



# Peculiar properties of water squeezed within nanoglasses

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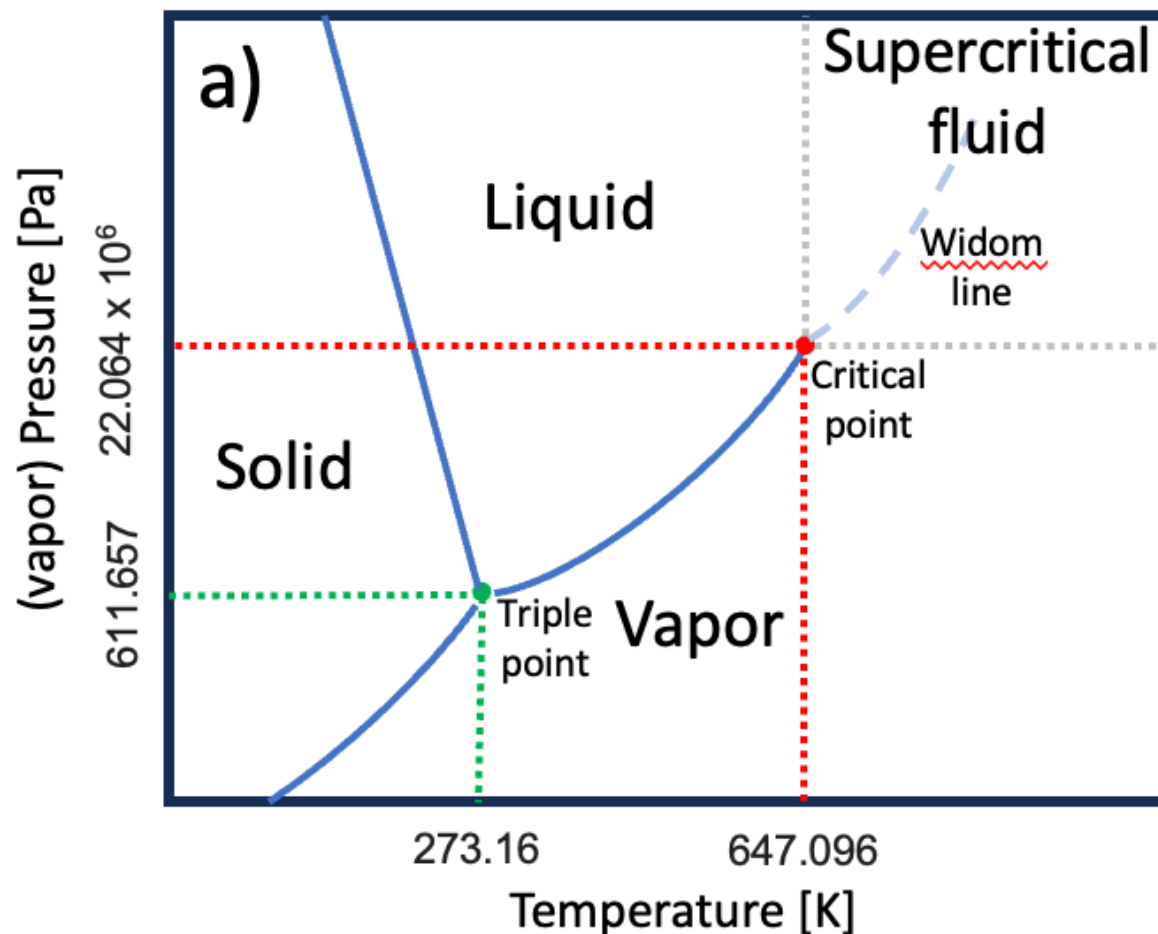
Alma Mater Studiorum, University of Bologna  
13 May 2025



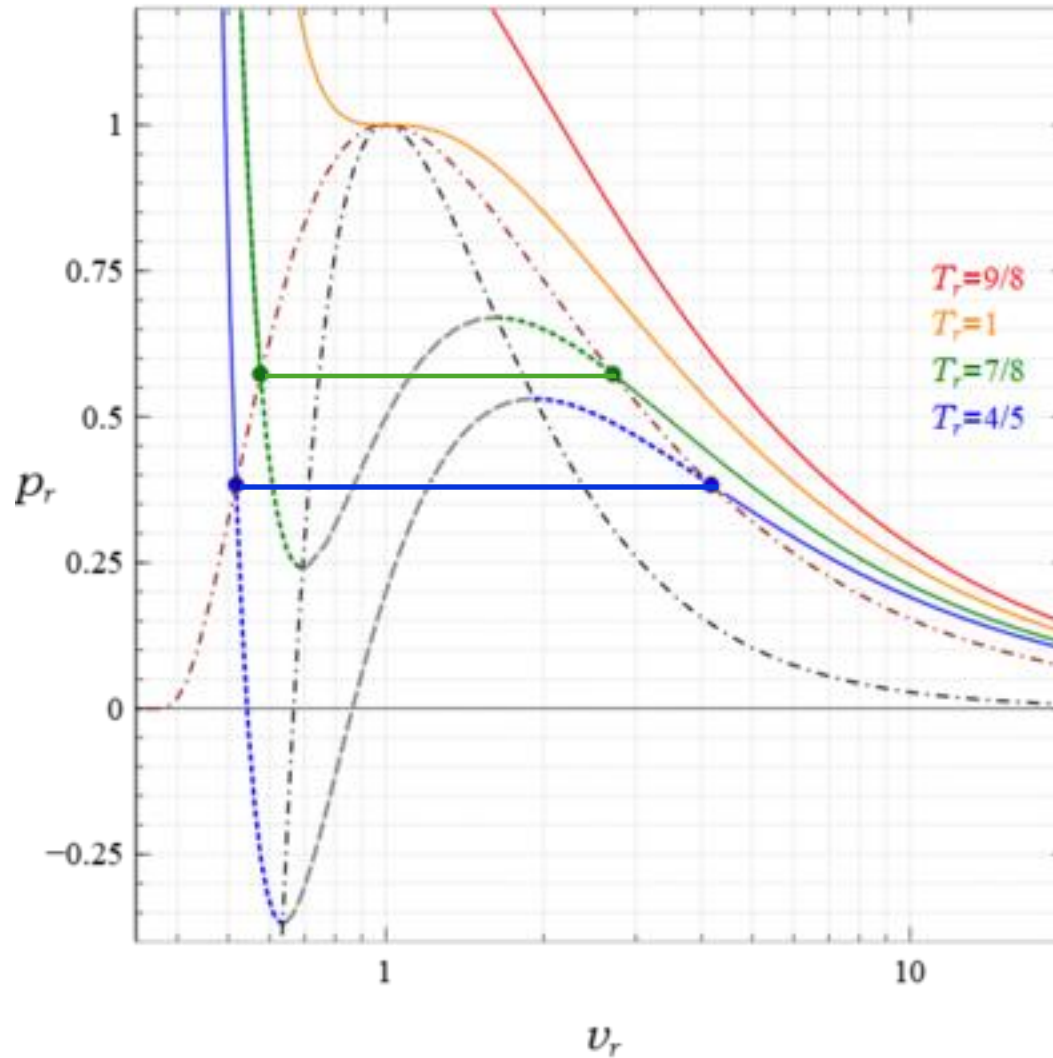
Funded by  
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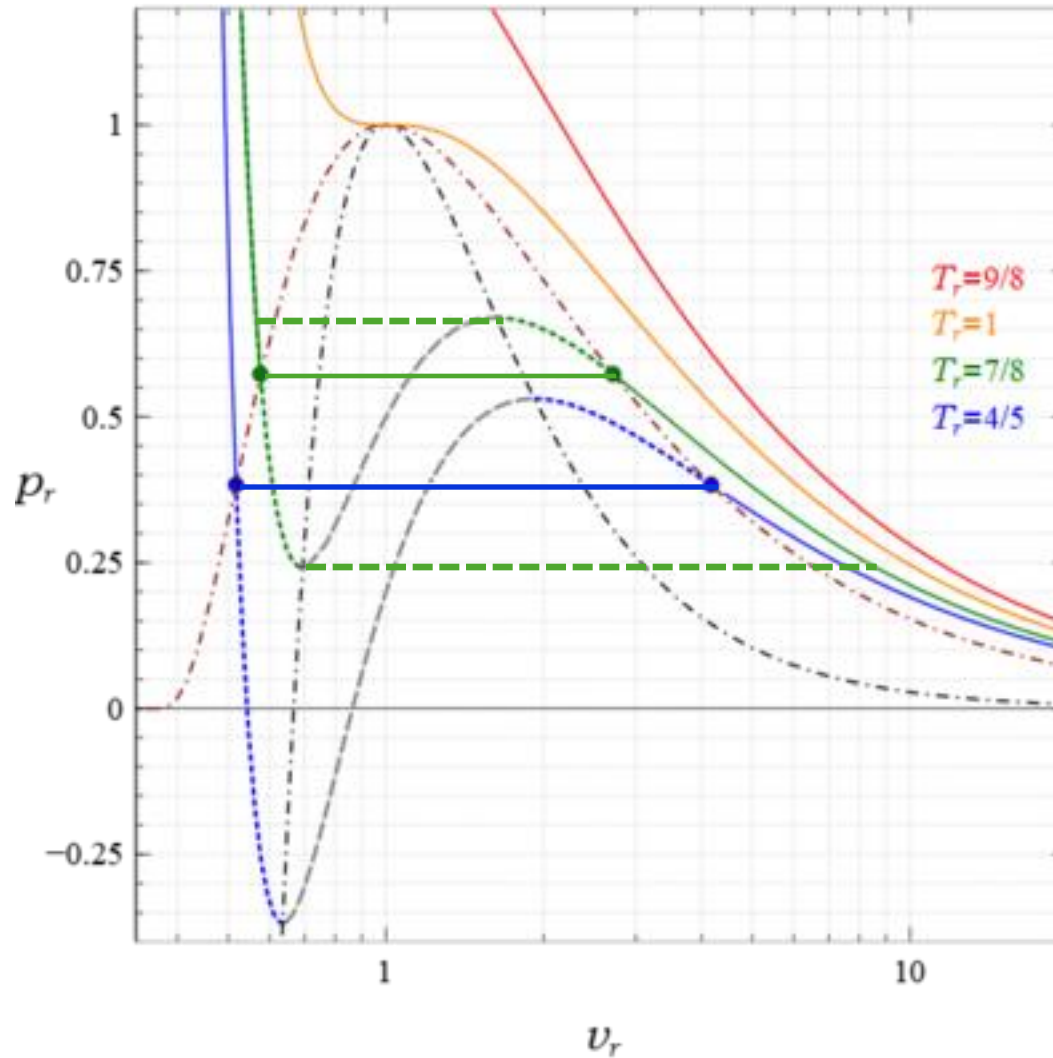
# Phase diagram of bulk water



# Liquid/vapor Phase transition

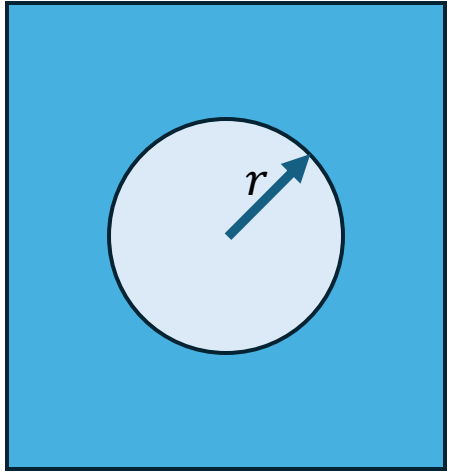


# Liquid/vapor Phase transition

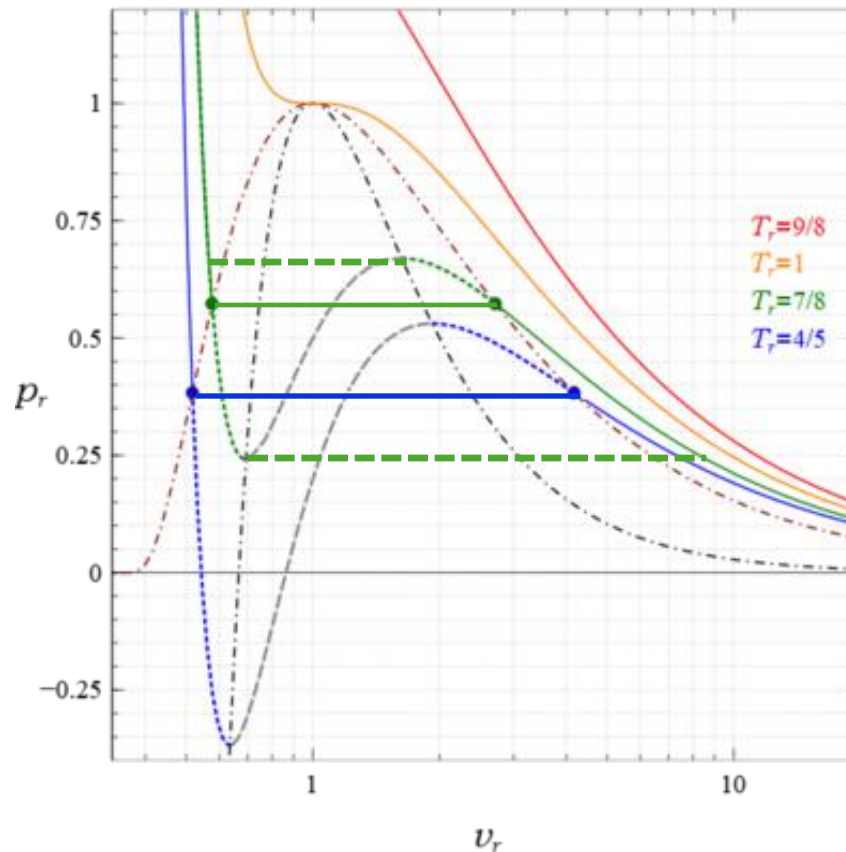
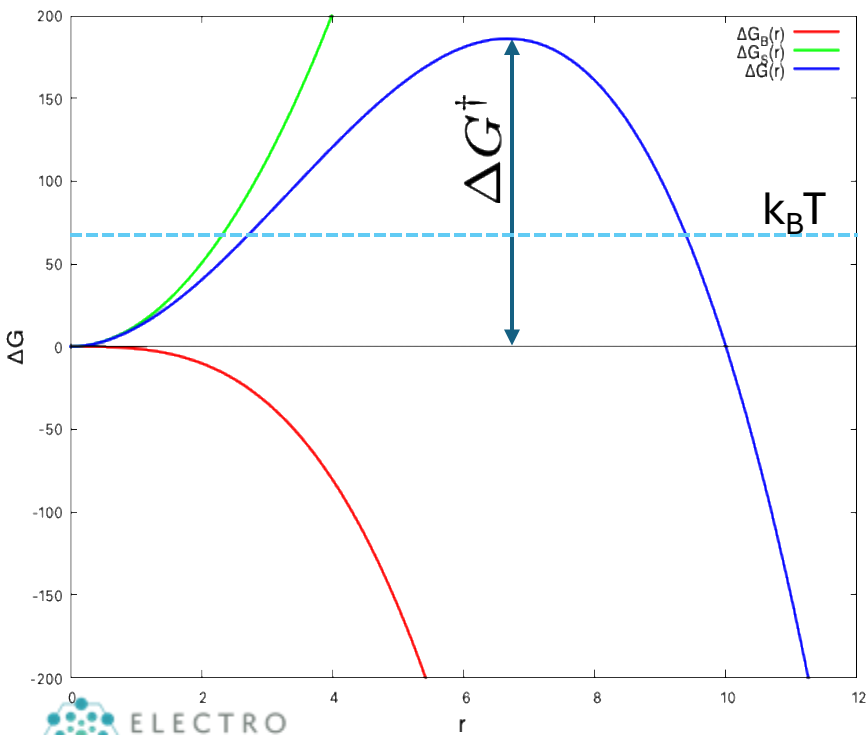




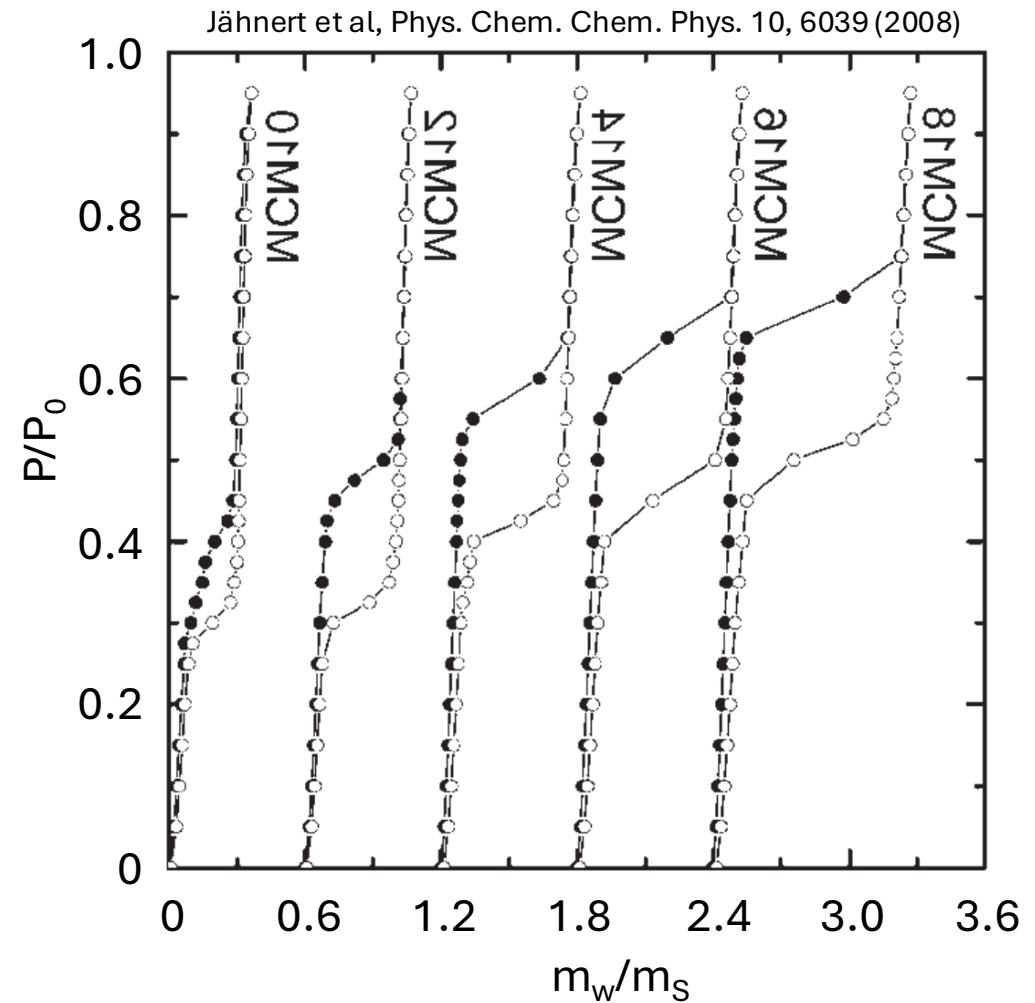
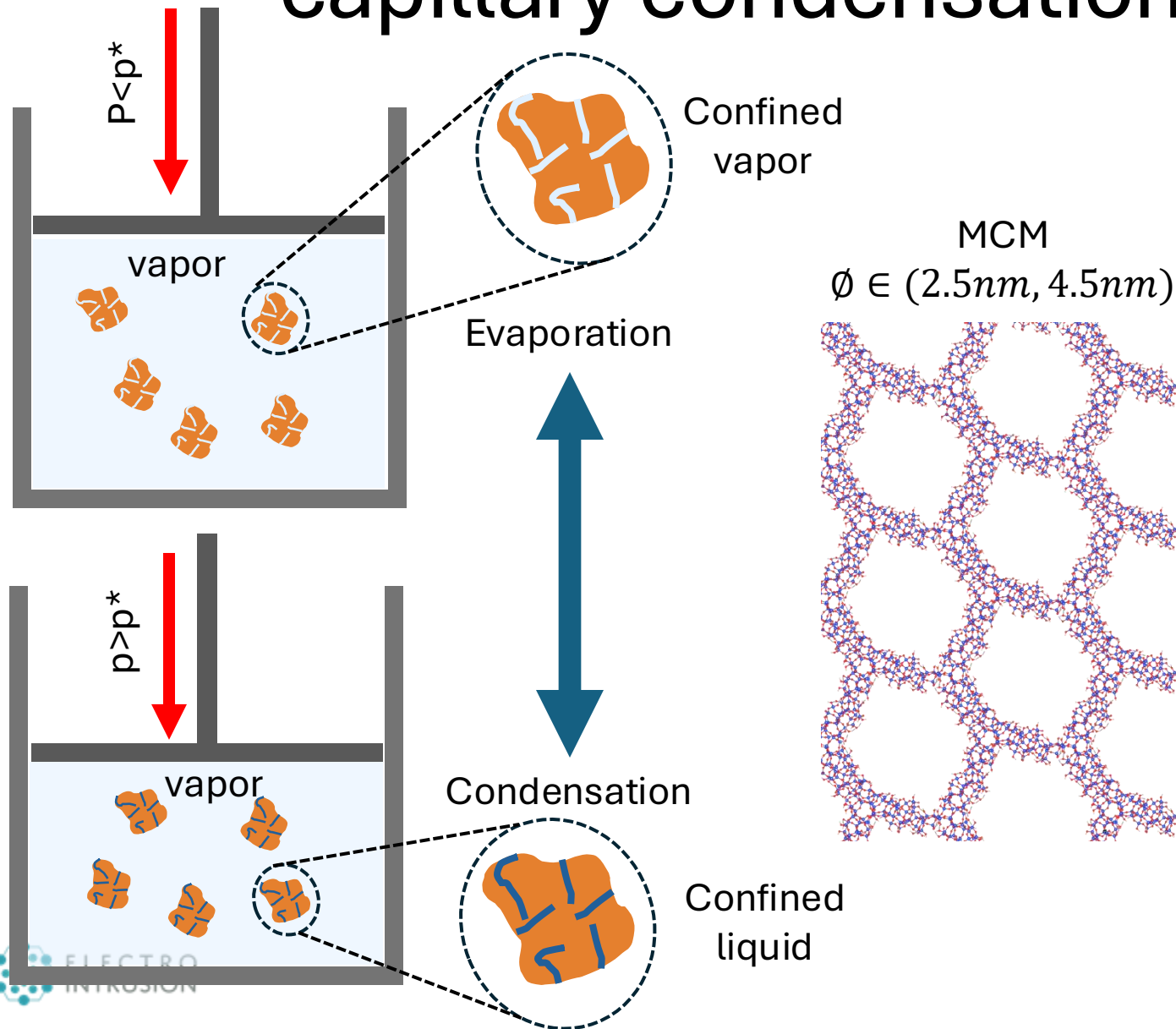
# Liquid/vapor Phase transition



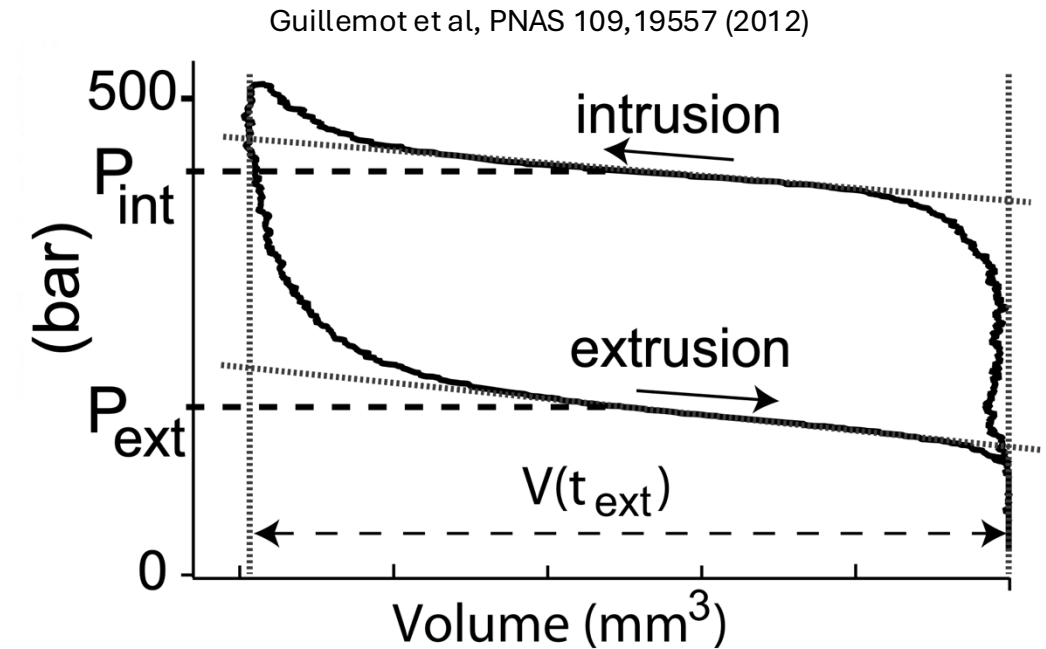
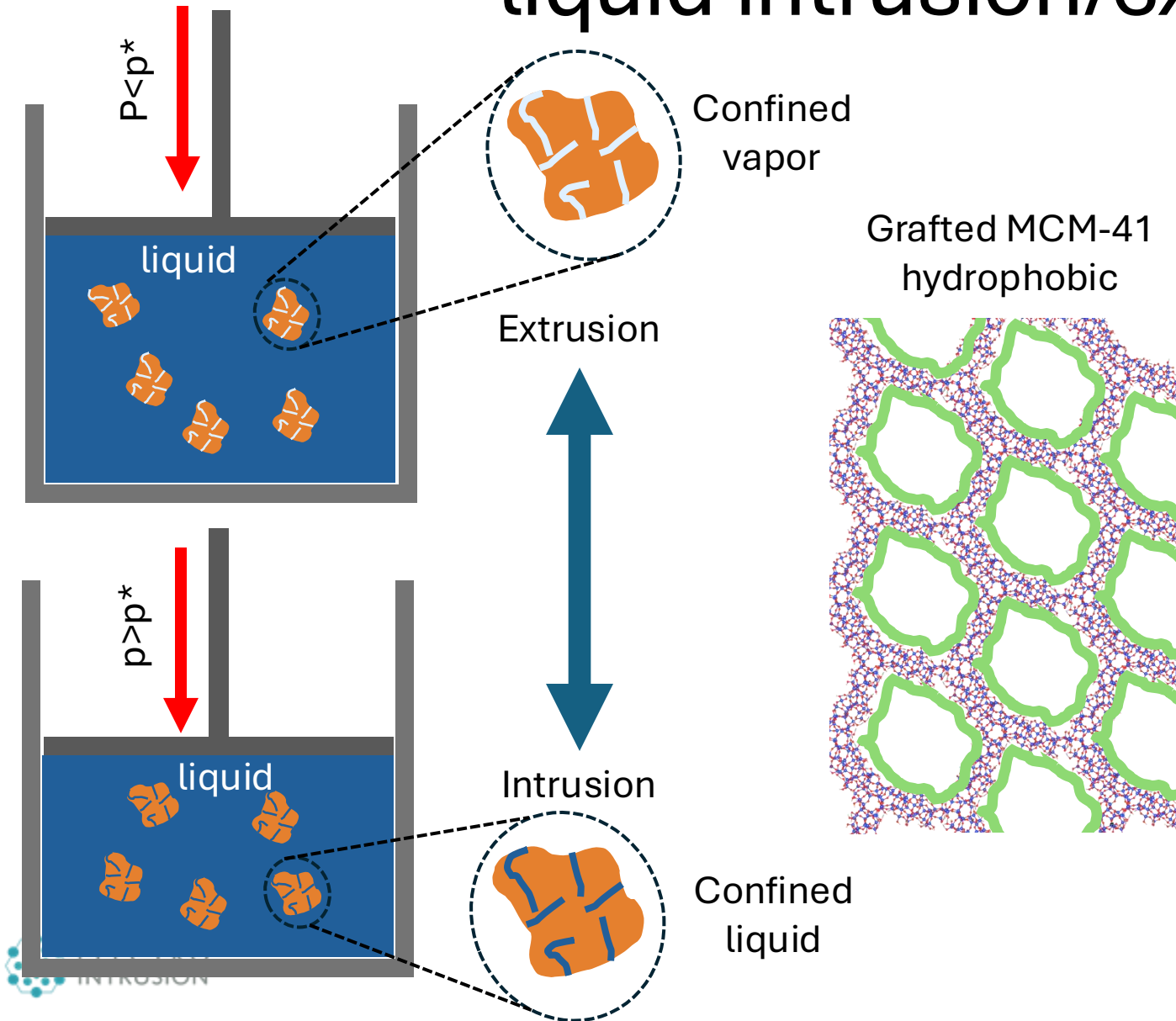
$$\Delta G(r) = \frac{4\pi r^3}{3\nu} \Delta\mu + 4\pi r^2 \gamma$$



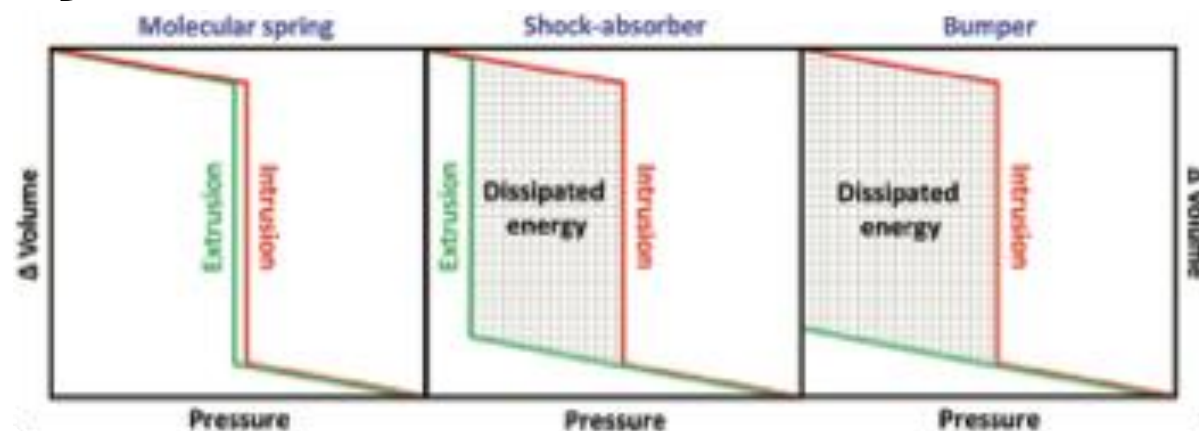
# Confined liquid-vapor phase transition: capillary condensation/evaporation



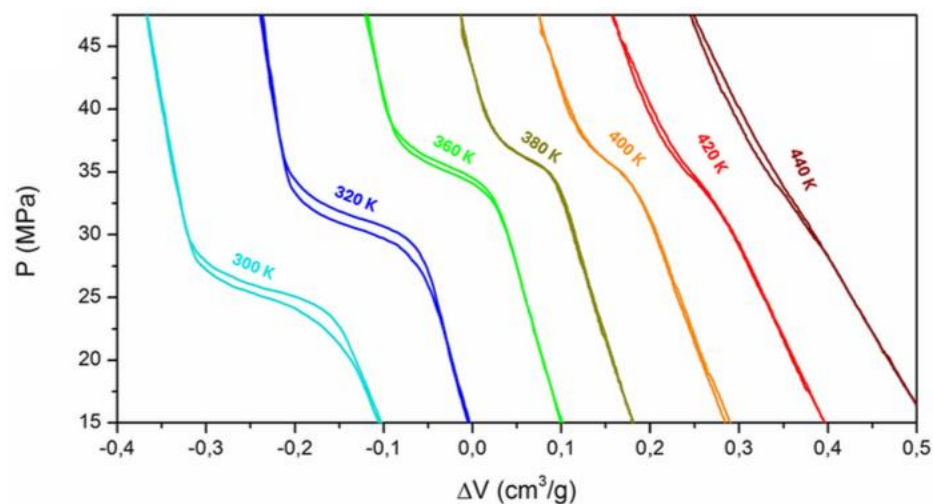
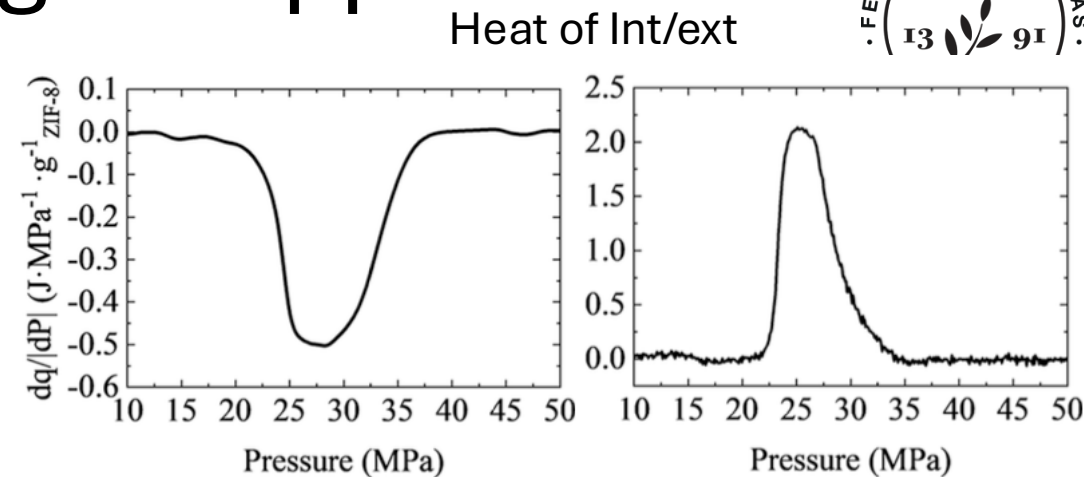
# Confined liquid-vapor phase transition: liquid intrusion/extrusion



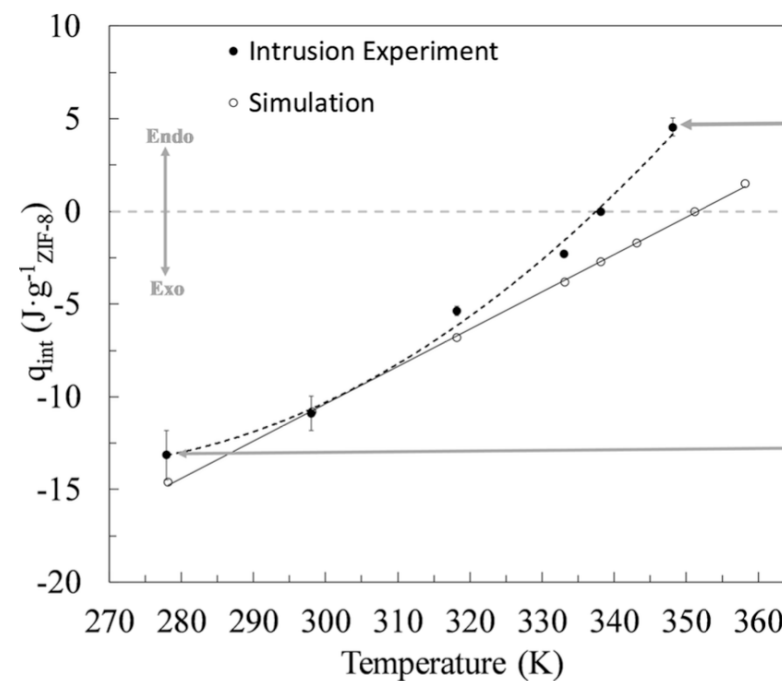
# Key characteristics for technological applications



Adv. Phys.: X, 7, 2052353, 2022



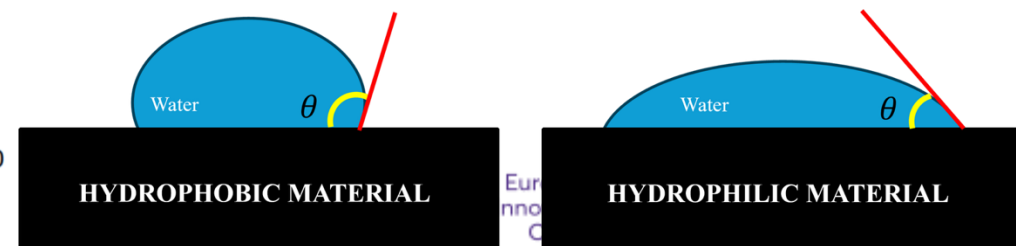
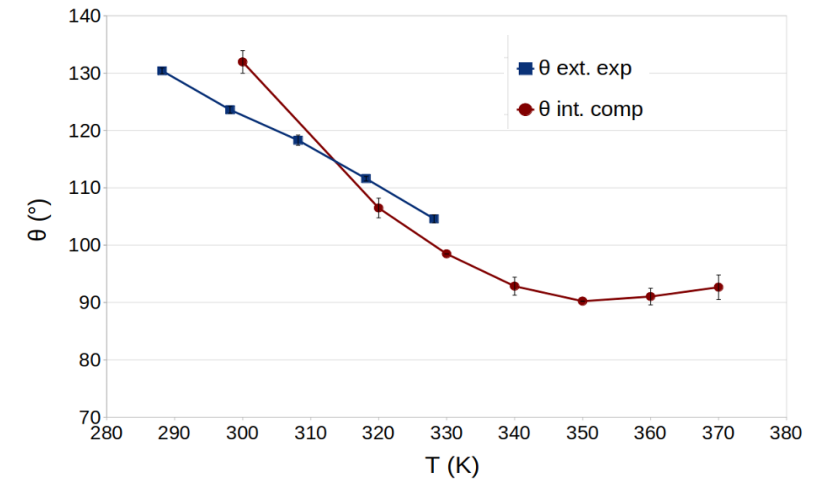
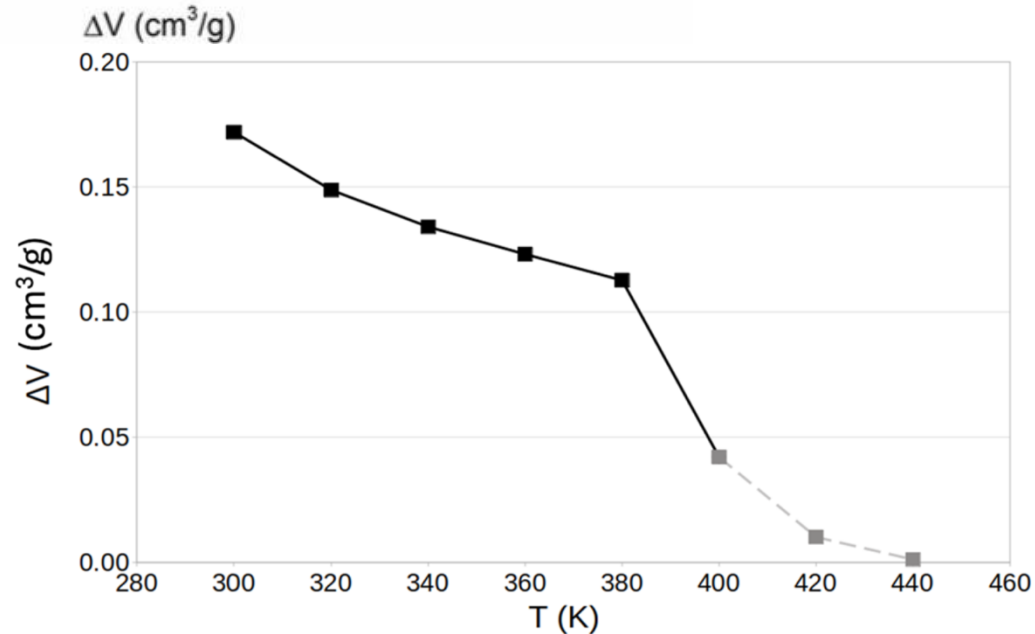
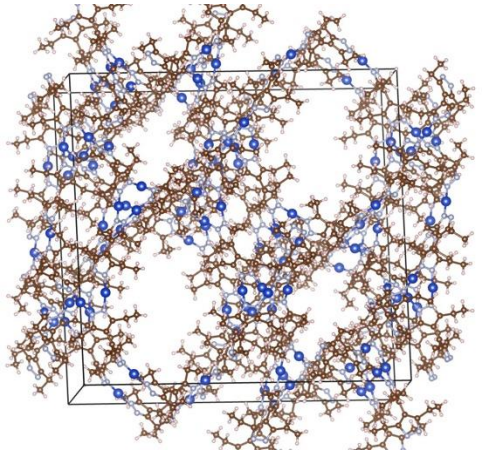
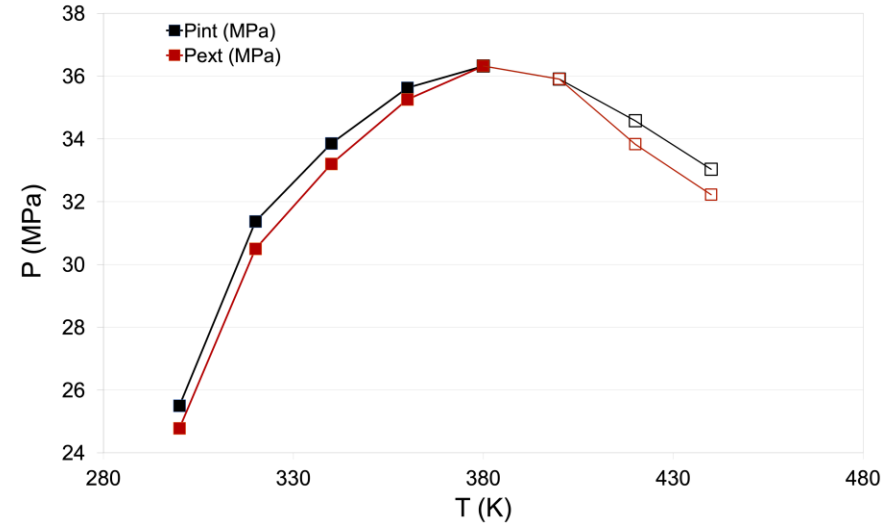
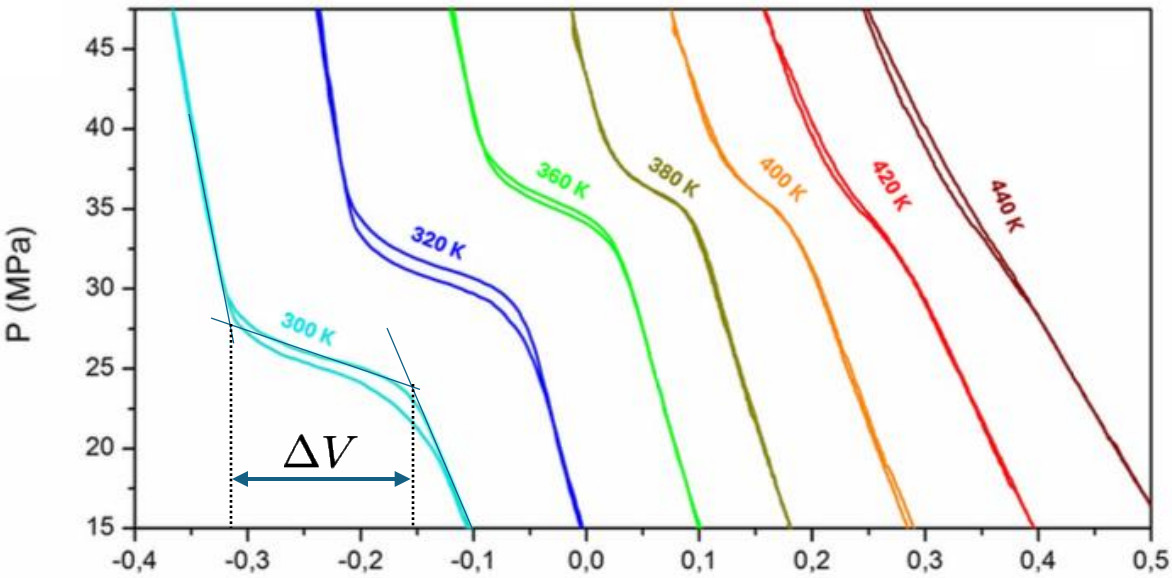
J. Am. Chem. Soc. 146, 13236, 2024



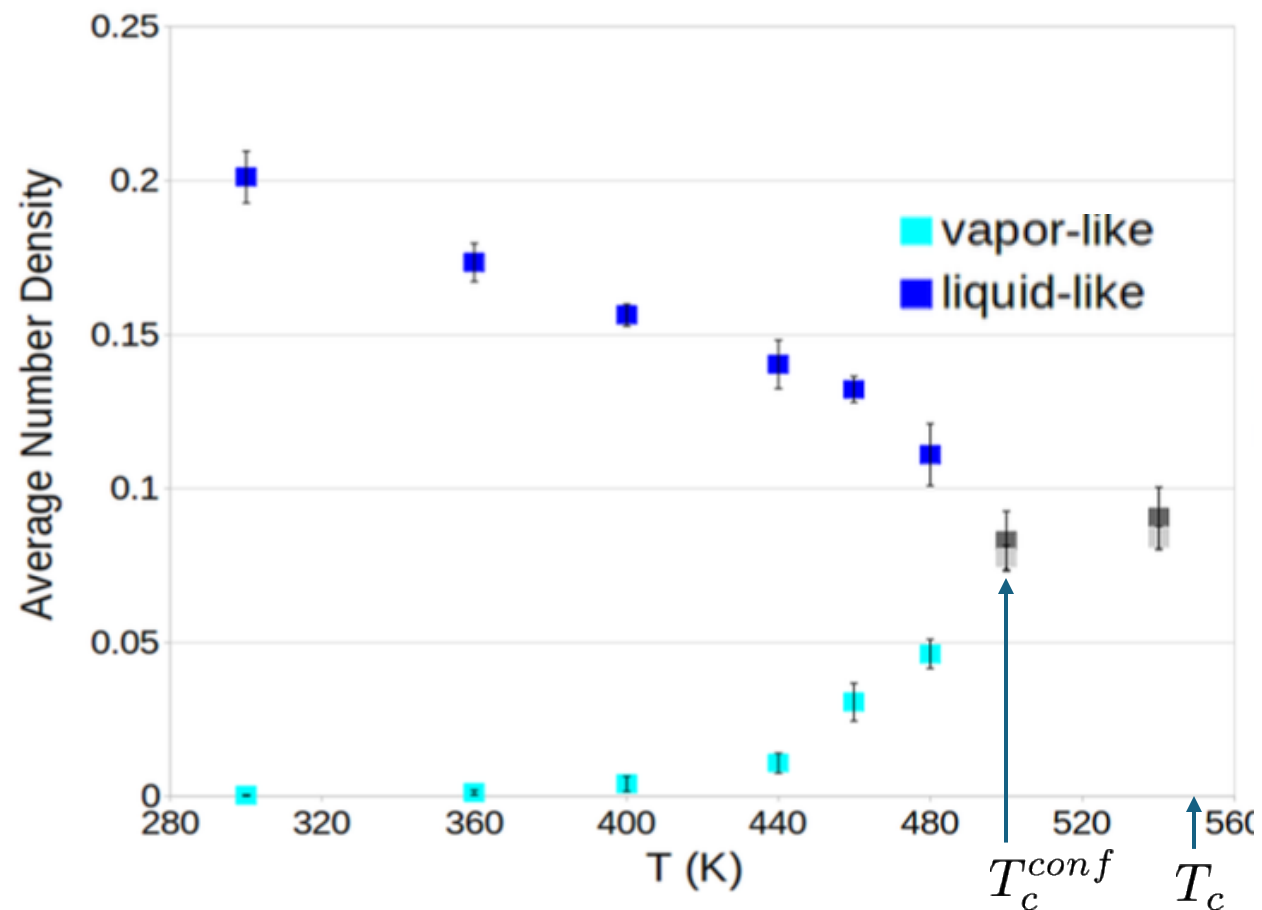
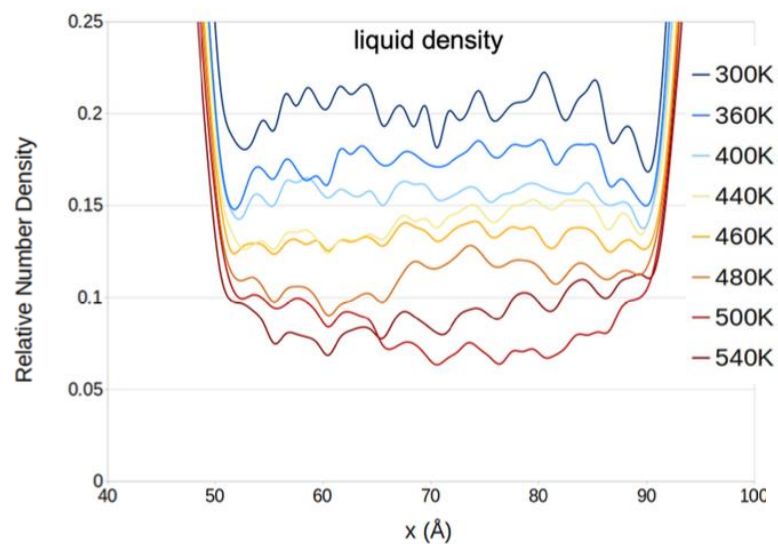
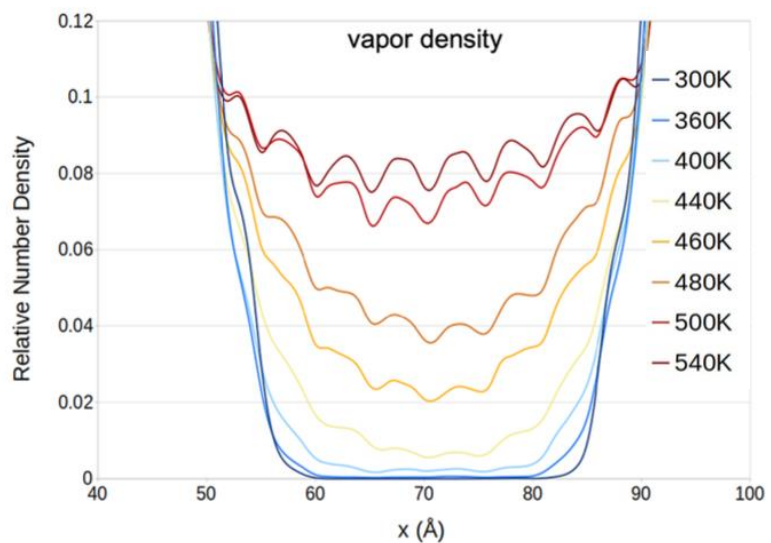
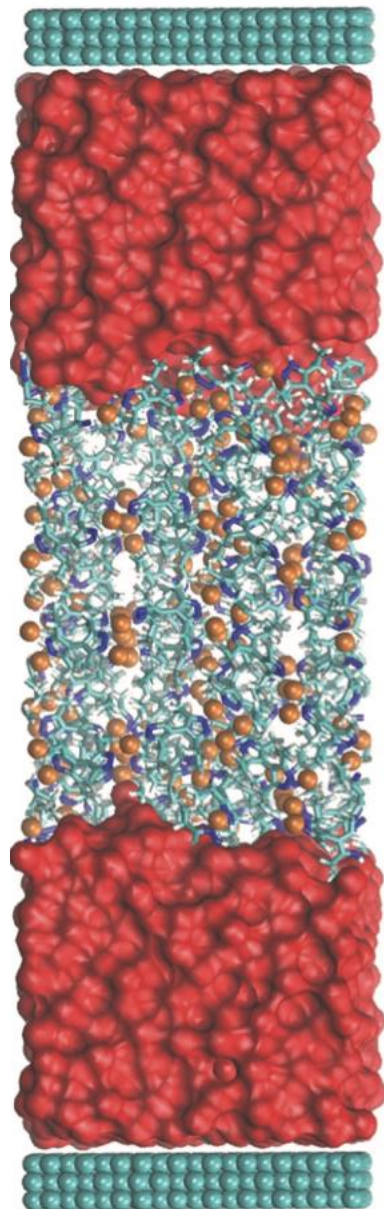
ACS Appl. Mater. Interfaces 16, 5286, 2024



# Effect of the temperature

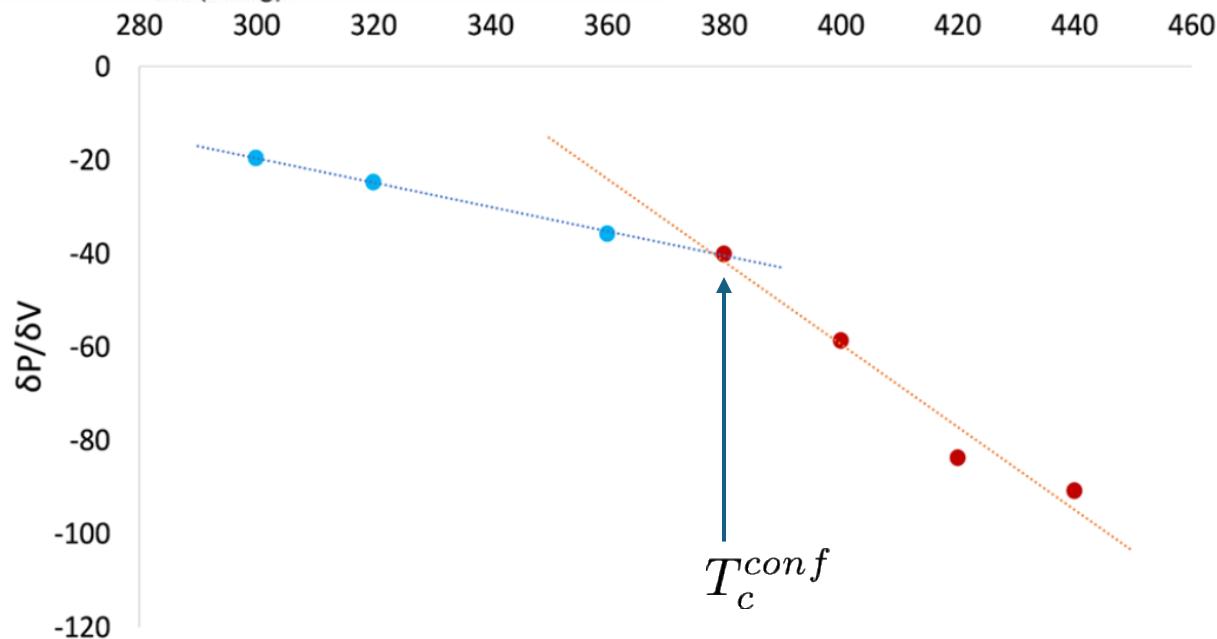
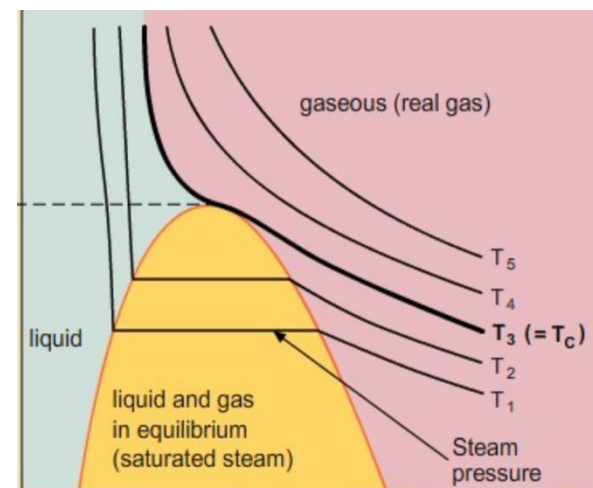
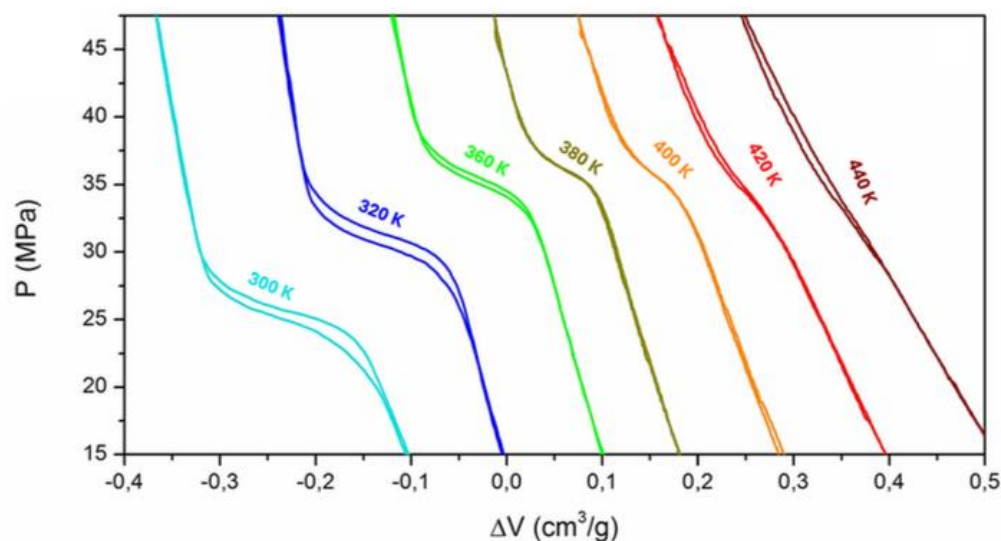


# Confined, Low-T, supercritical water

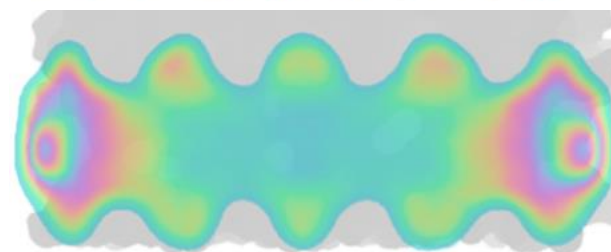
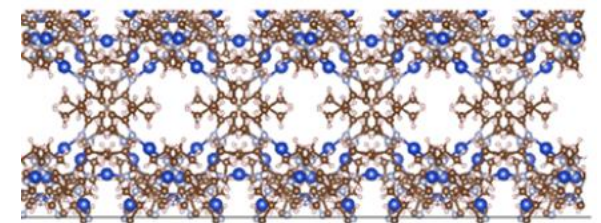
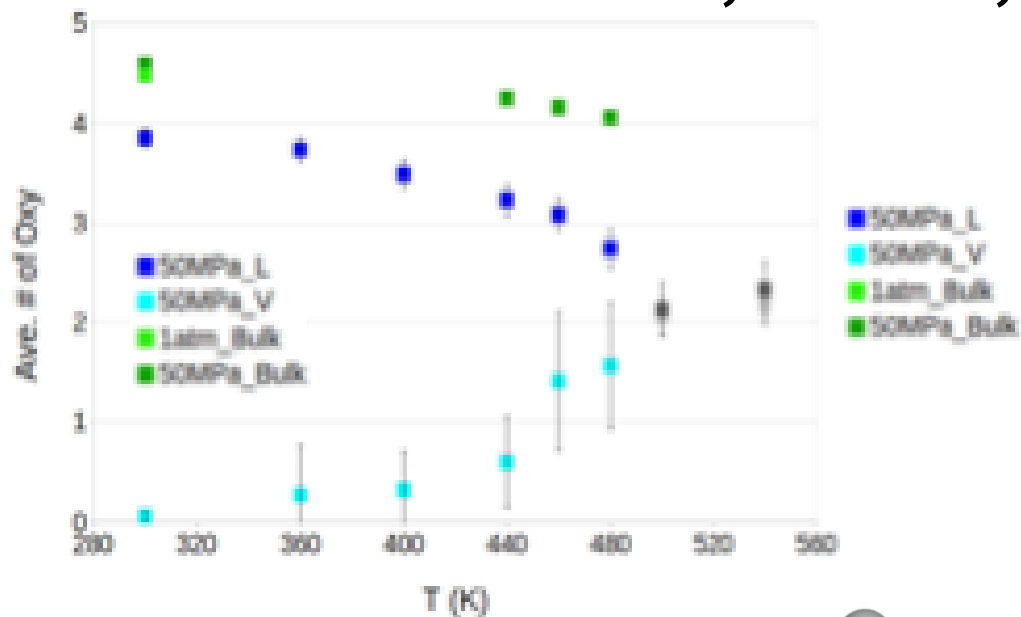




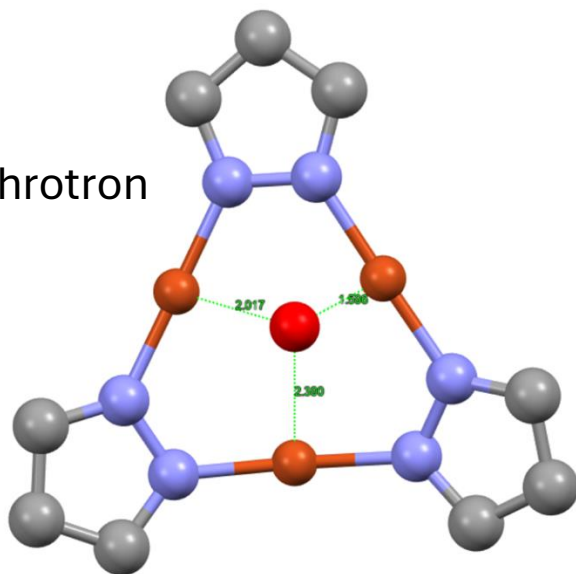
# Confined, Low-T, supercritical water



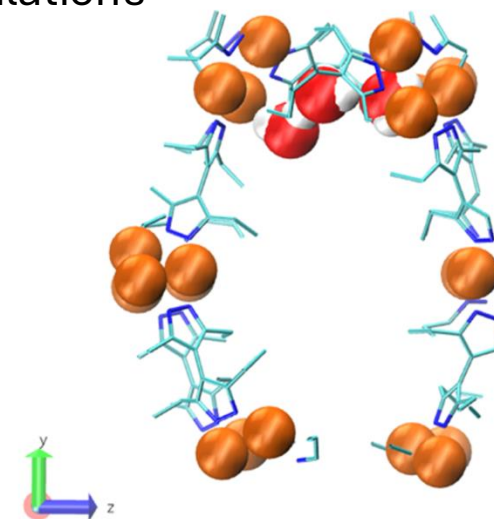
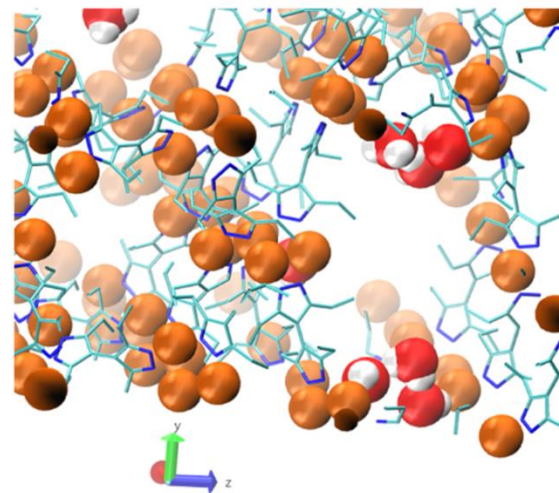
# Confined, Low-T, supercritical water



Synchrotron

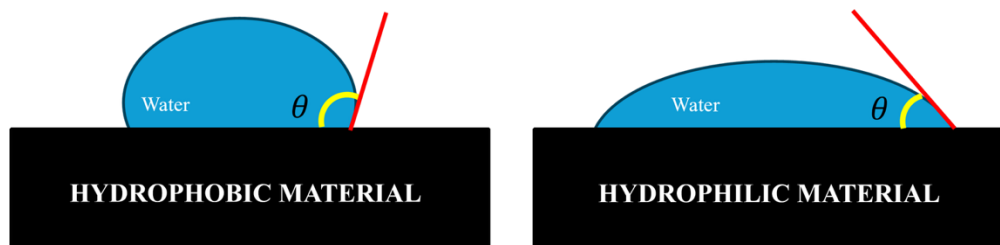
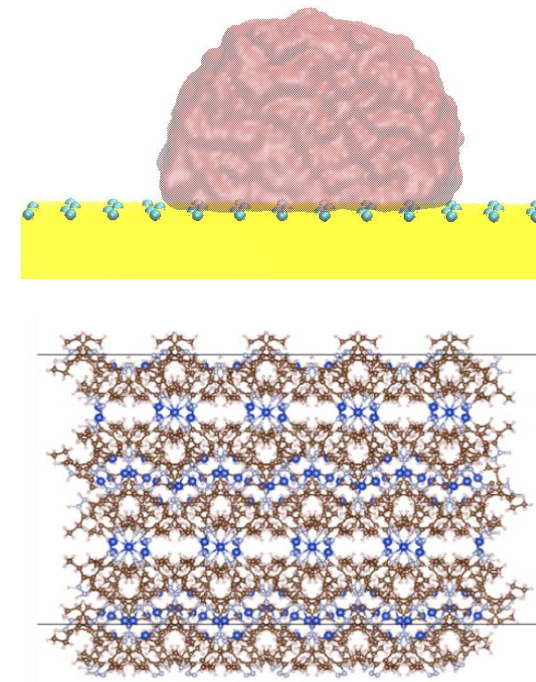
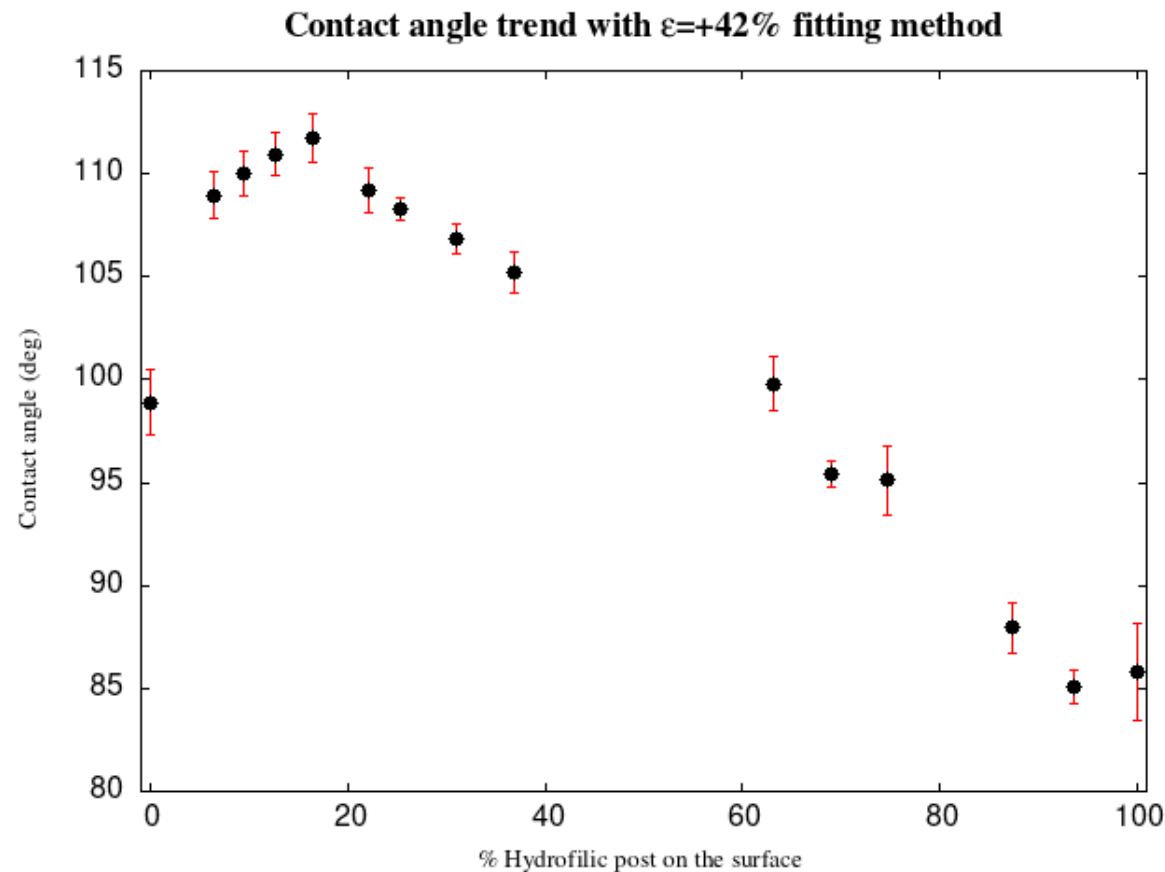
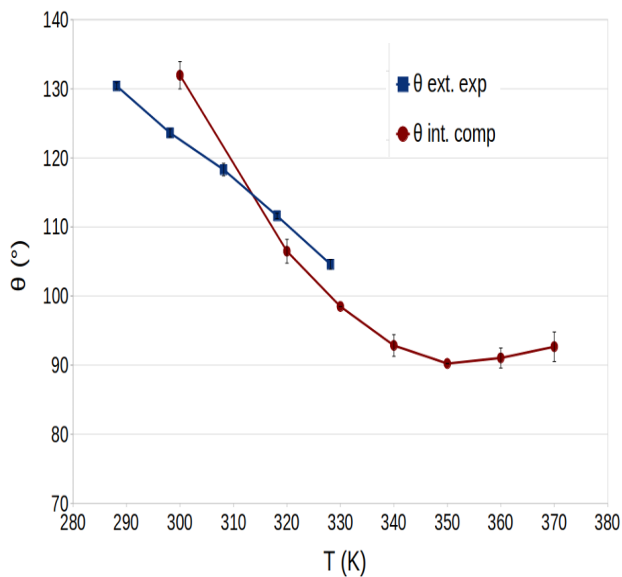


Simulations

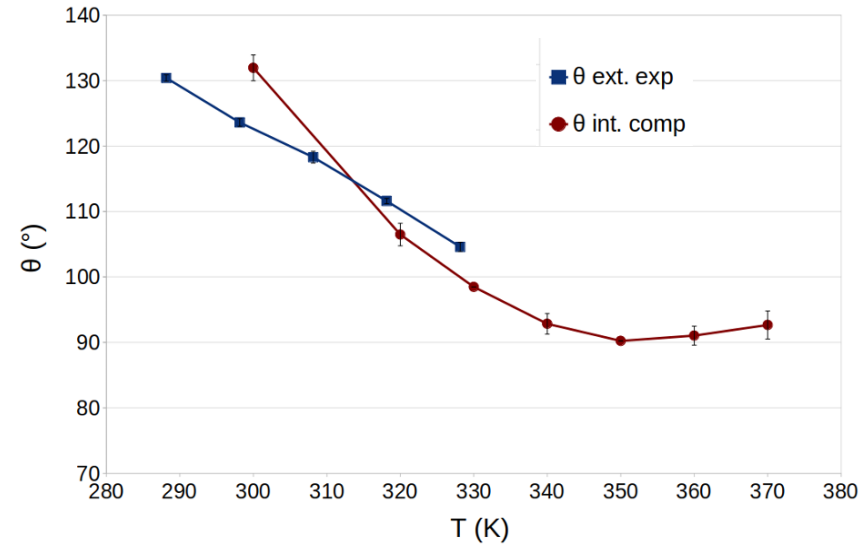
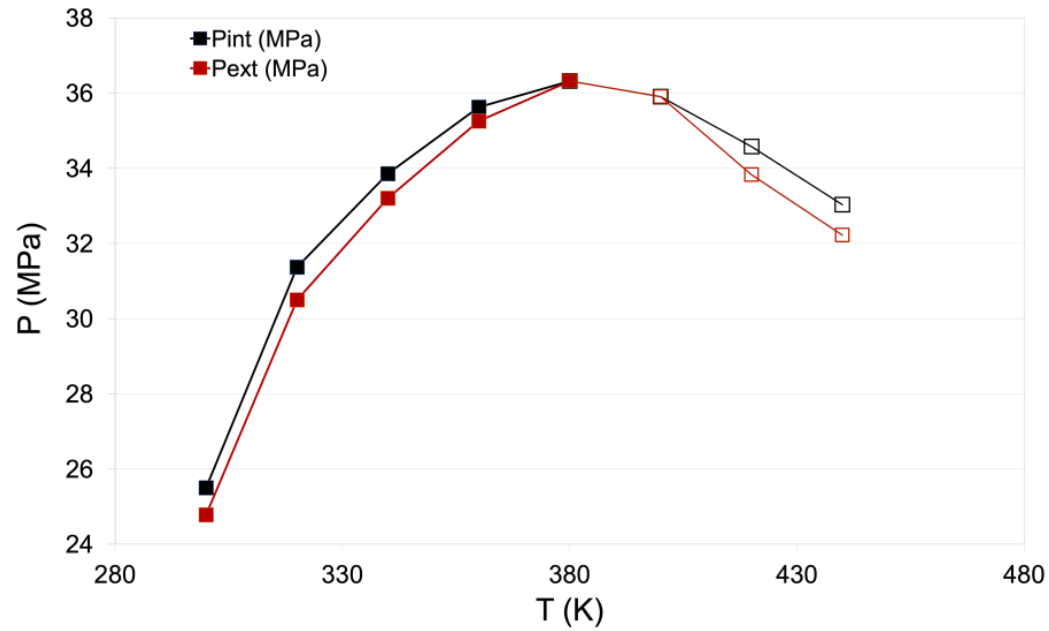




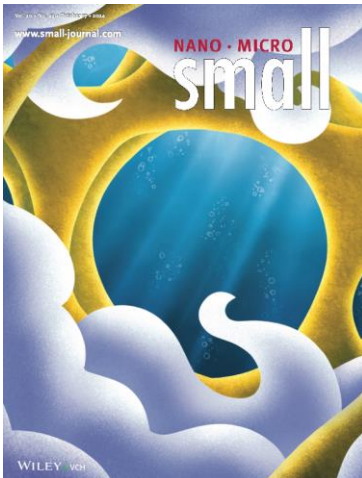
# The unusual chemistry of $\text{Cu}_2(\text{tebpz})$ : highly hydrophobic but with hydrophilic spots



# Effect of the temperature: reprised



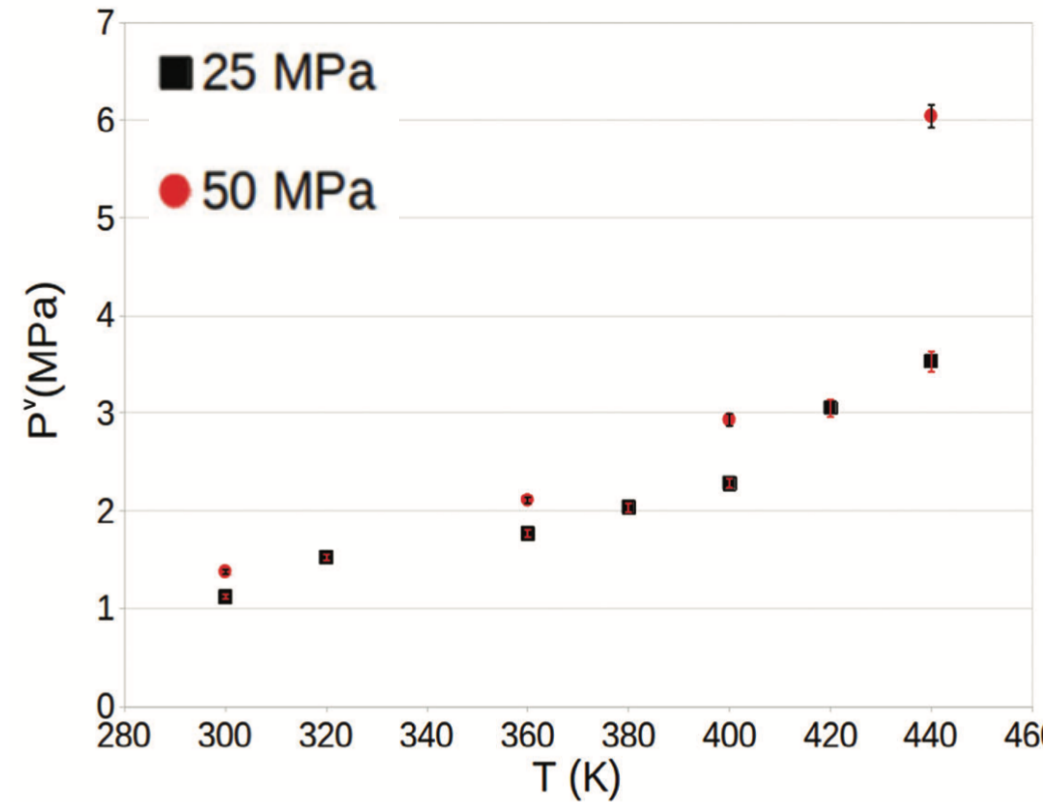
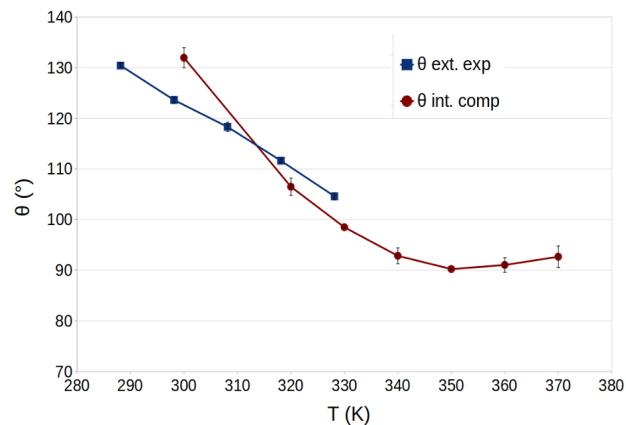
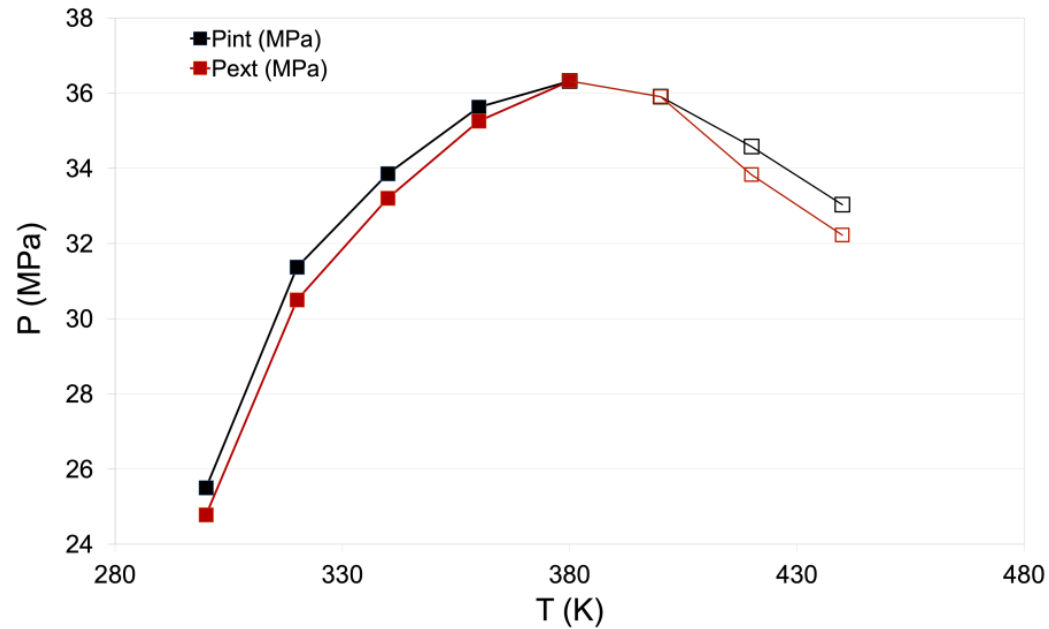
$$P^i = -2\gamma \cos \vartheta / a$$



*Small* 2024, 20, 2402173

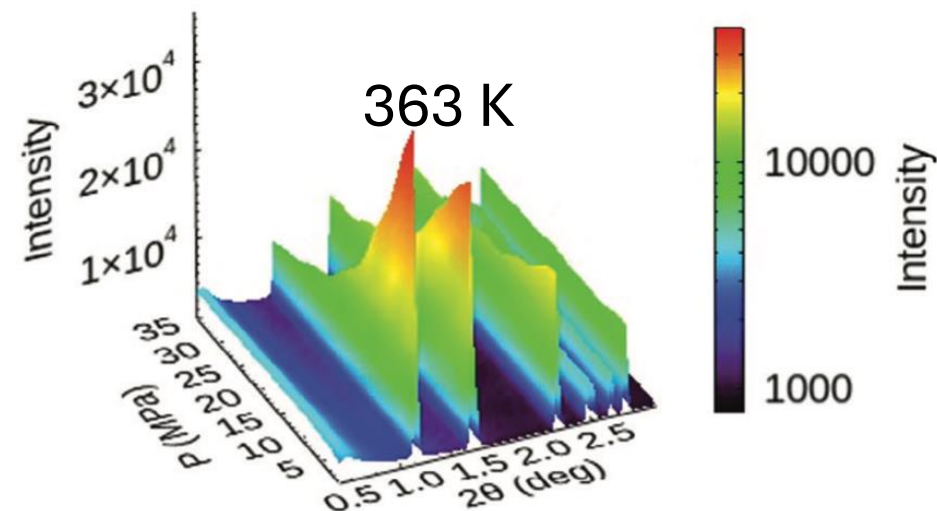
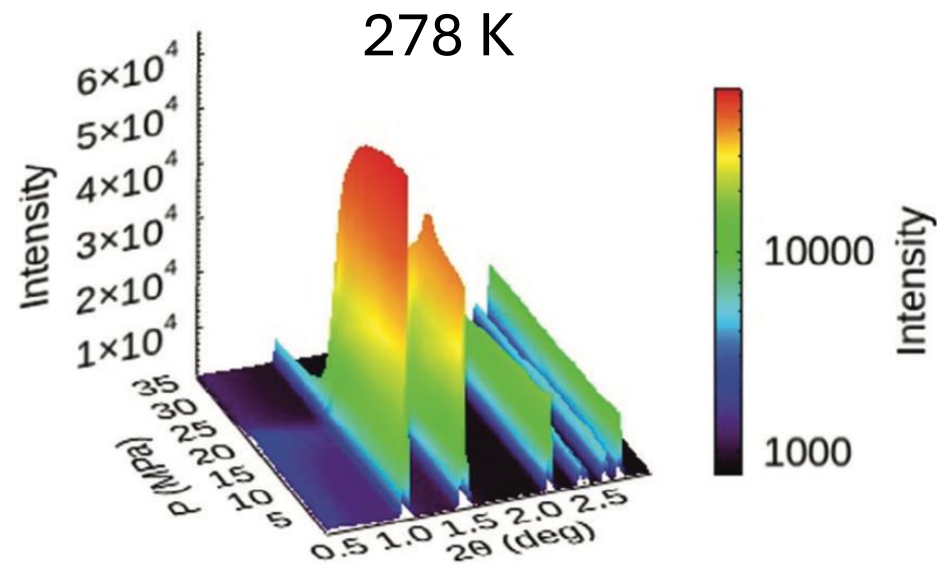
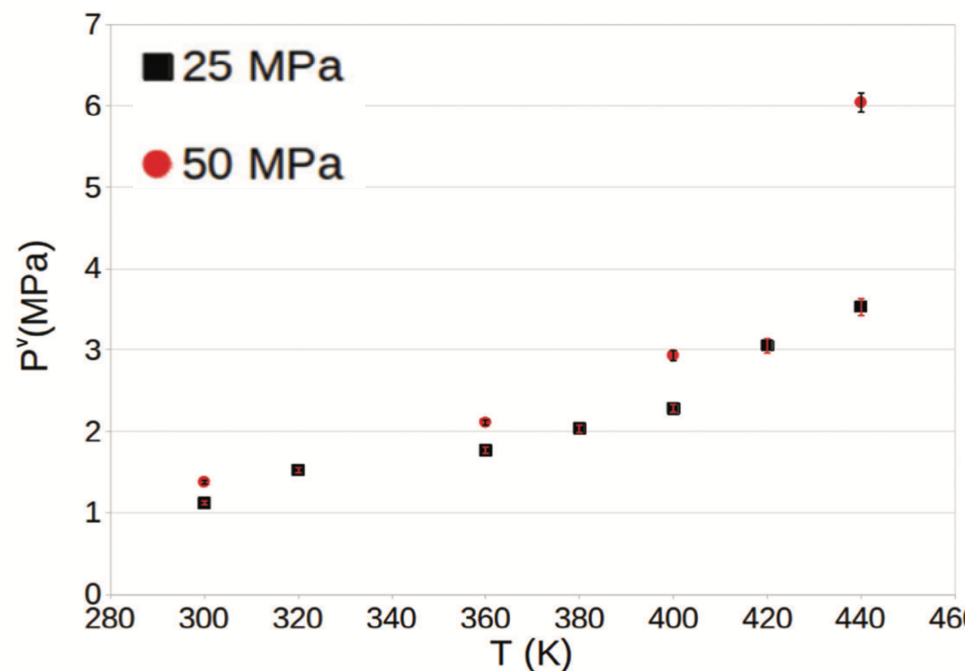


# Effect of the temperature: reprised



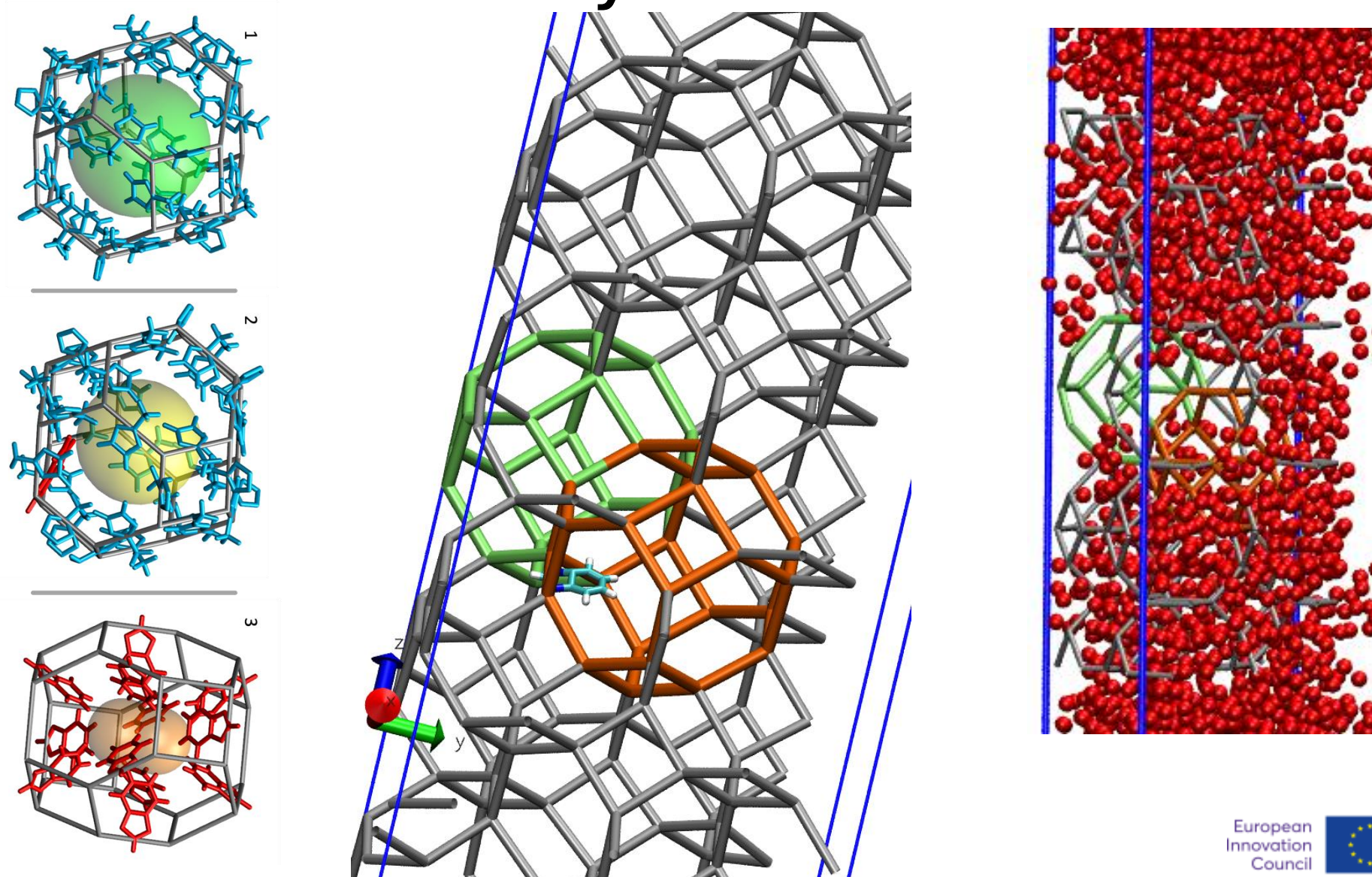
$$P^i = -2\gamma \cos \vartheta / a + P^v$$

# Effect of the temperature: reprised

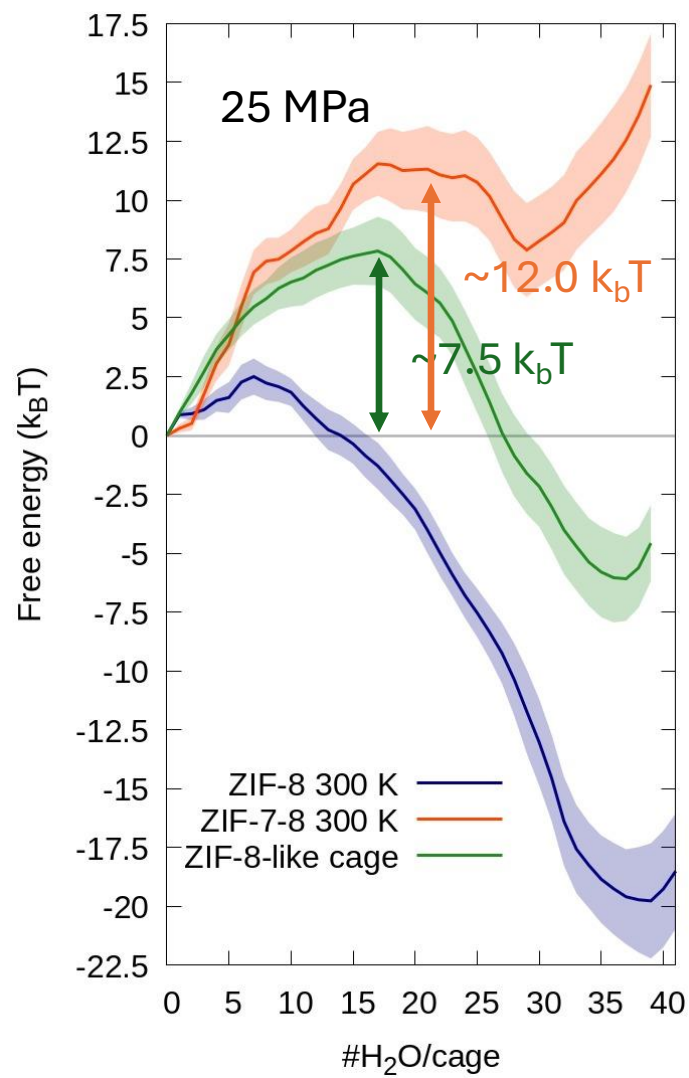




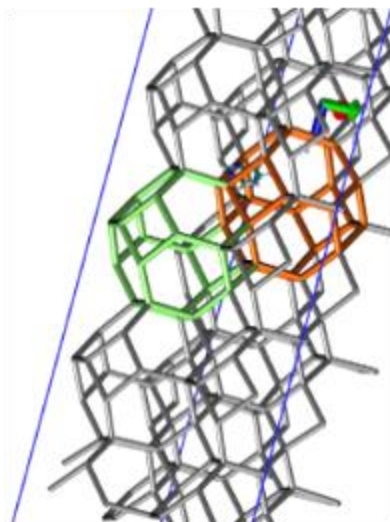
# Tuning critical temperature by reducing the liquid density: the ZIF case



# Tuning critical temperature by reducing the liquid density: the ZIF case



	$E^\ddagger [k_B T]$	at	$E_{\text{wet}} [k_B T]$	at	wet neigh.
<b>ZIF-8</b>	2.50	7	-19.78	39	5
<b>ZIF-8-like-cage</b>	7.84	17	-6.09	37	6
<b>ZIF-7-8</b>	11.55	17	7.88	29	5





# 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.
- A supercritical phase exists as well (all props of bulk SC water?)
- The porous material plays a role beyond the classical physics picture: it is not an inert confining medium.
- Low-T supercriticality 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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