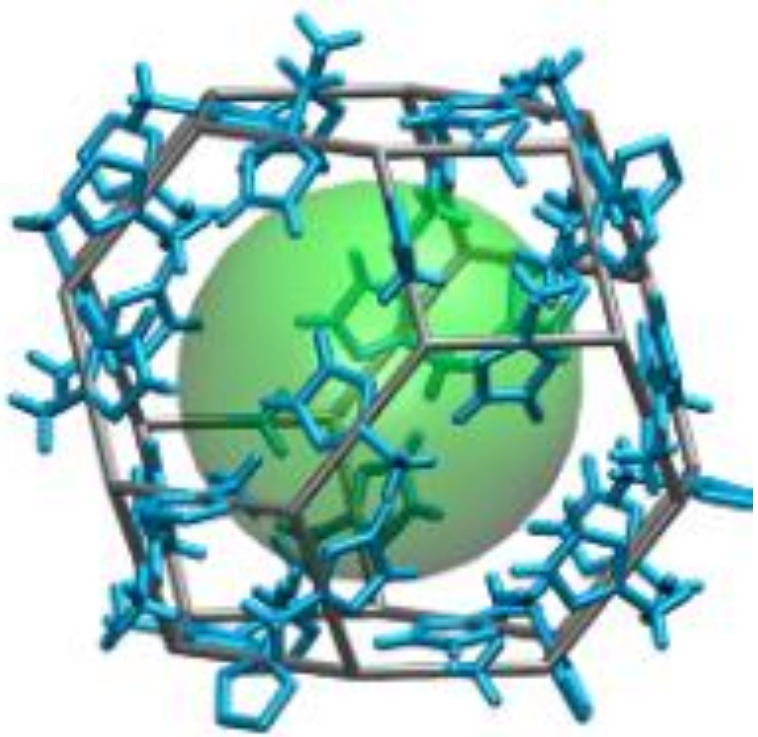
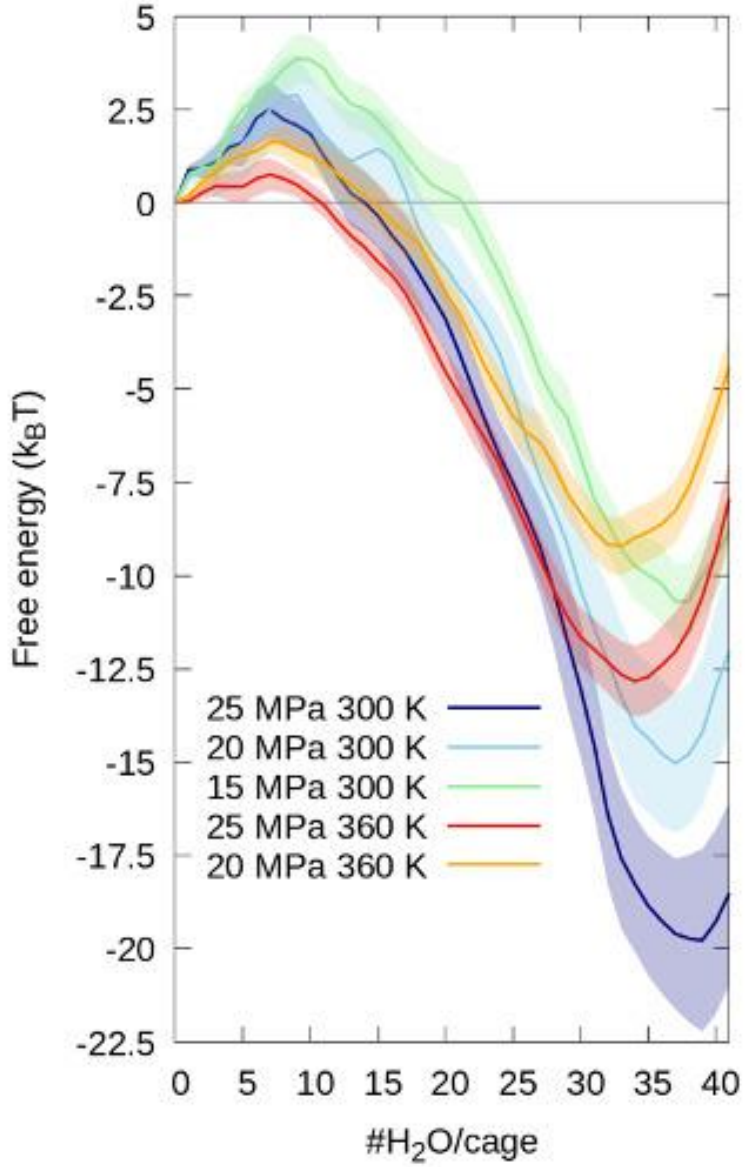
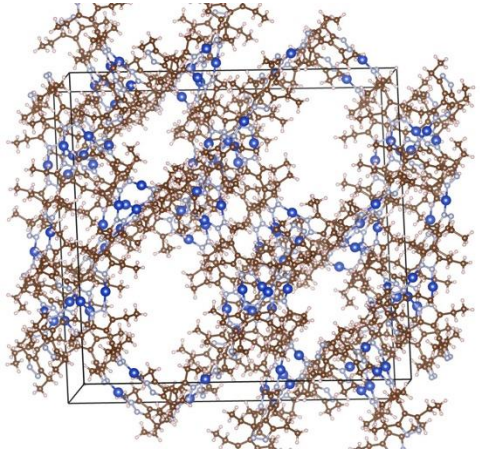


# Water under extreme confinement

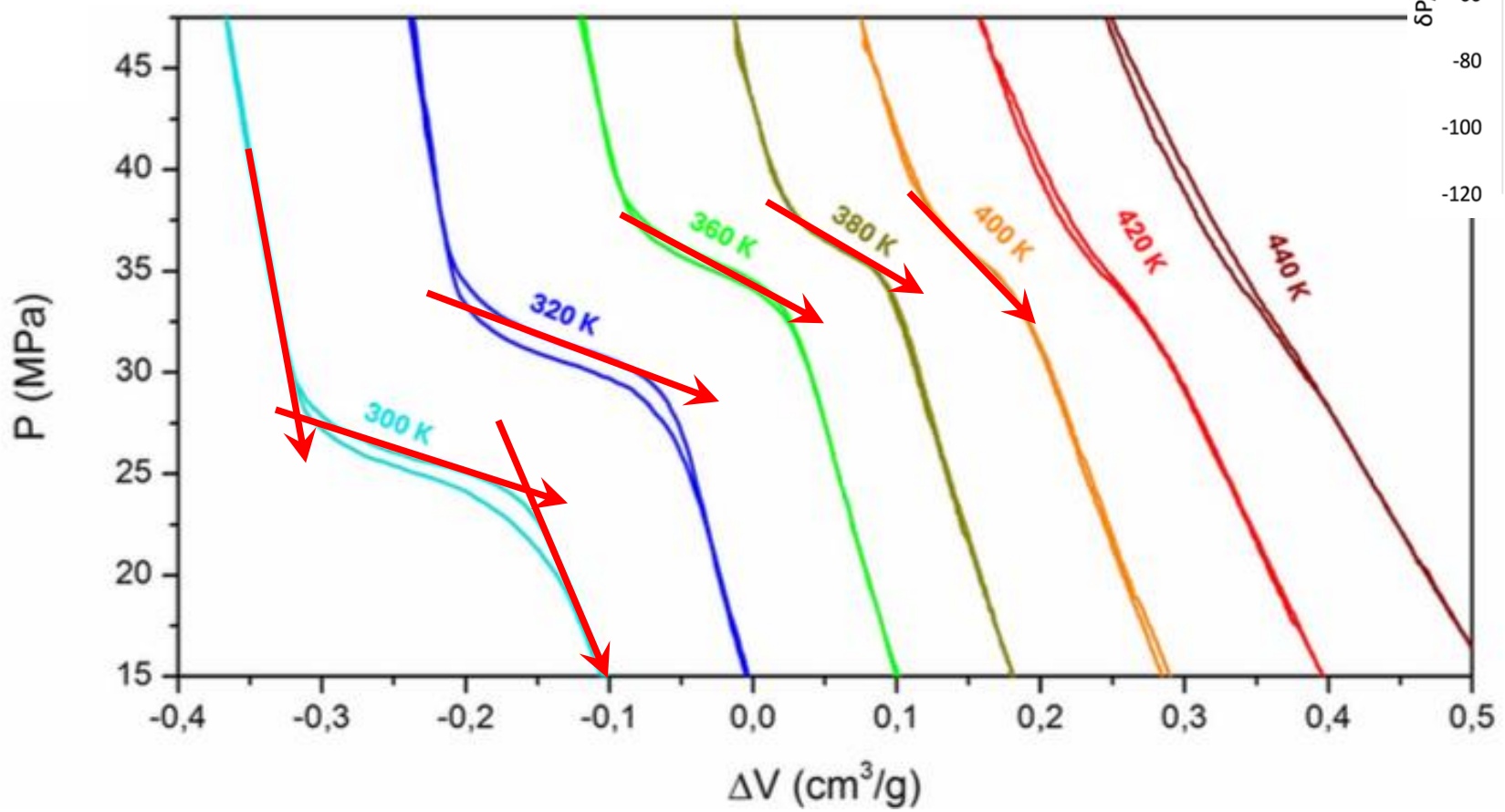


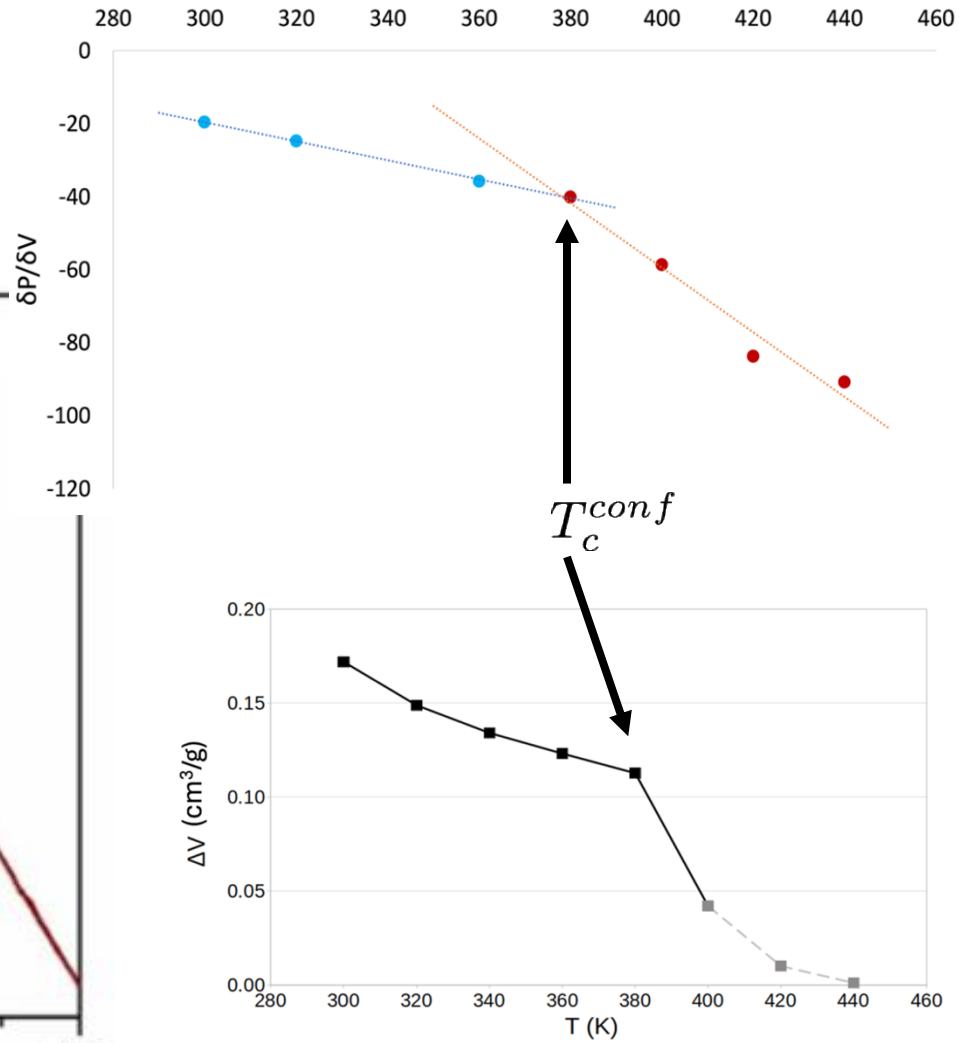
ZIF-8 cage



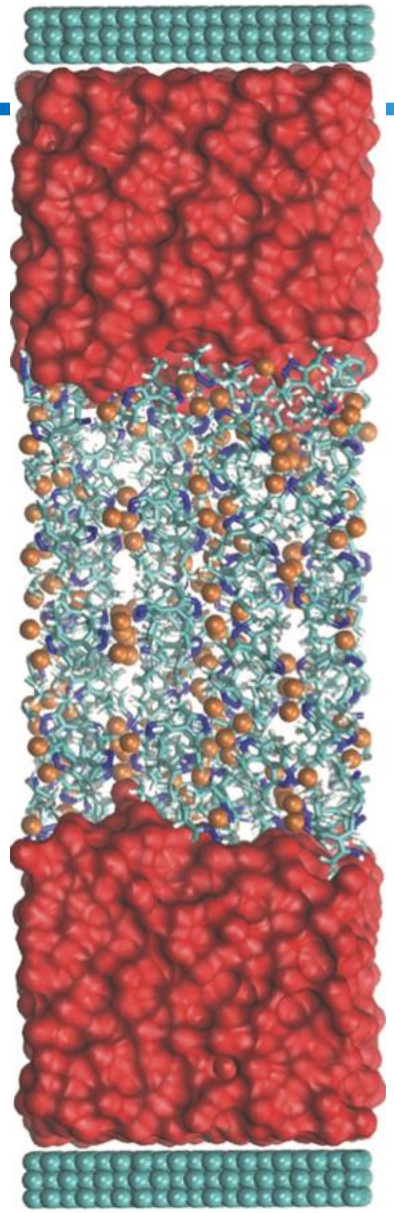
# Phase diagram of confined water

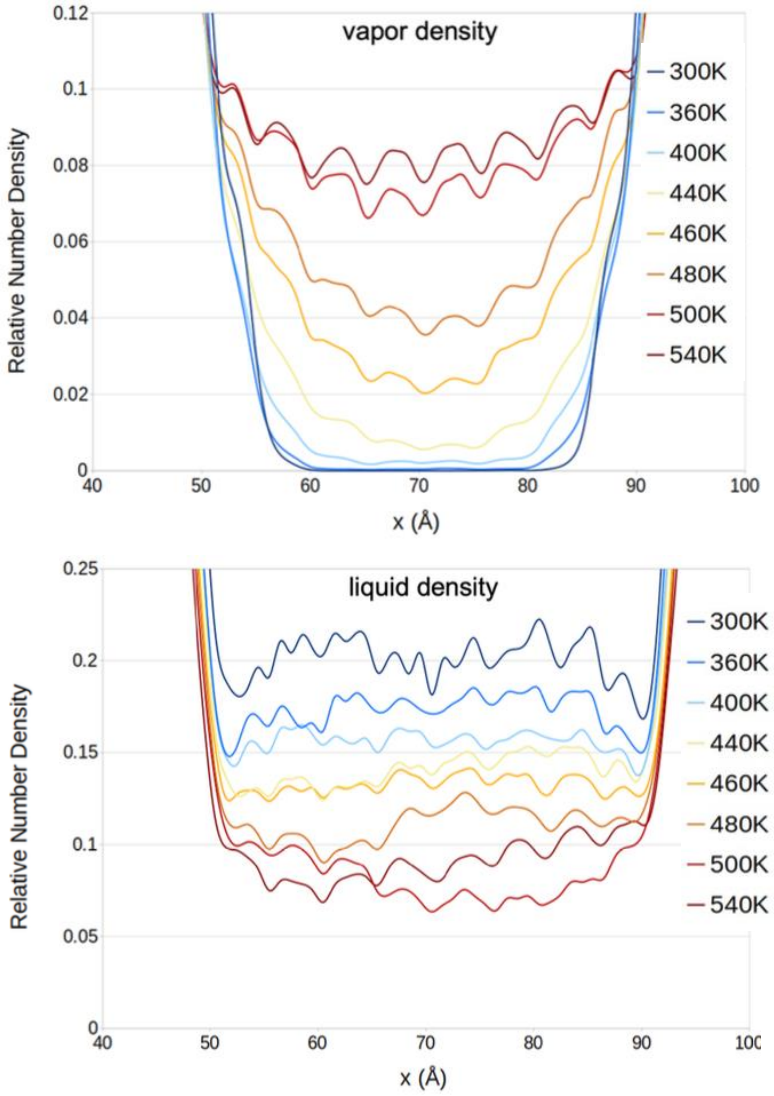


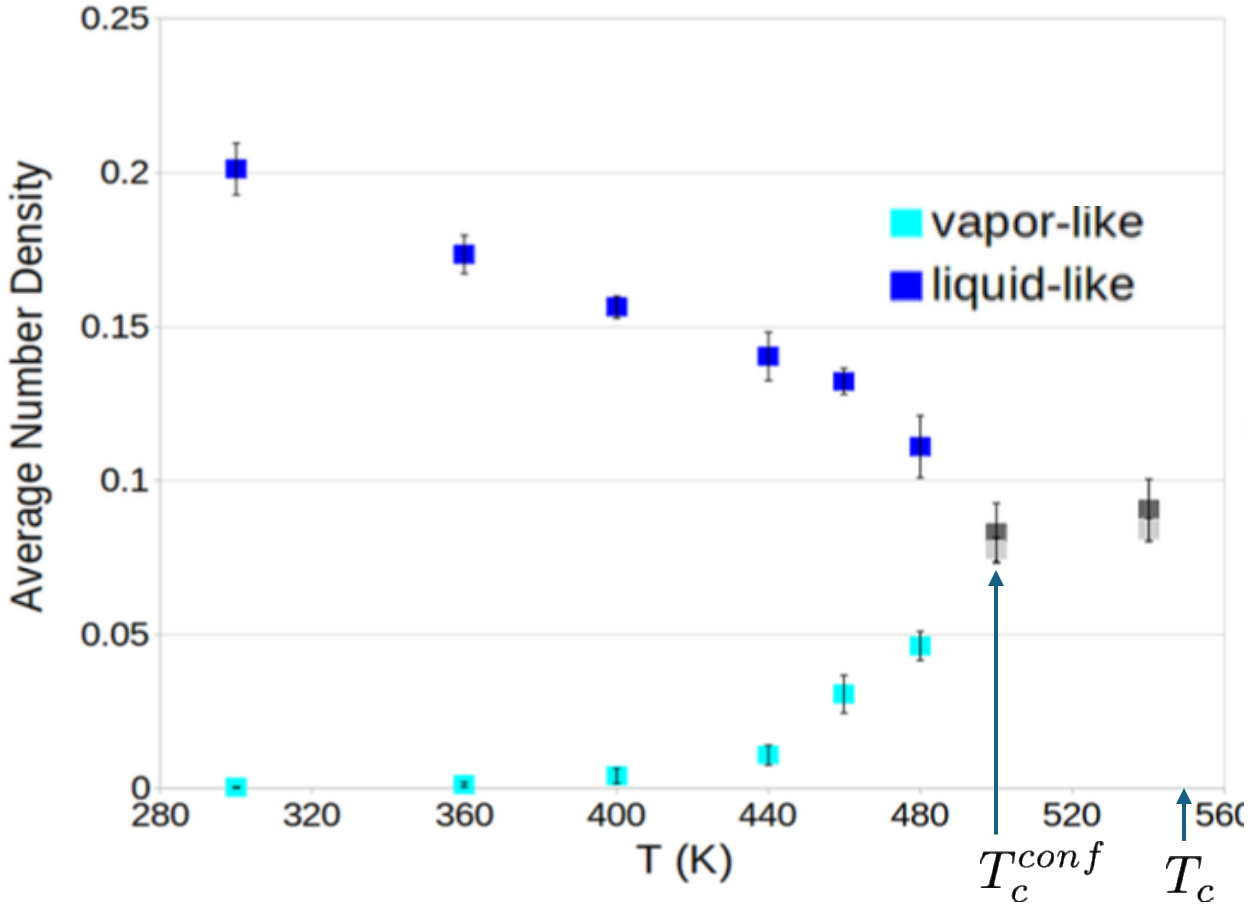




*J. Am. Chem. Soc.* 146, 13236, 2024; Small 2402173, 2024

# Mild, confined supercritical water



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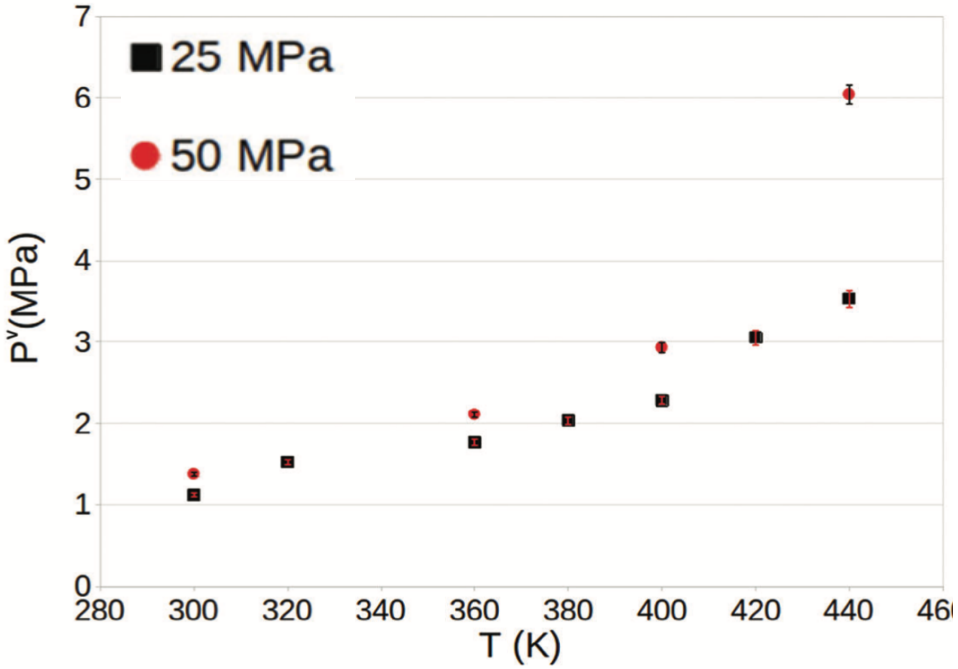
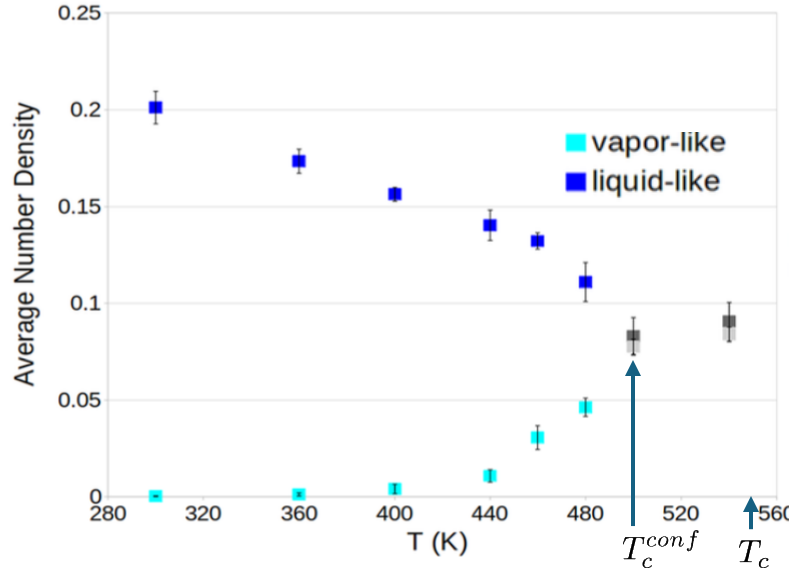
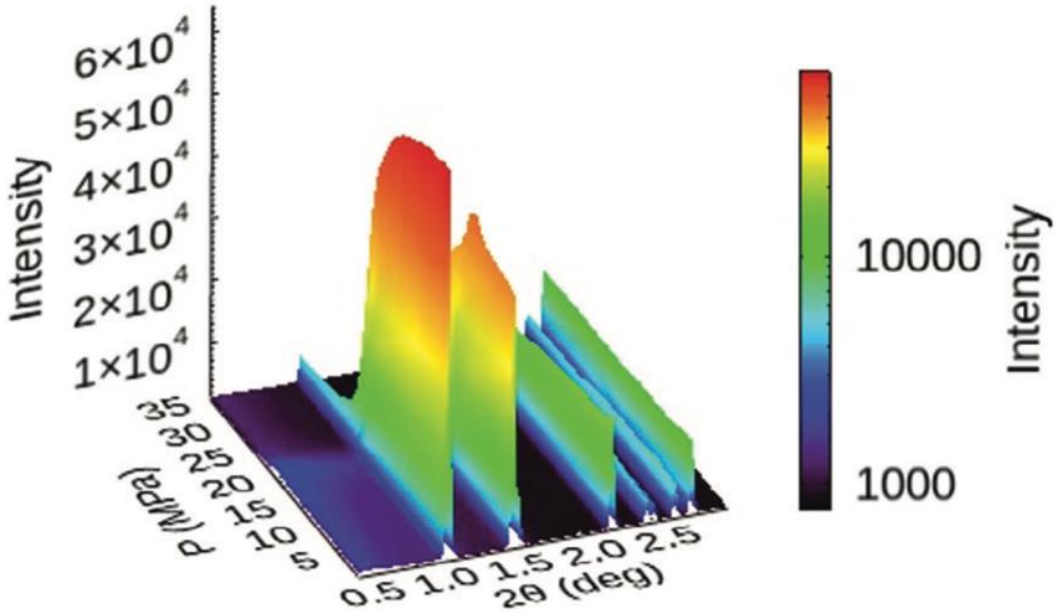
# High vapor pressure

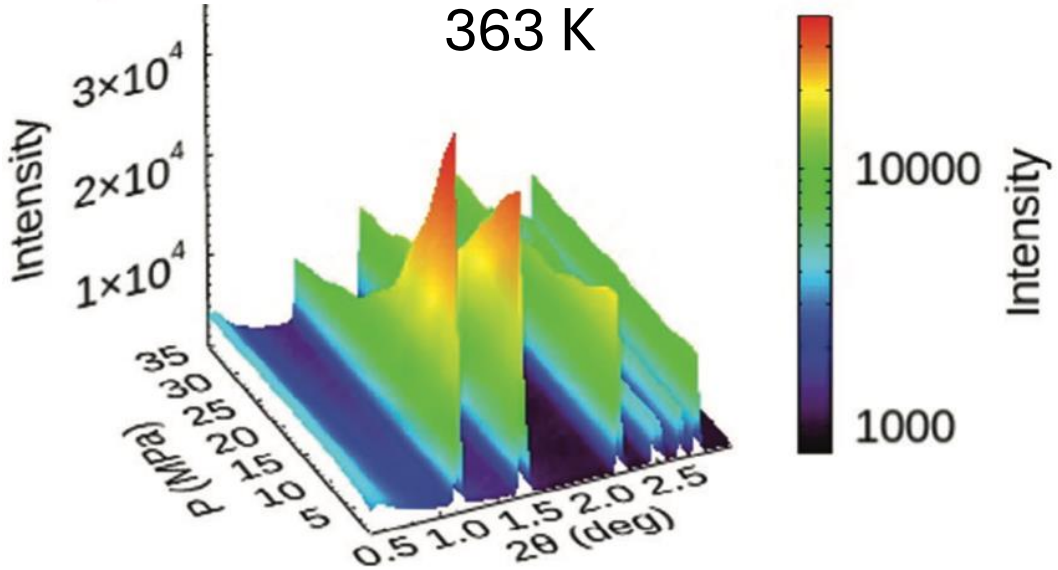



278 K

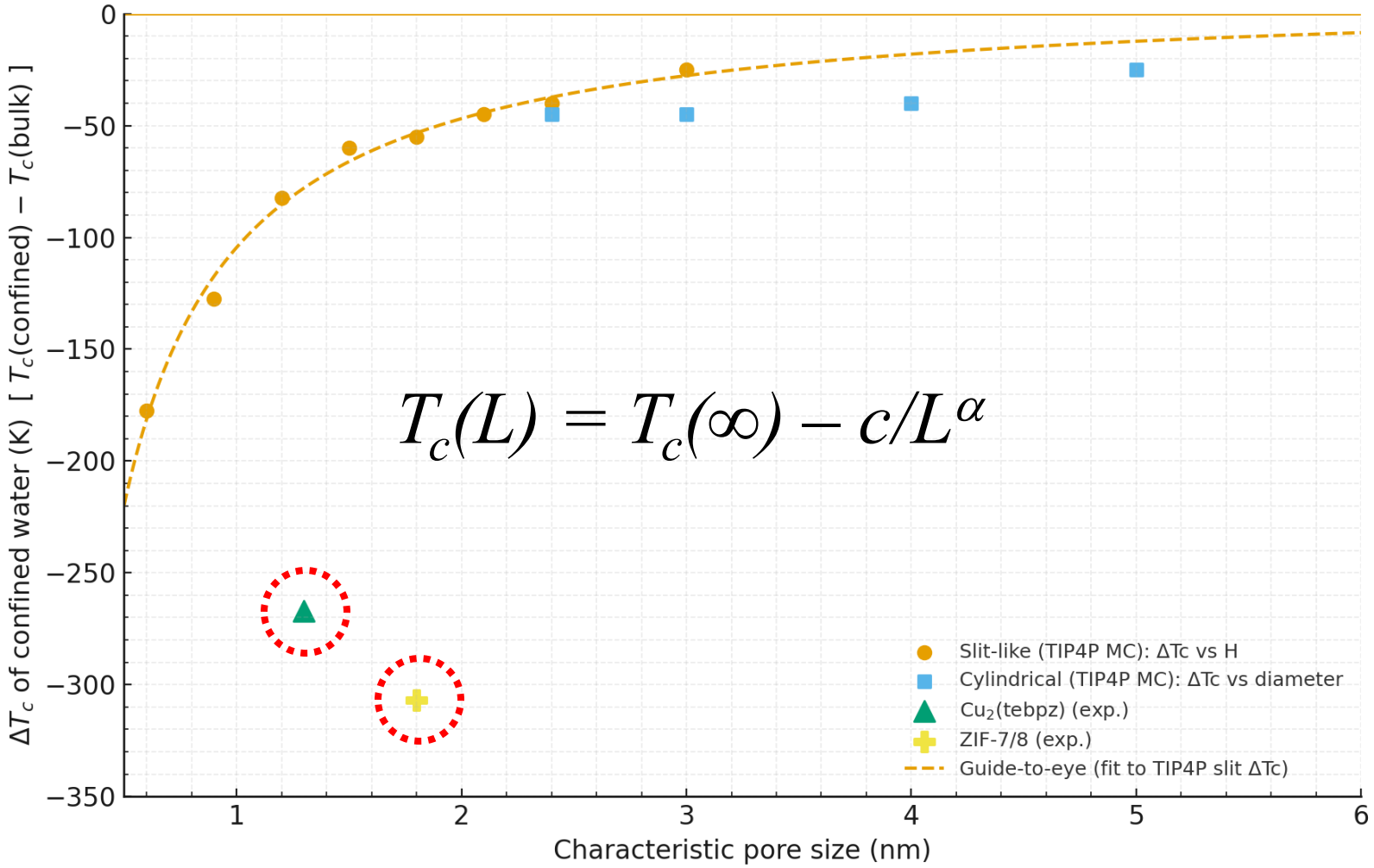



363 K




*J. Am. Chem. Soc.* 146 (2024) 13236,; Small (2024 ) 2402173

# Effect of confinement on $T_c$



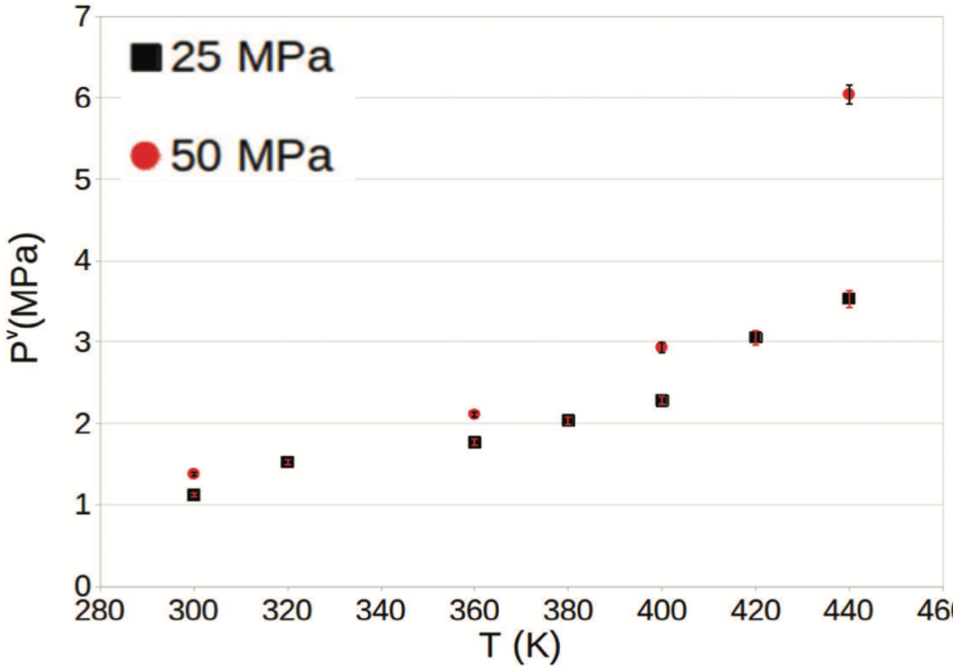


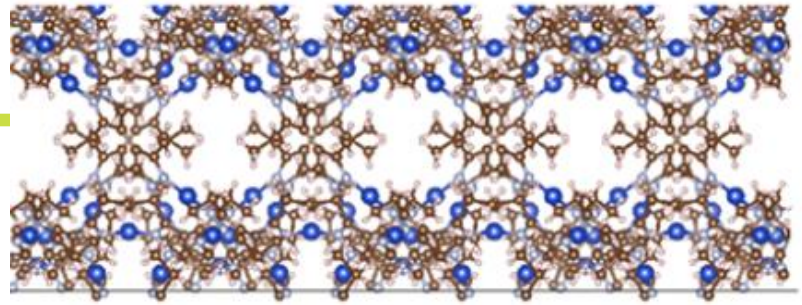
J. Phys.: Condens. Matter 16 (2004) S5345

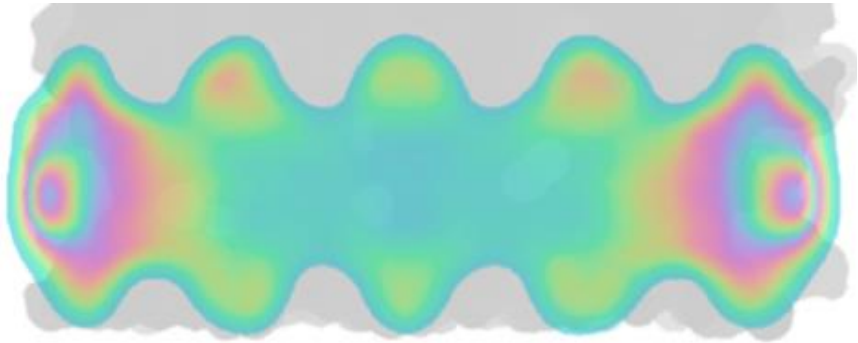
J. Chem. Phys. 120 (2004) 1958

J. Am. Chem. Soc. 146 (2024) 13236

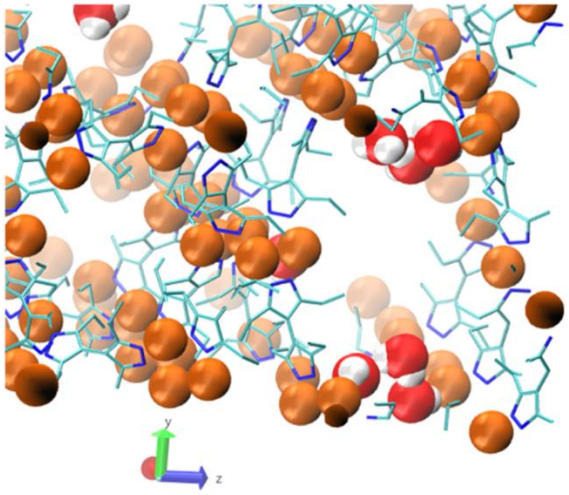
# High vapor pressure

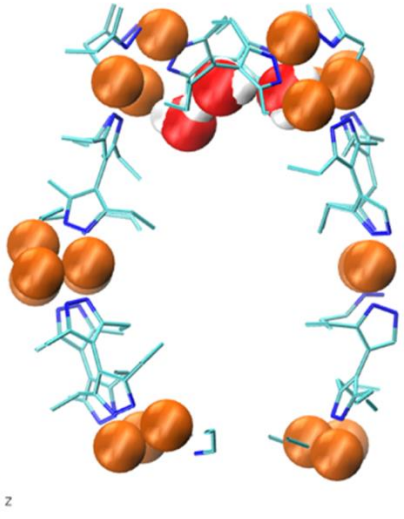


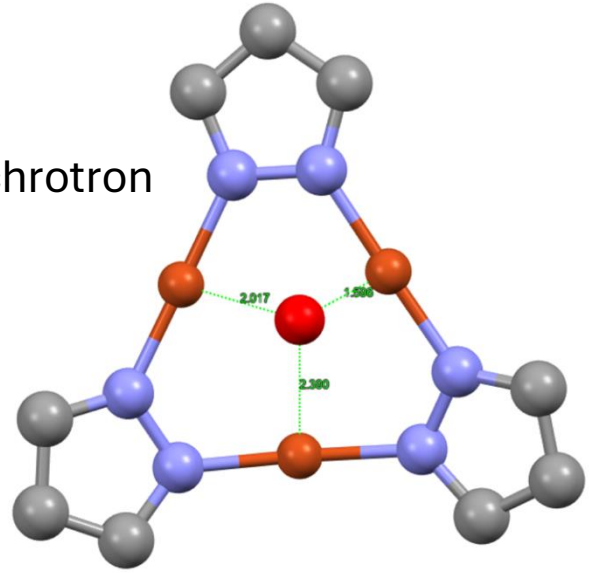


Simulations





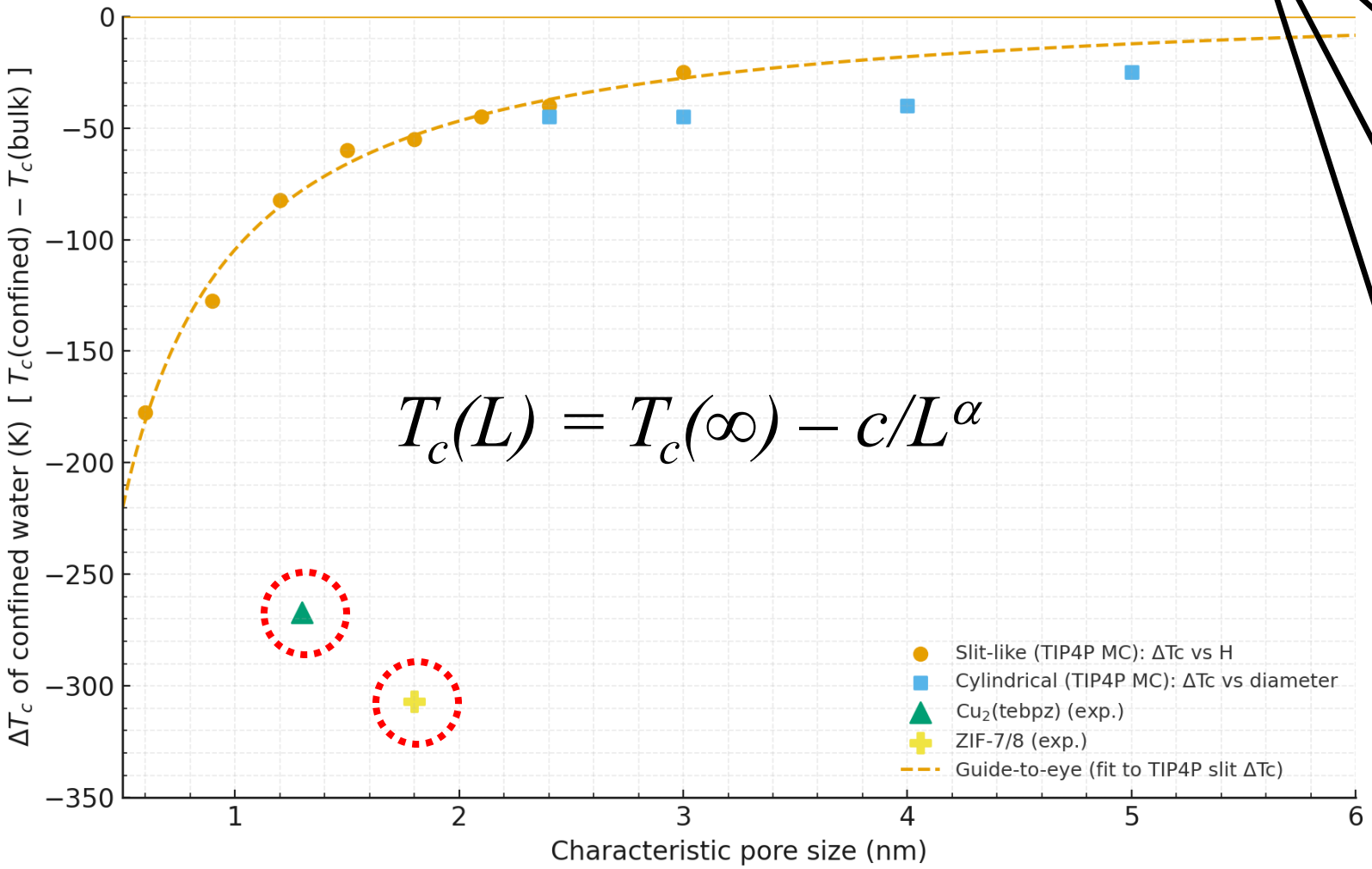
Synchrotron

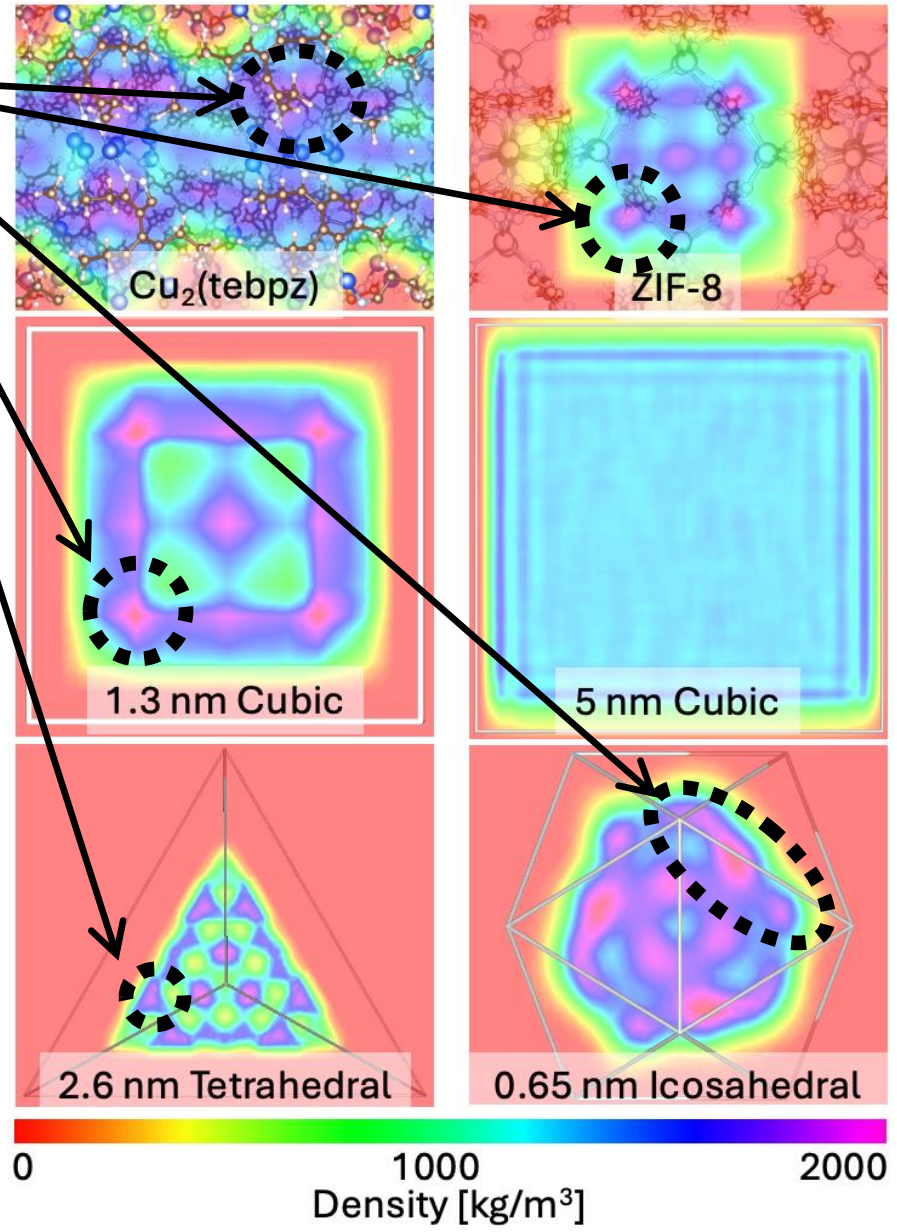



*J. Am. Chem. Soc.* 146 (2024) 13236,; Small (2024 ) 2402173

# Effect of confinement on $T_c$

Smeller than the confining cavities



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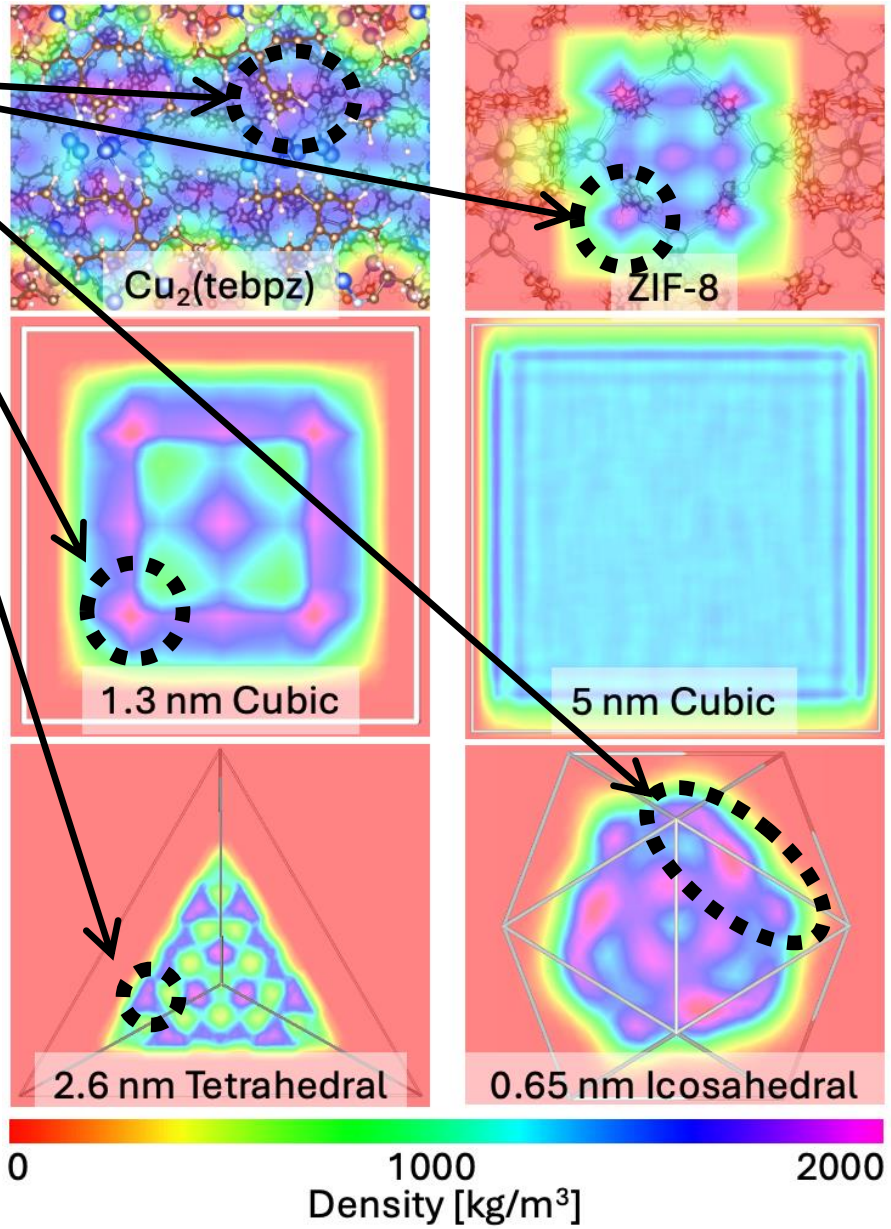


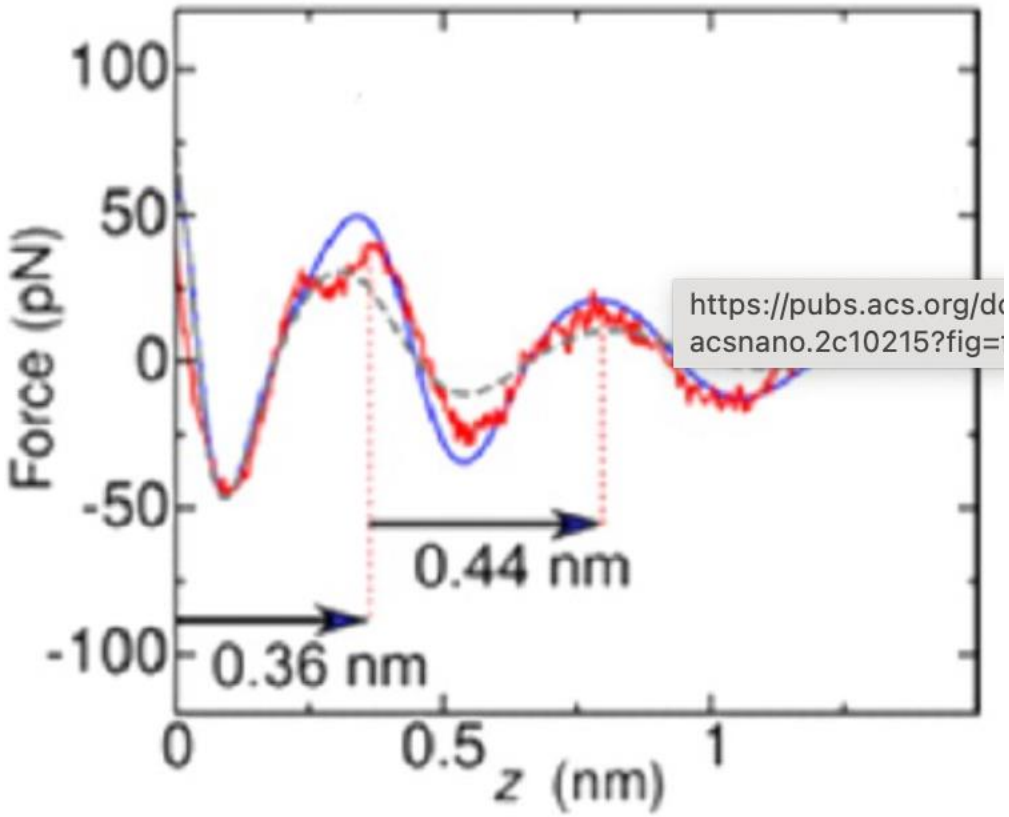


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# Conclusions and outlook

- The ordinary fluid phases of water, liquid(-like) and vapor(-like) exist also under extreme confinement, down to 1 nm pore size.
- However, the porous material plays a role beyond the classical physics picture: it is not an inherit confining medium.
- Many questions remain to be addressed, e.g., the relation between hysteresis and confined critical T, how to control int/ext pressure and hysteresis, etc.
- Exploitability for technological applications in energy storage, dissipation, conversion (not discussed, here)…
- …Moreover, low-T hysteresis opens new perspective in sensible thermal energy storage, supercritical solvents for chemistry. Additionally, the existence of (confined) supercritical water and bulk water at the same P/T allows to dream of a all-water fluid/fluid chromatography

# Acknowledgements


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