
Peculiar properties of water
squeezed within nanoglasses
Simone.meloni@unife.it
AQTIVATE Workshop,
Jülich, 3-5 February 2025
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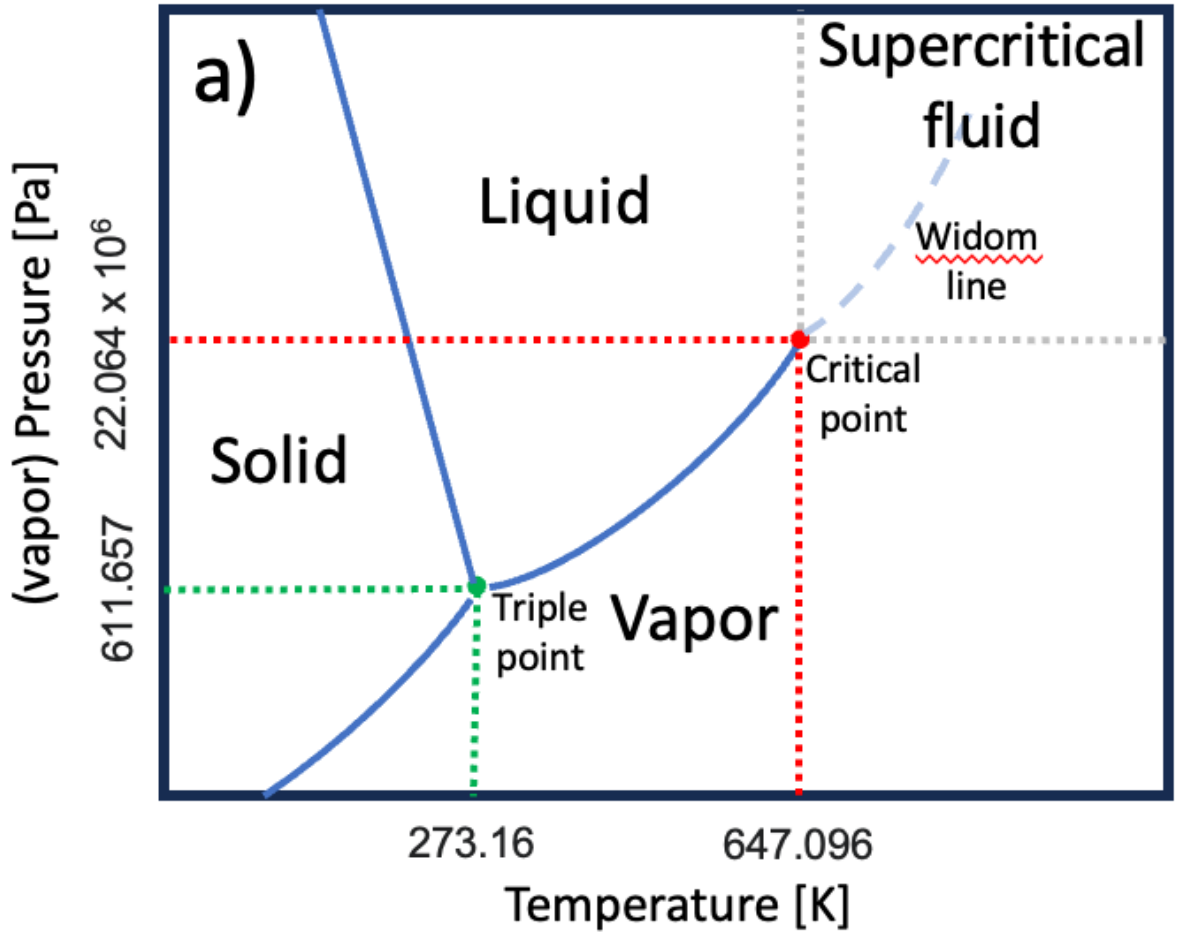
Phase diagram of bulk water



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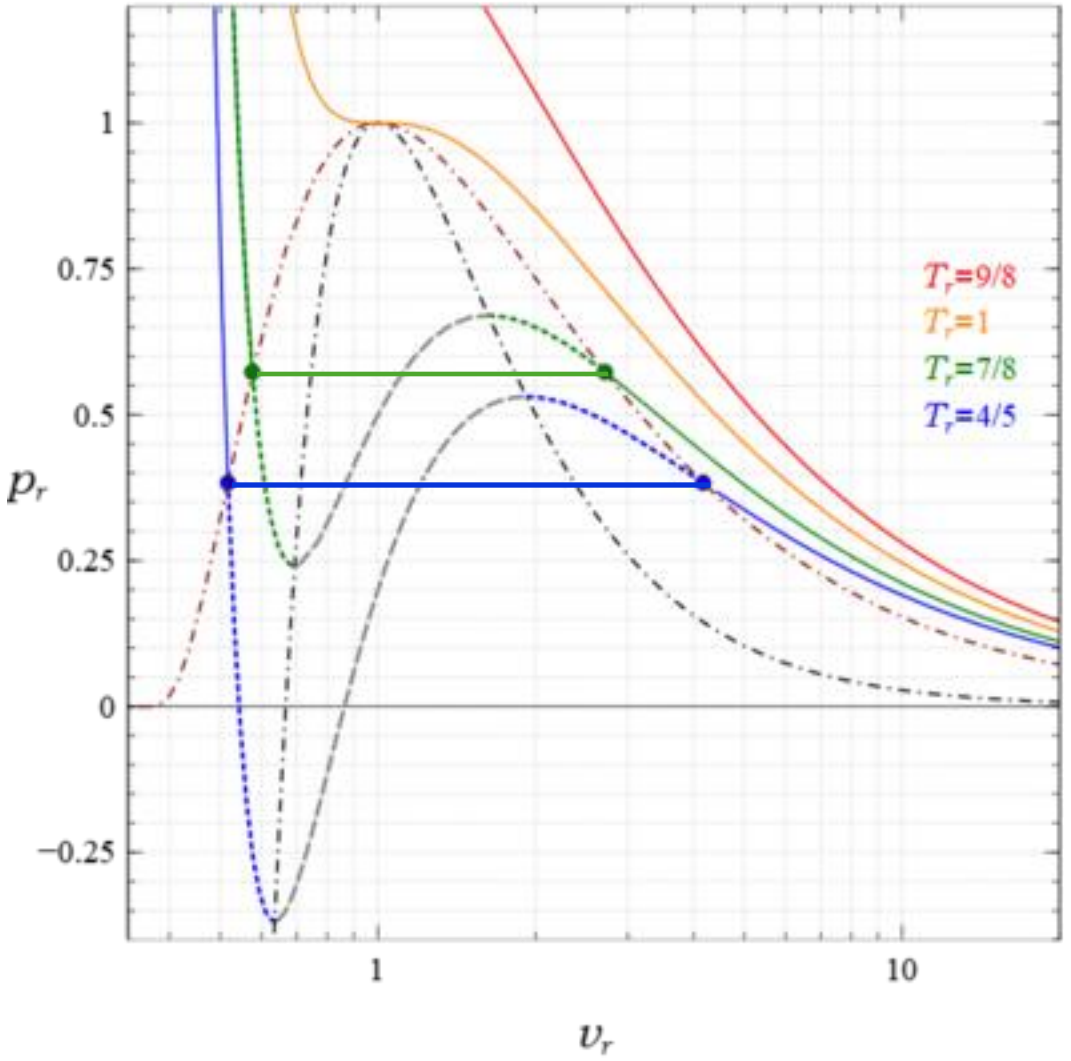
Liquid/vapor Phase transition



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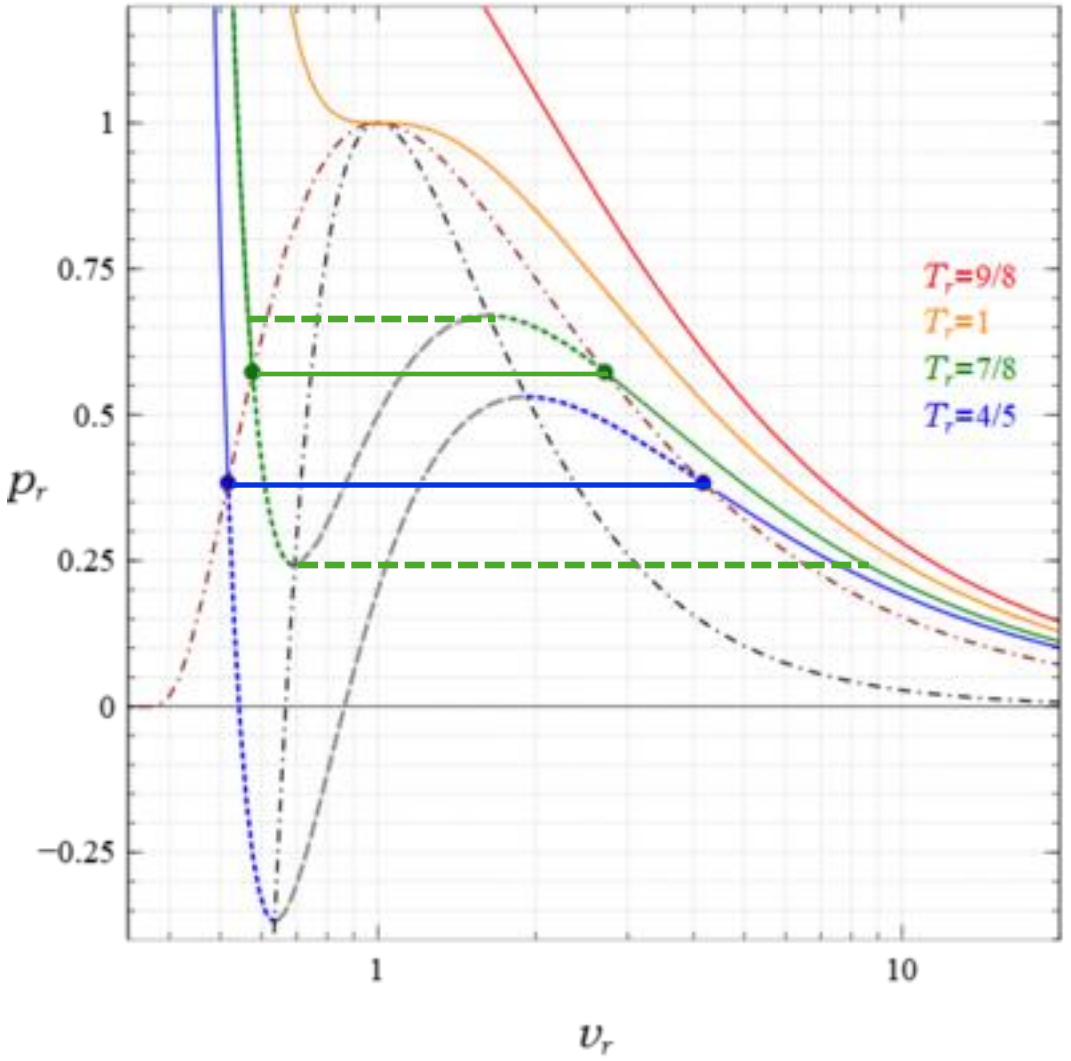
Liquid/vapor Phase transition



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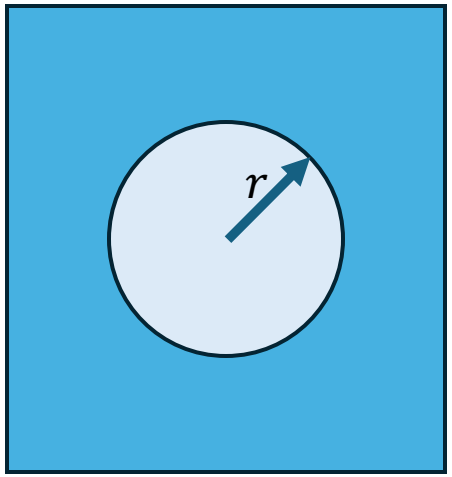
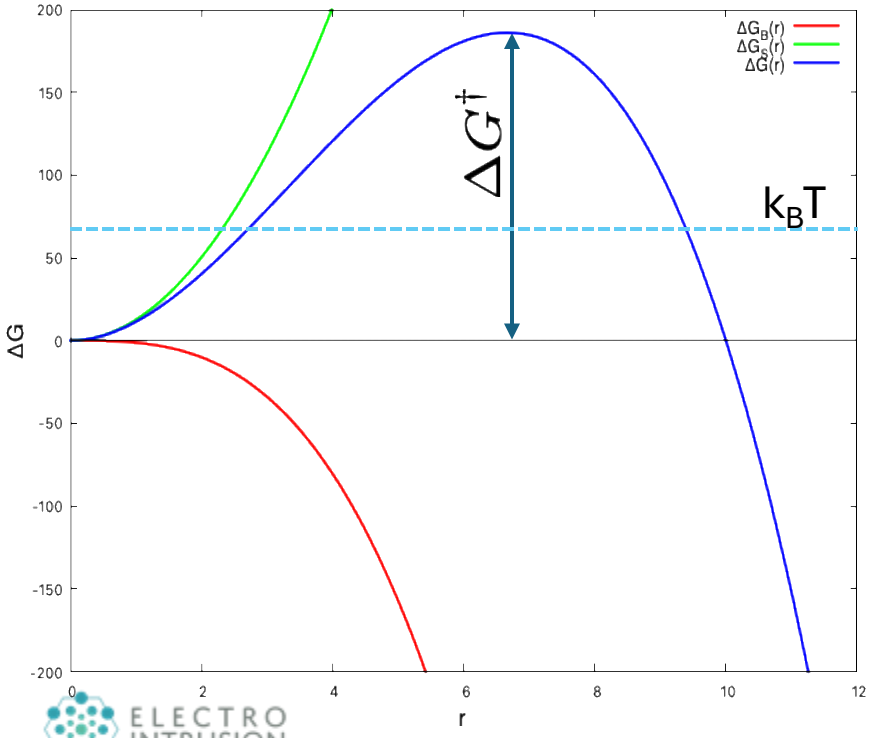
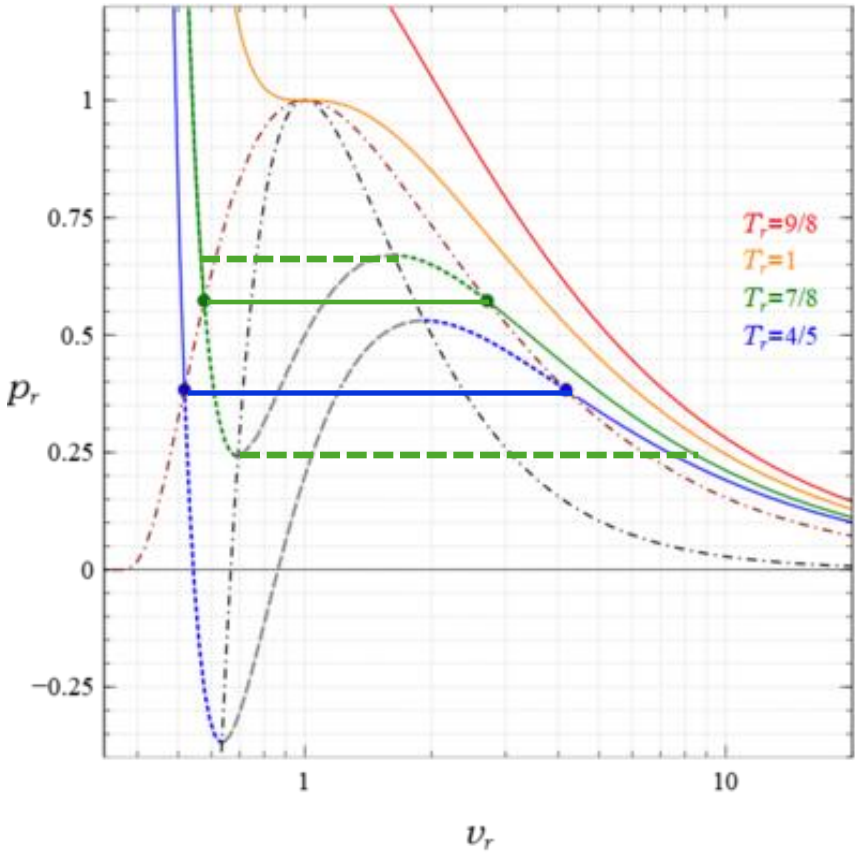
Liquid/vapor Phase transition



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





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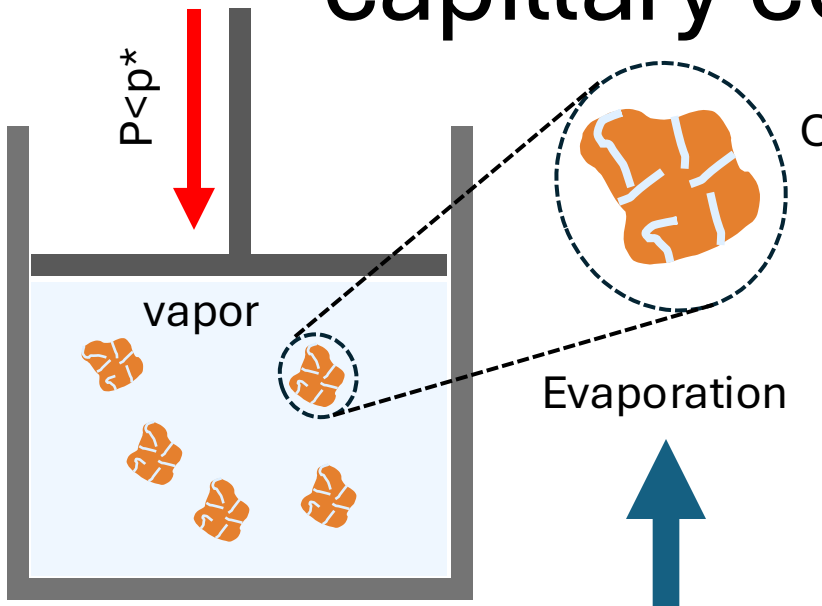
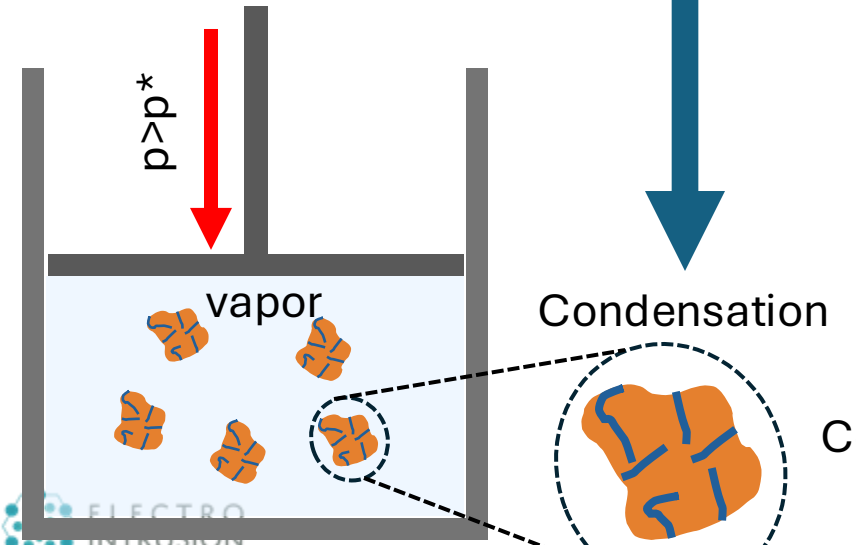
Confined liquid-vapor phase transition: capillary condensation/evaporation



Confined vapor

Evaporation

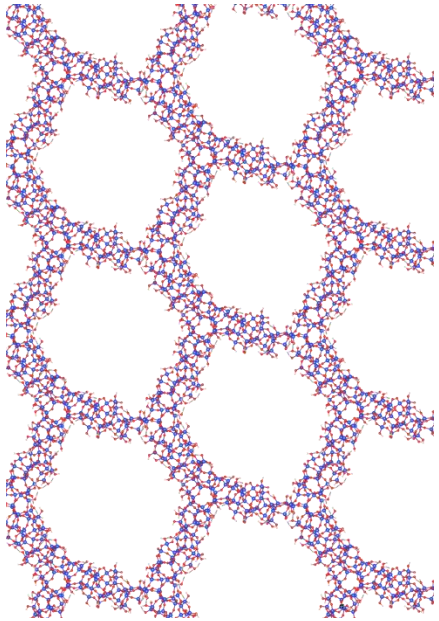


Condensation

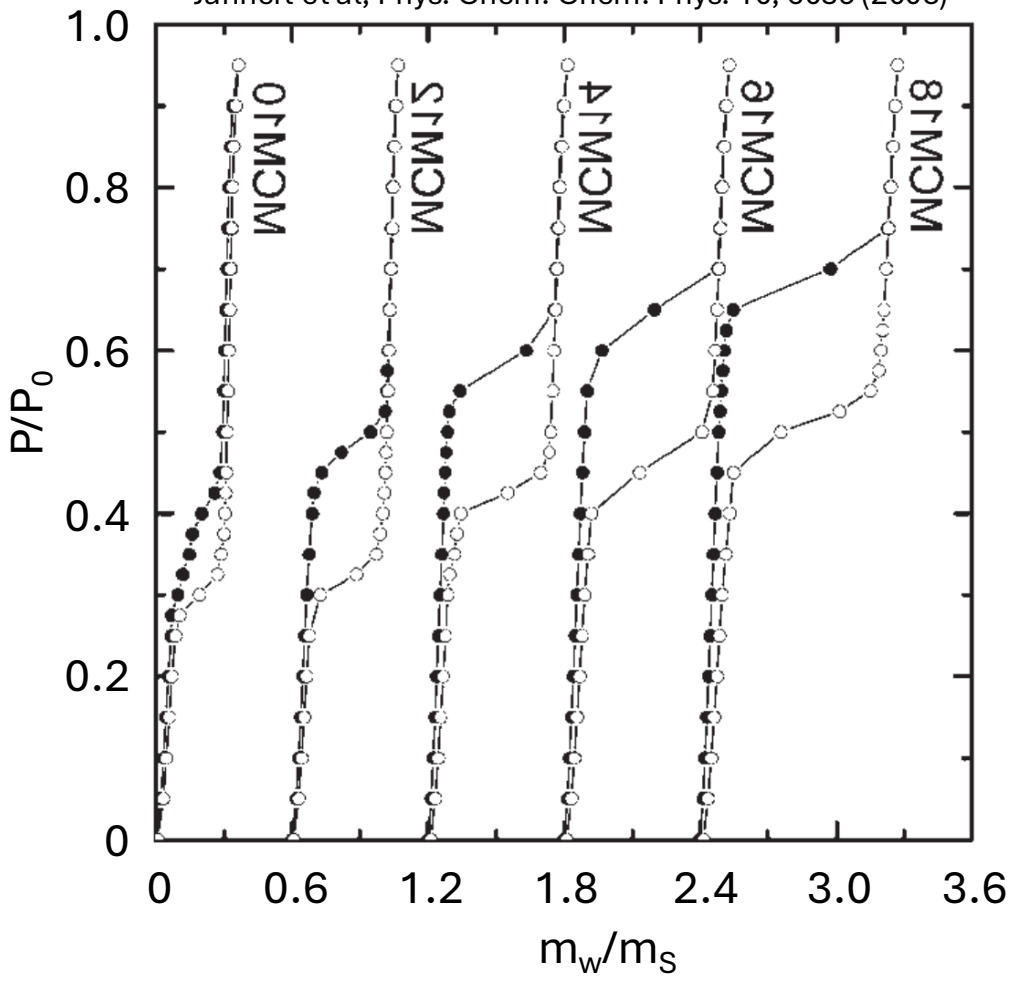
Confined liquid

MCM

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



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



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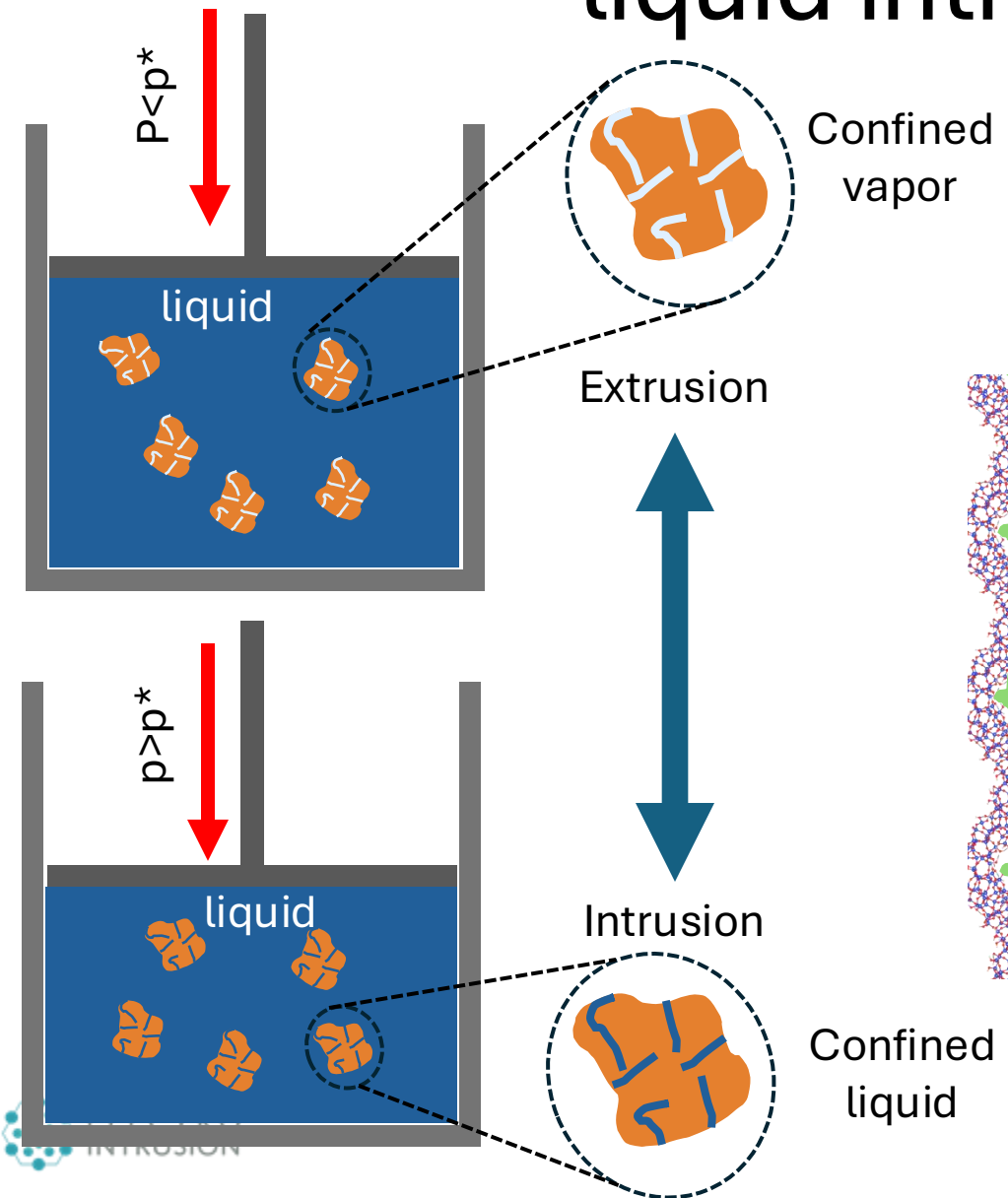
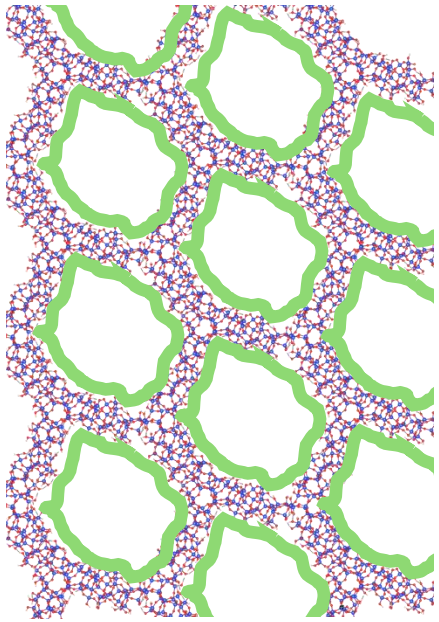
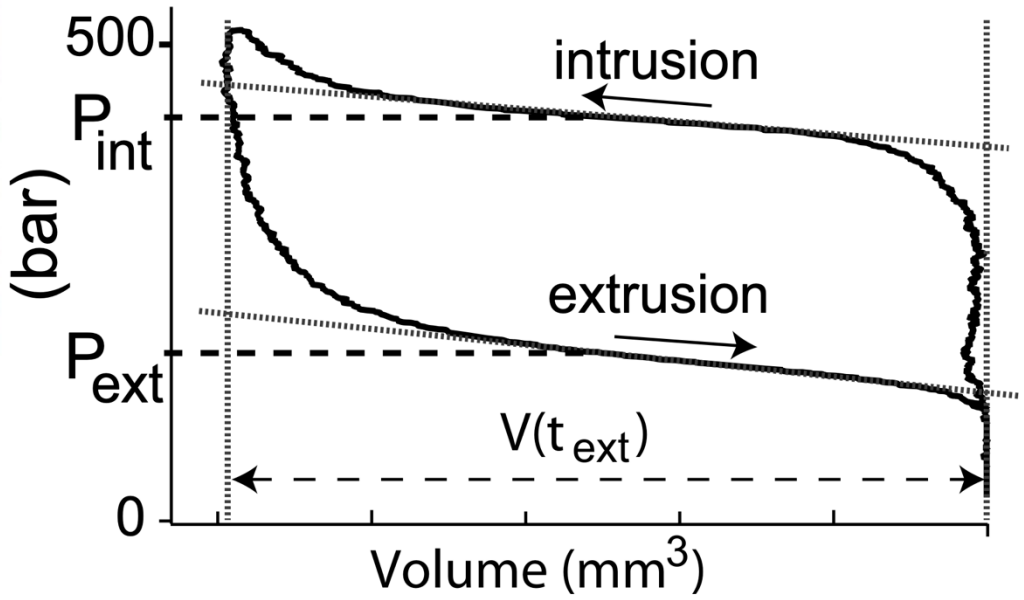
Confined liquid-vapor phase transition: liquid intrusion/extrusion



Grafted MCM-41 hydrophobic



Guillemot et al, PNAS 109,19557 (2012)



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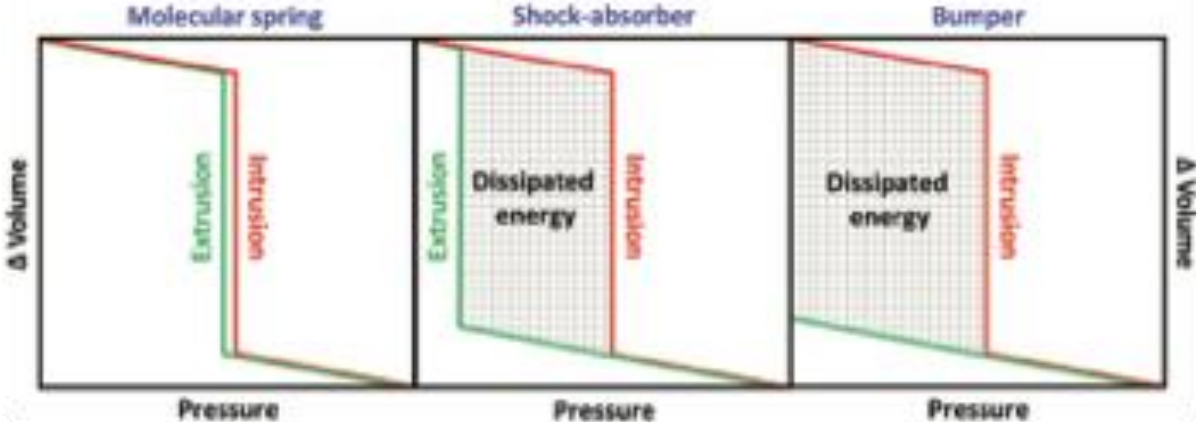
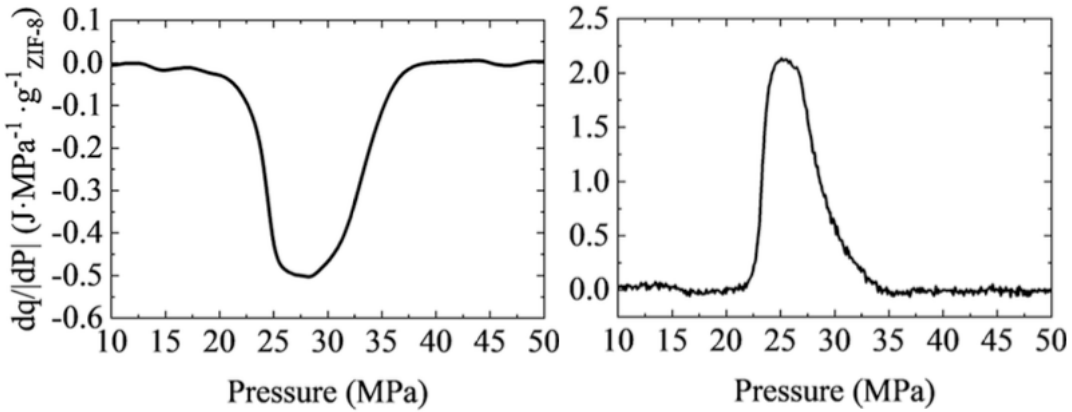
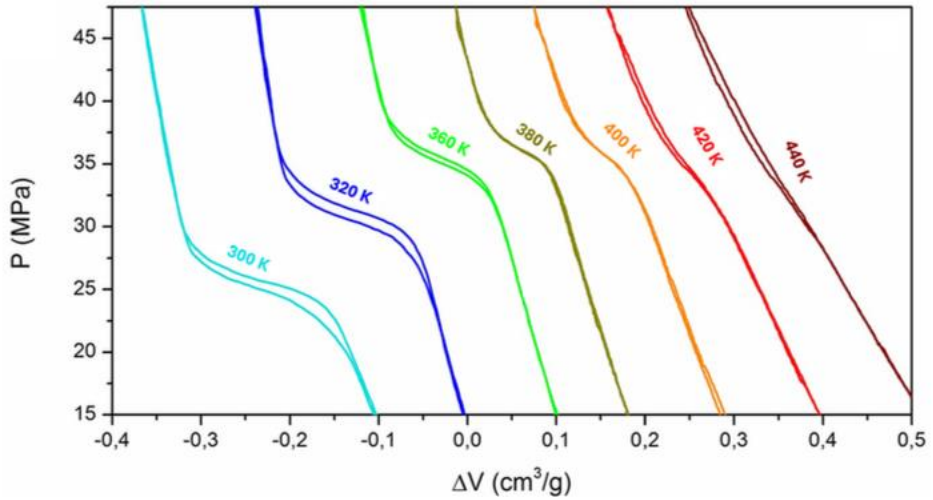
Key characteristics for technological applications



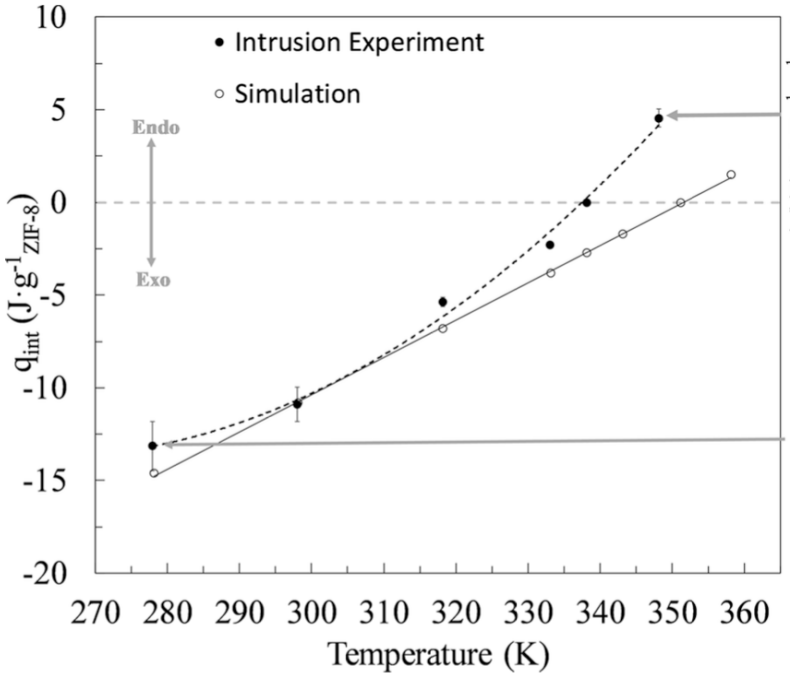
Adv. Phys.: X, 7, 2052353, 2022

Heat of Int/ext





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



ACS Appl. Mater. Interfaces 16, 5286, 2024

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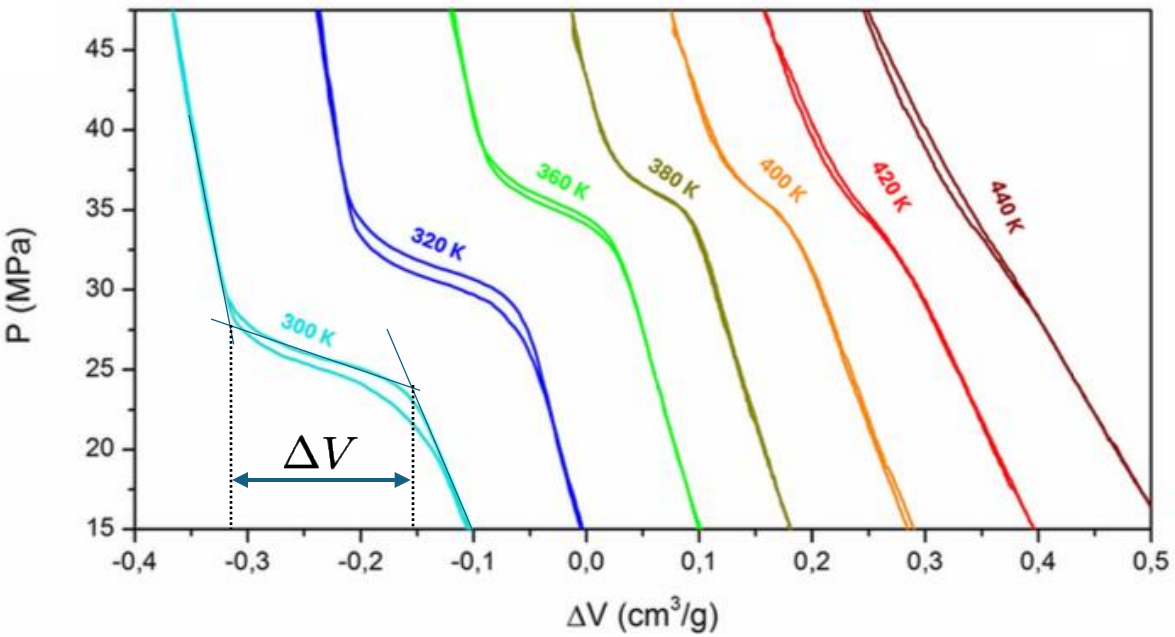
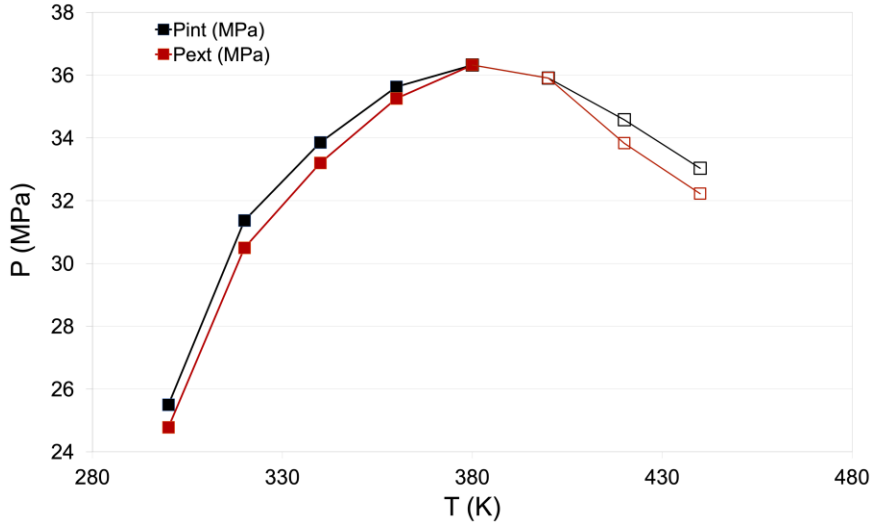
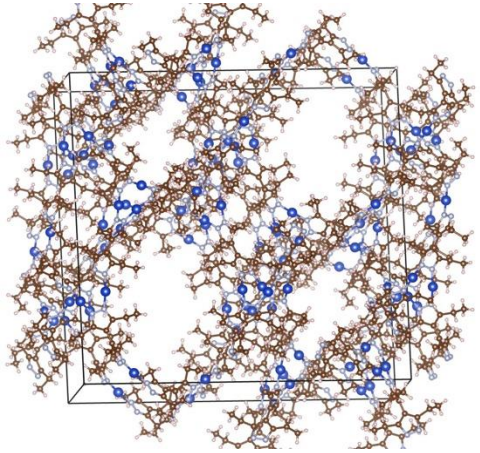
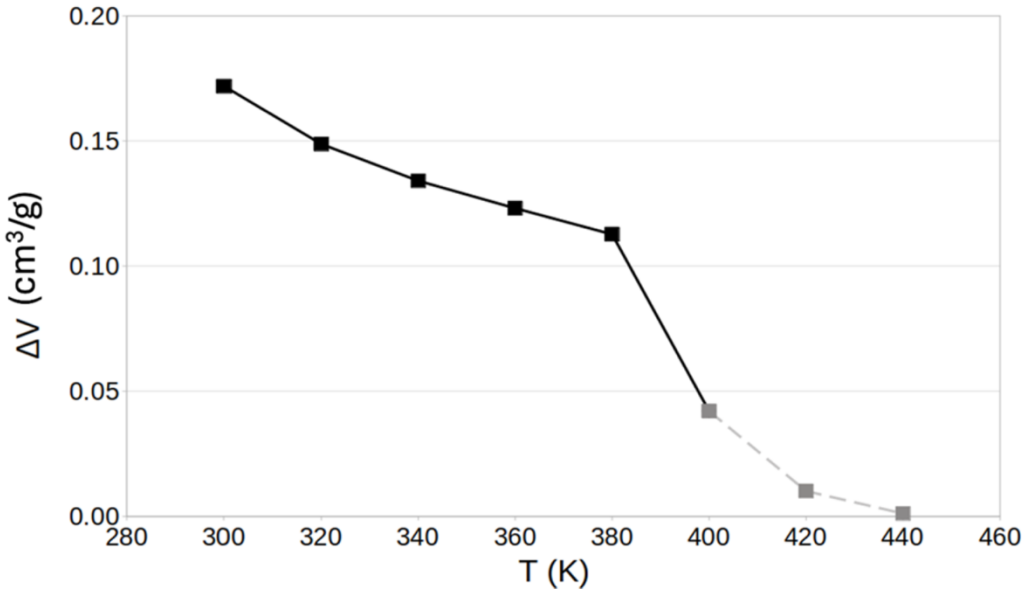
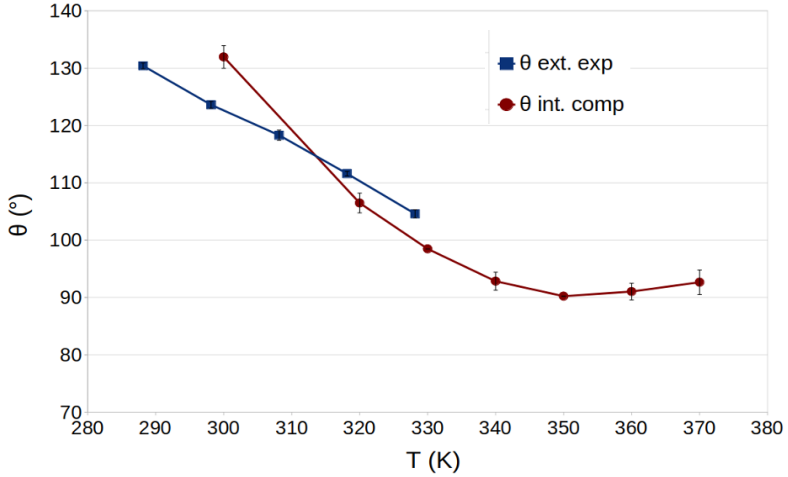
Effect of the temperature

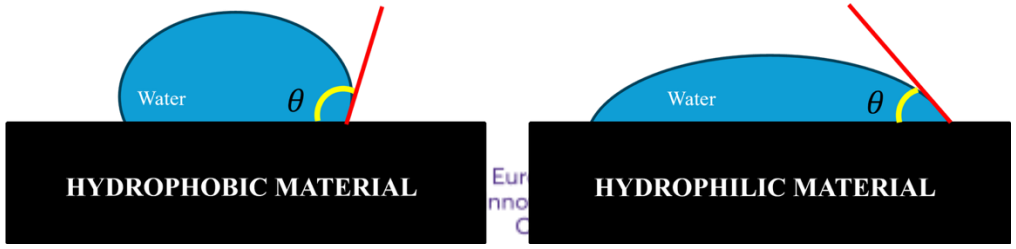












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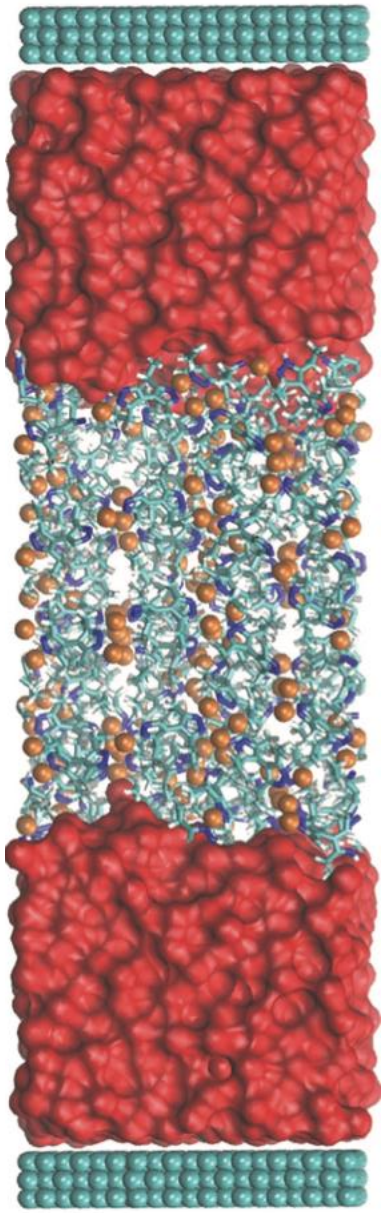
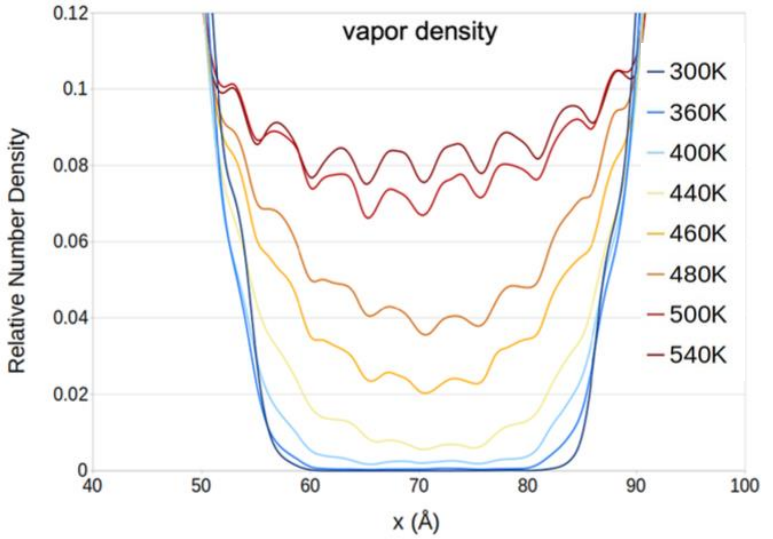
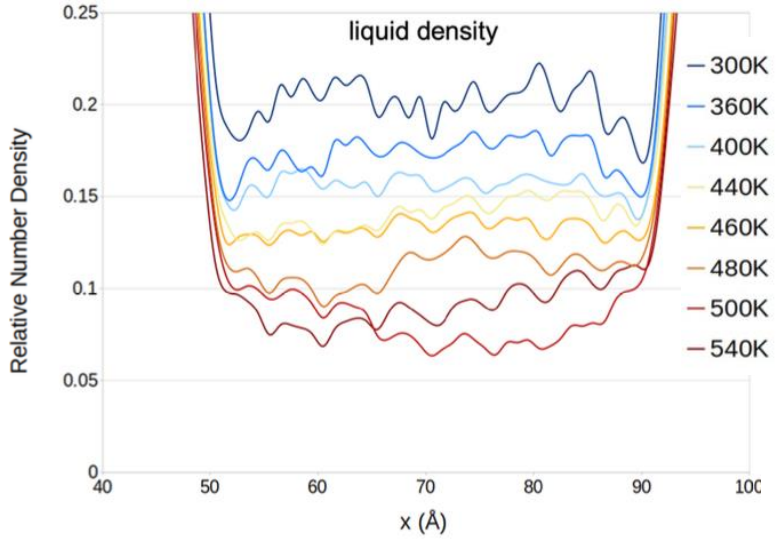
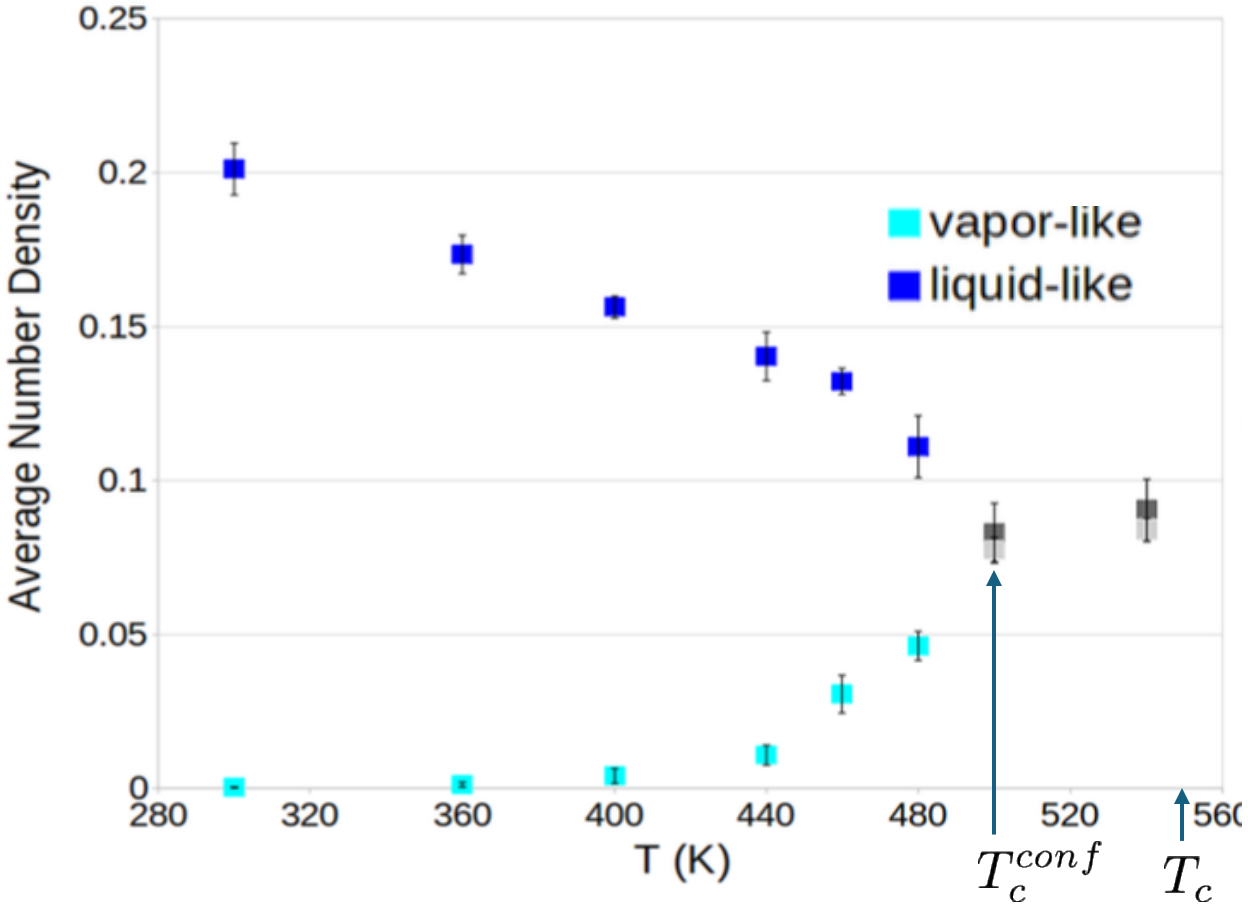
J. Am. Chem. Soc. 146, 13236, 2024; Small 2402173, 2024

Confined, Low-T, supercritical water









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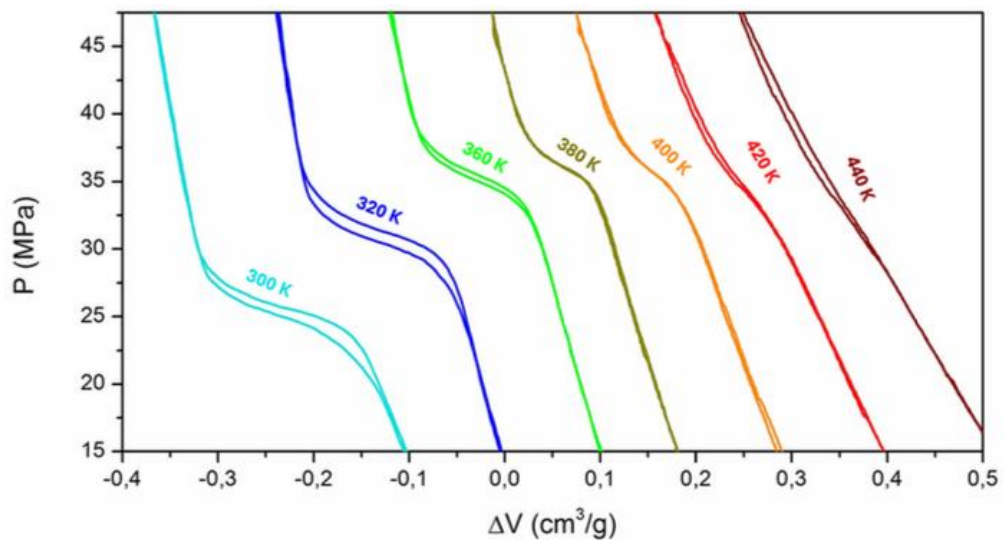
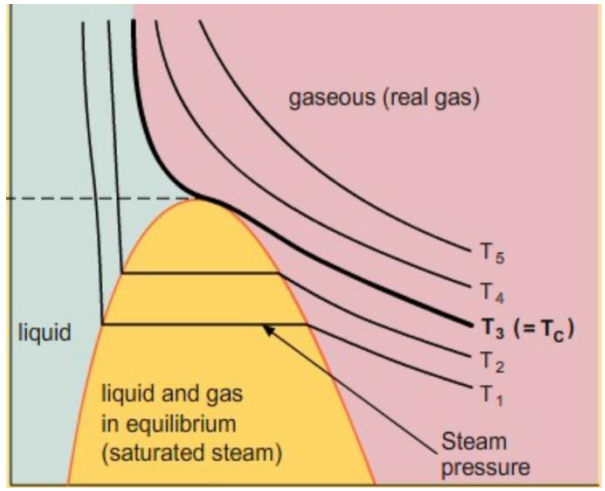
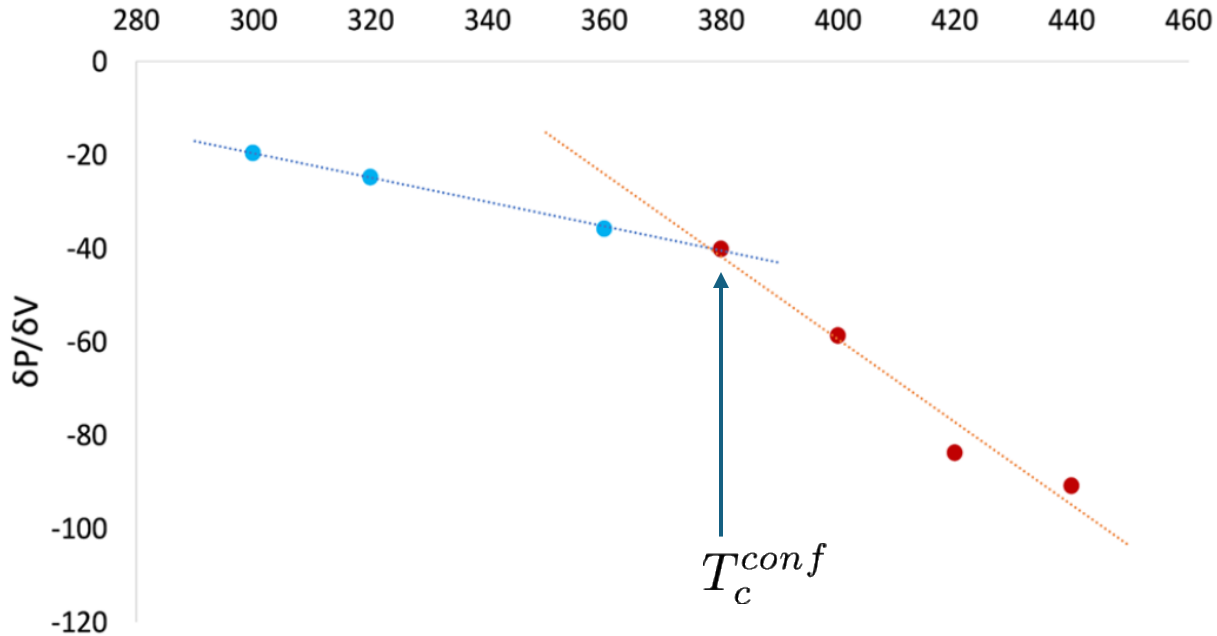
Confined, Low-T, supercritical water







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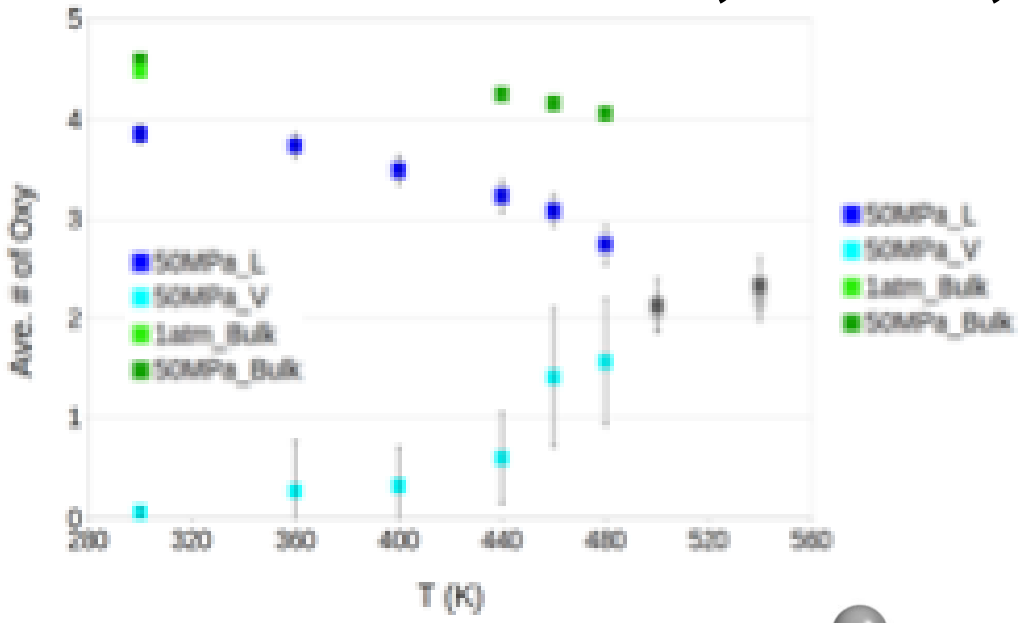
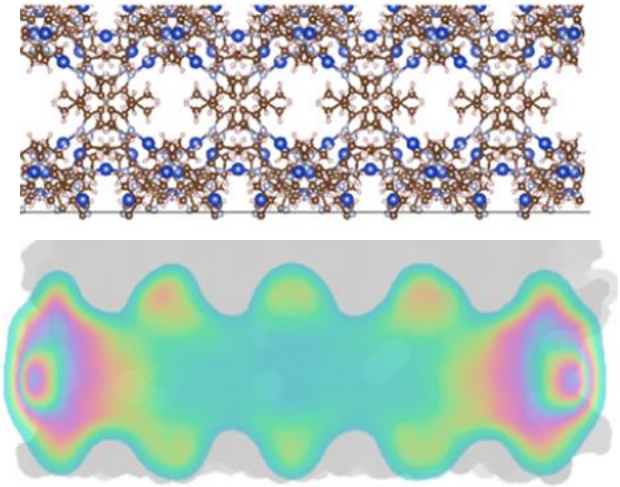
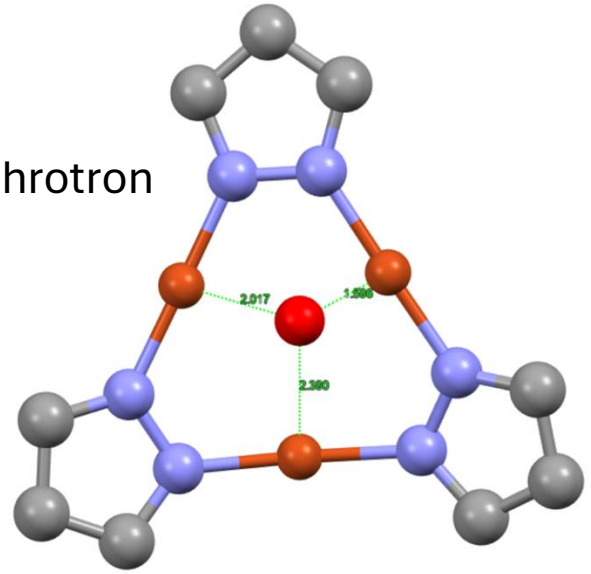
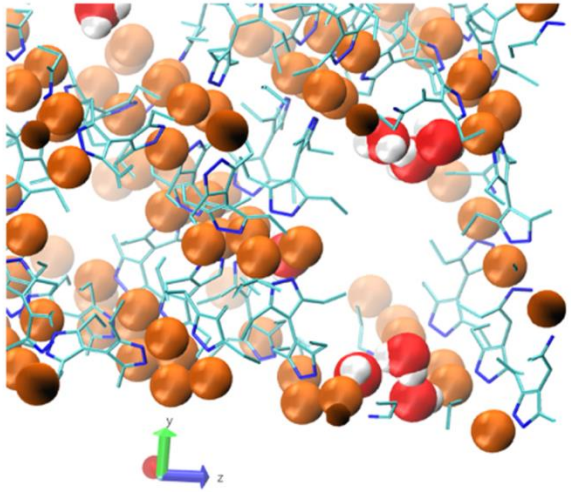


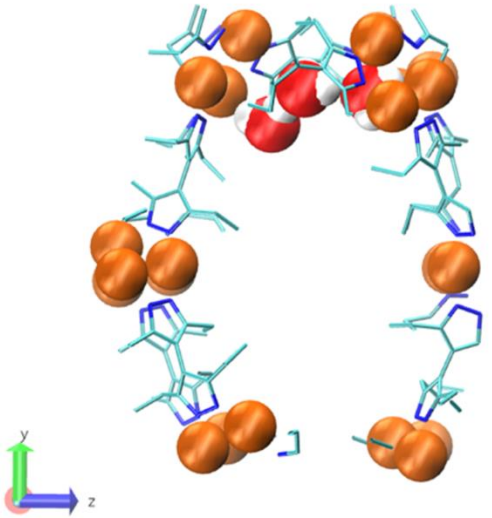


Synchrotron



Simulations





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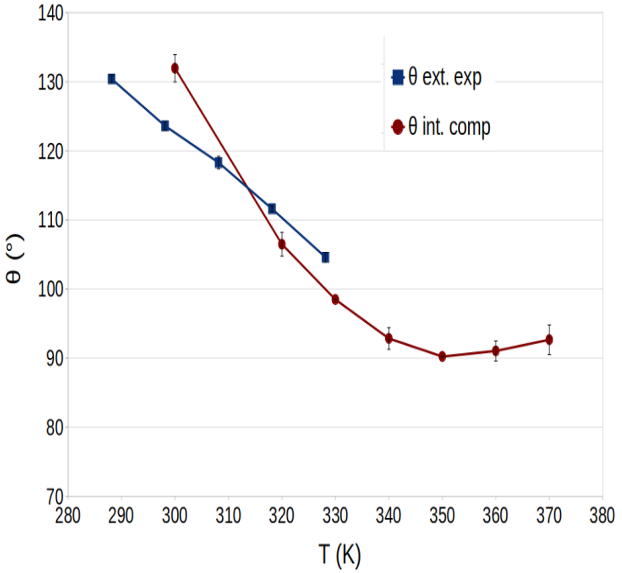
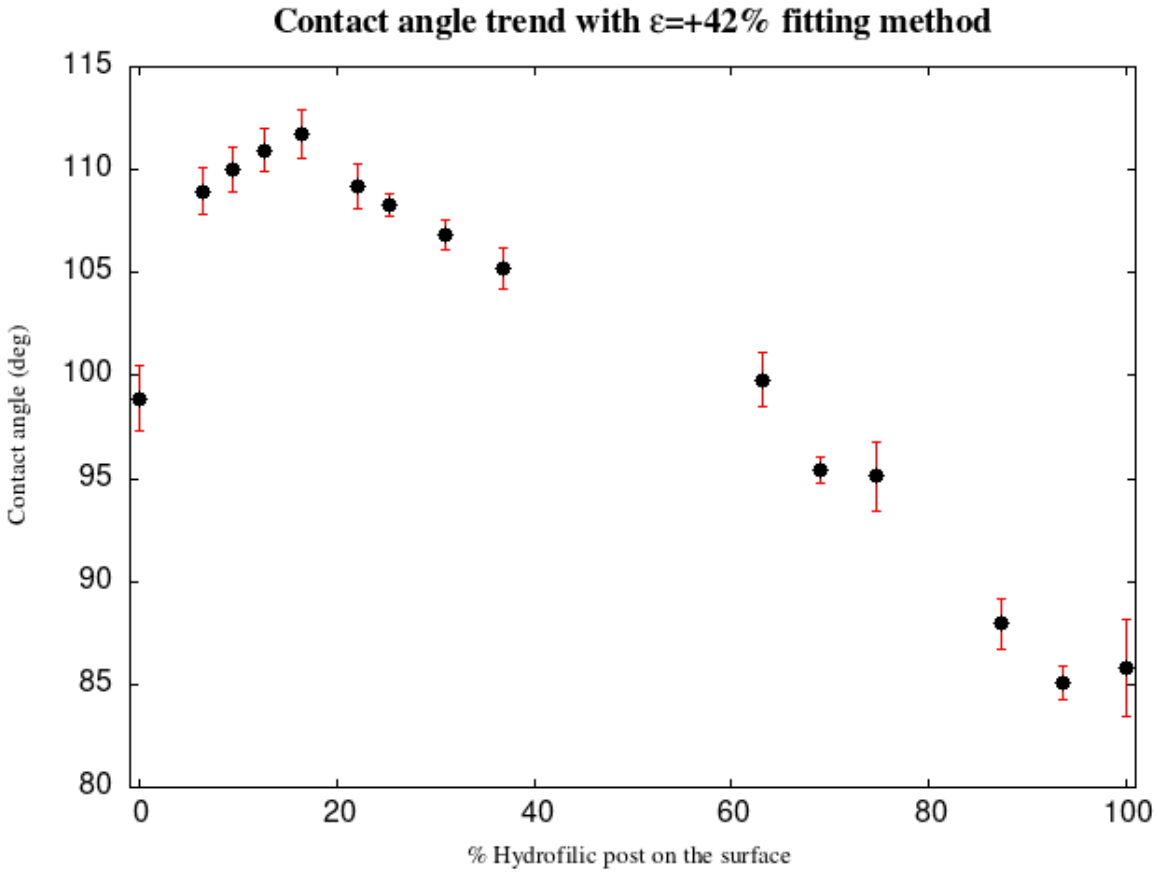
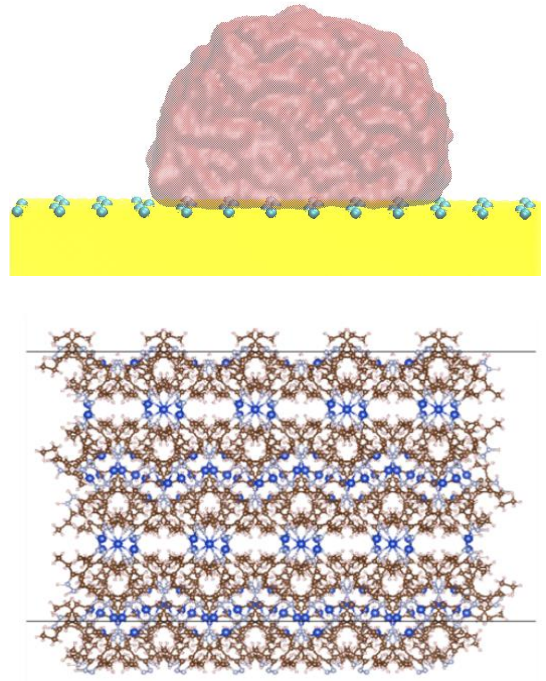
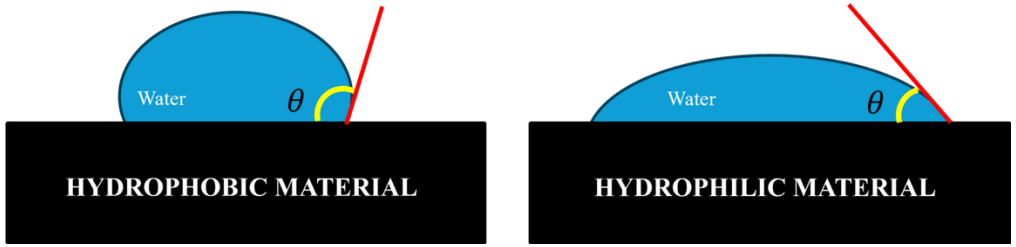
The unusual chemistry of Cu_2(tebpz): highly hydrophobic but with hydrophilic spots









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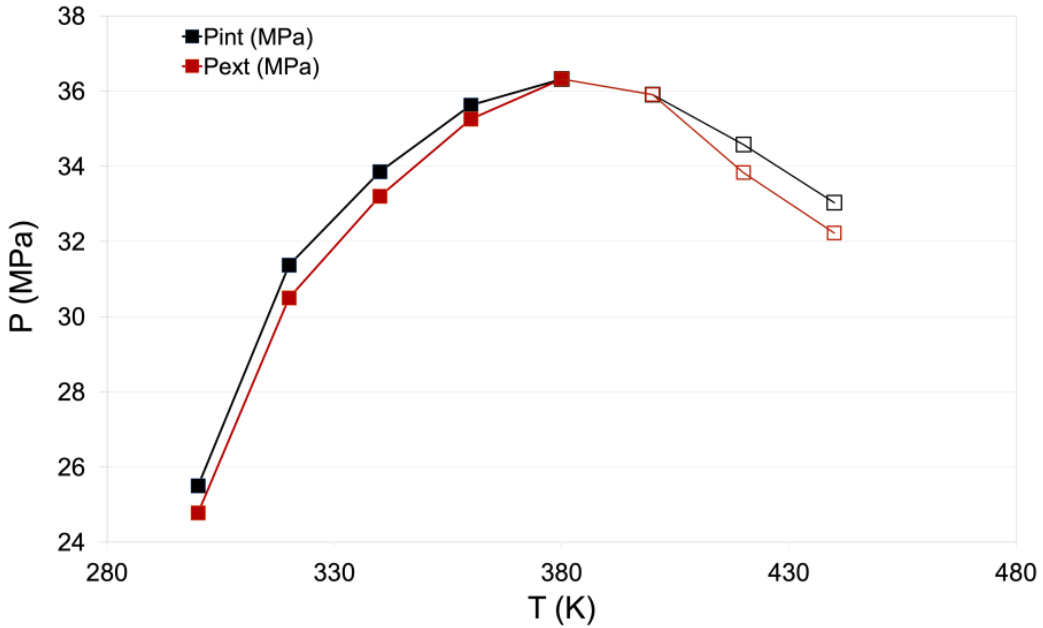
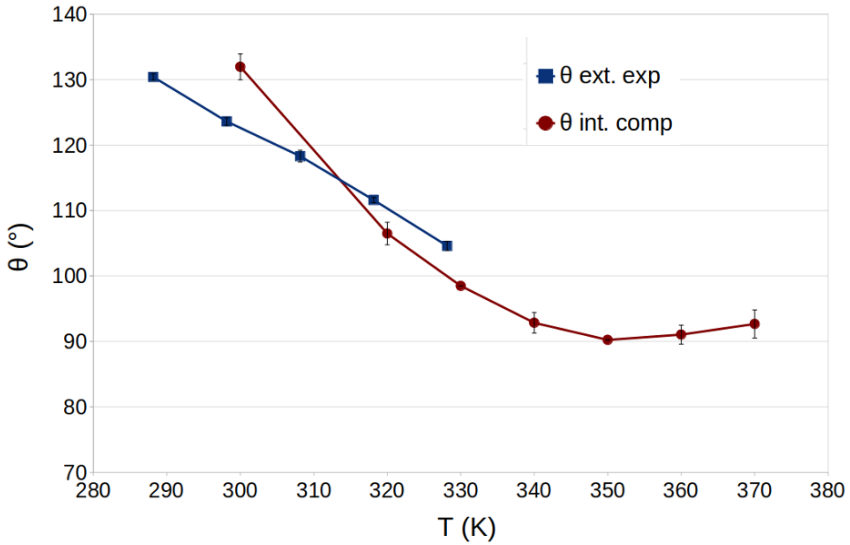
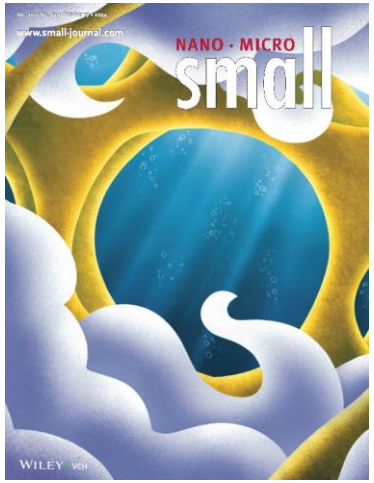
Effect of the temperature: reprised





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



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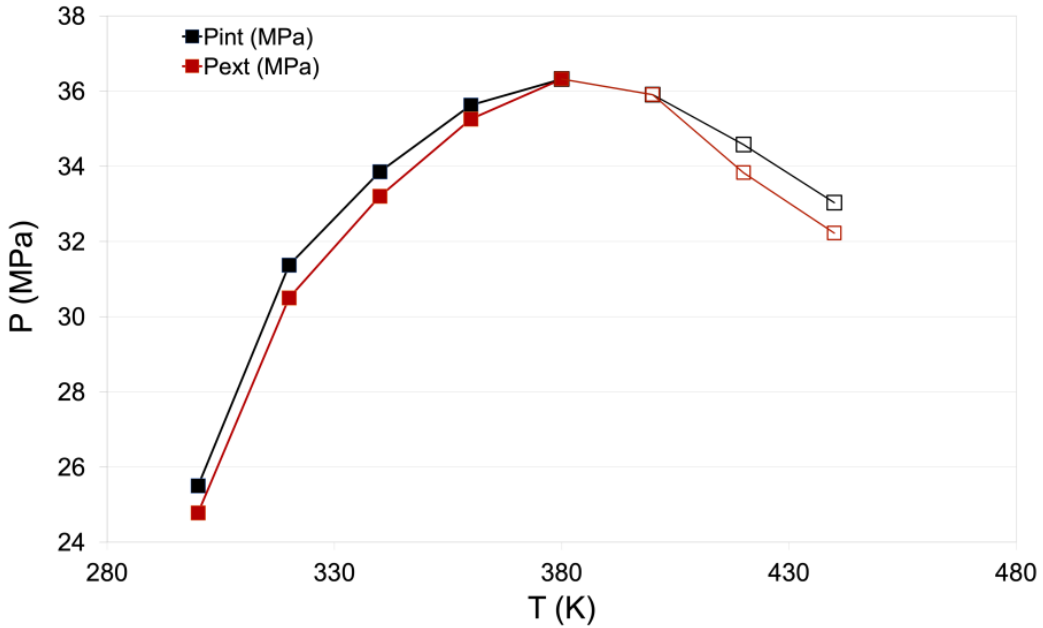
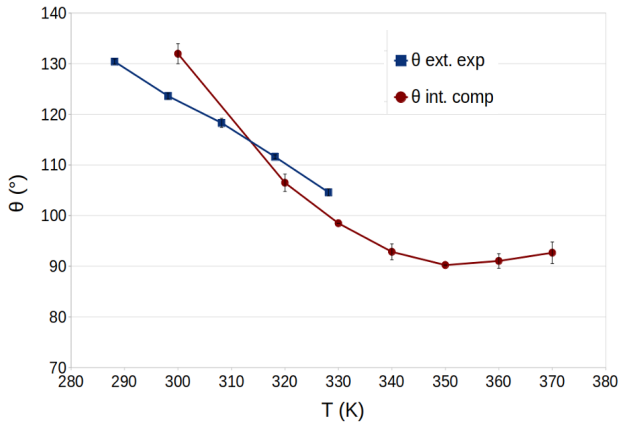
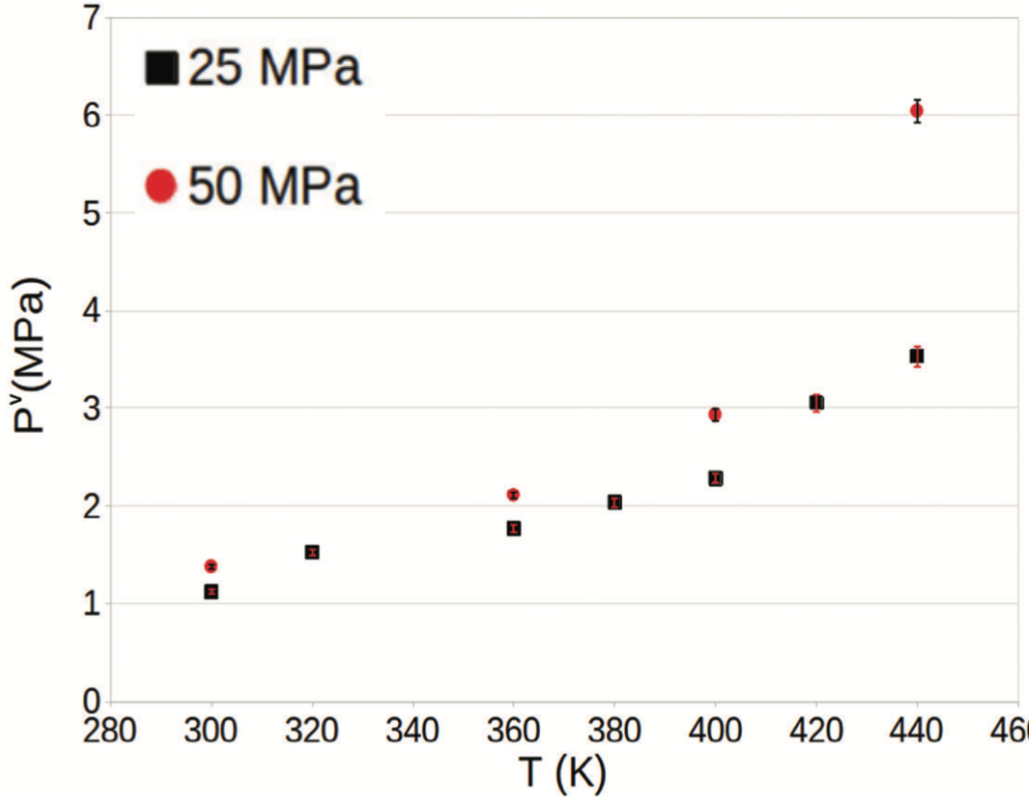
Effect of the temperature: reprised







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

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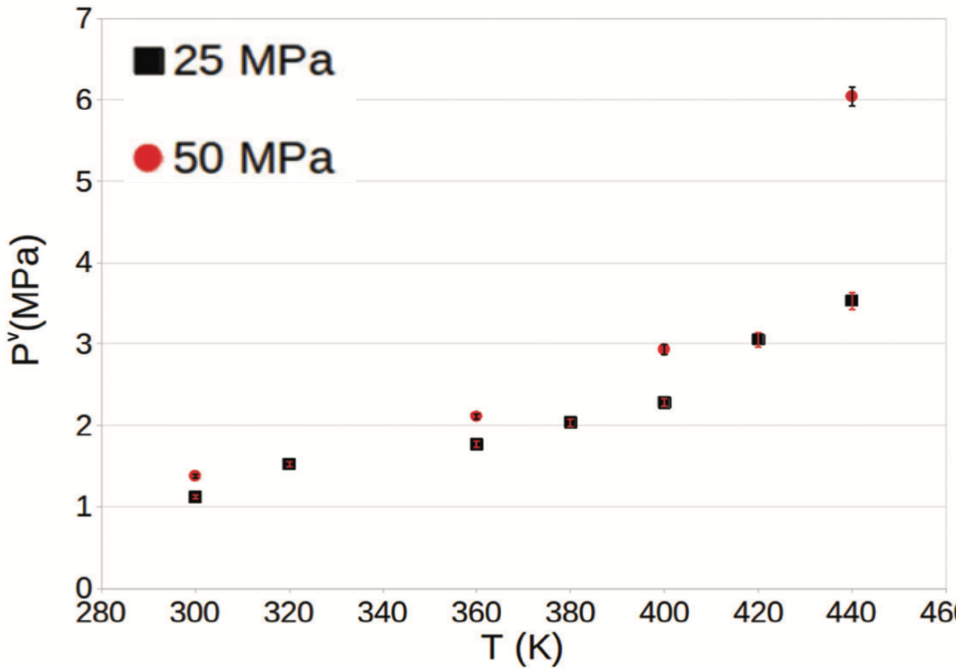
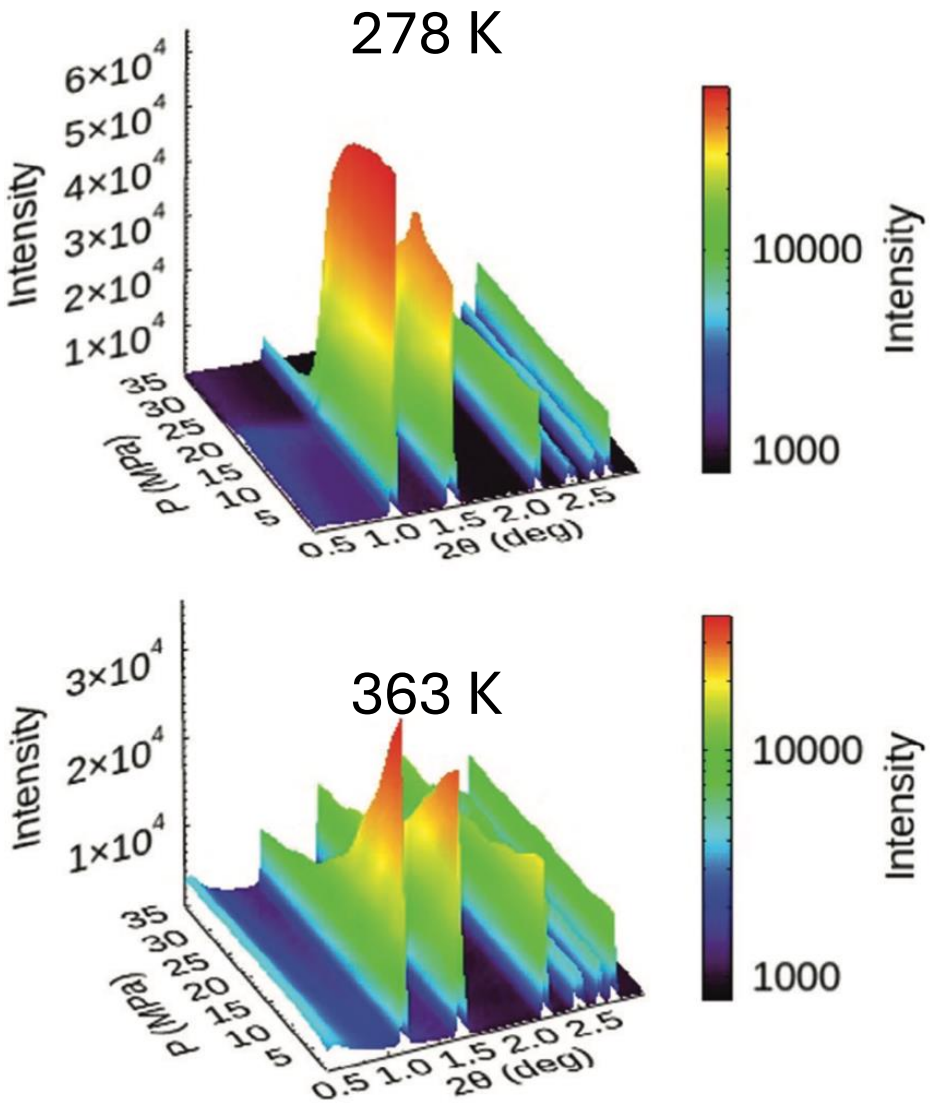
Effect of the temperature: reprised





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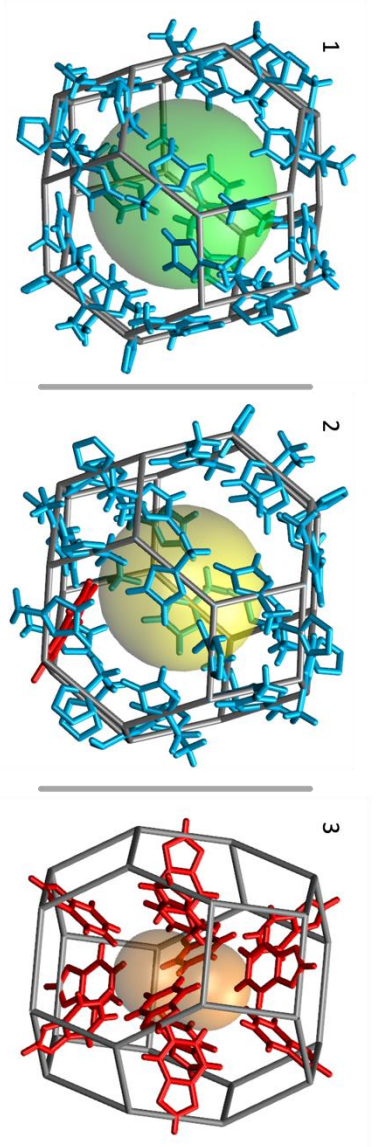
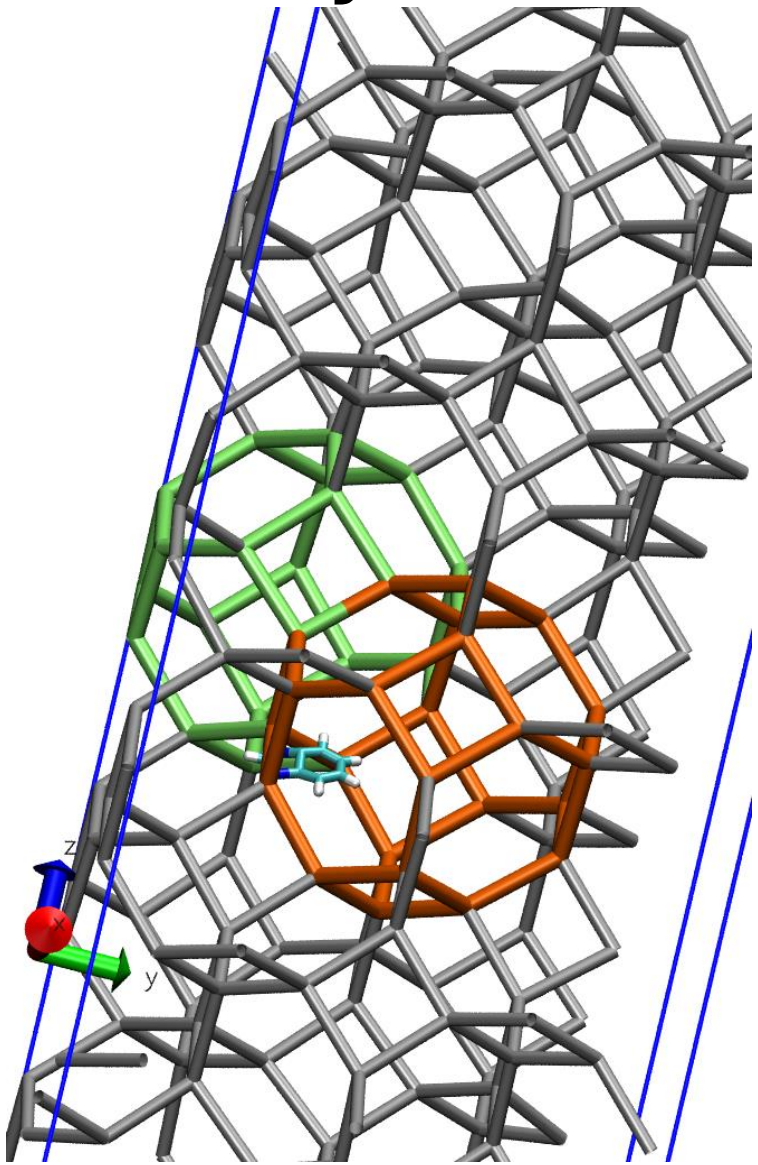
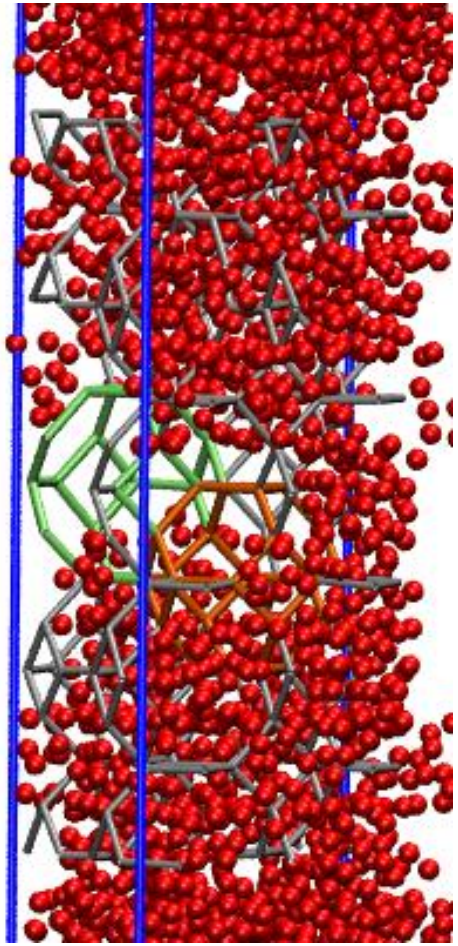
Tuning critical temperature by reducing the liquid density: the ZIF case







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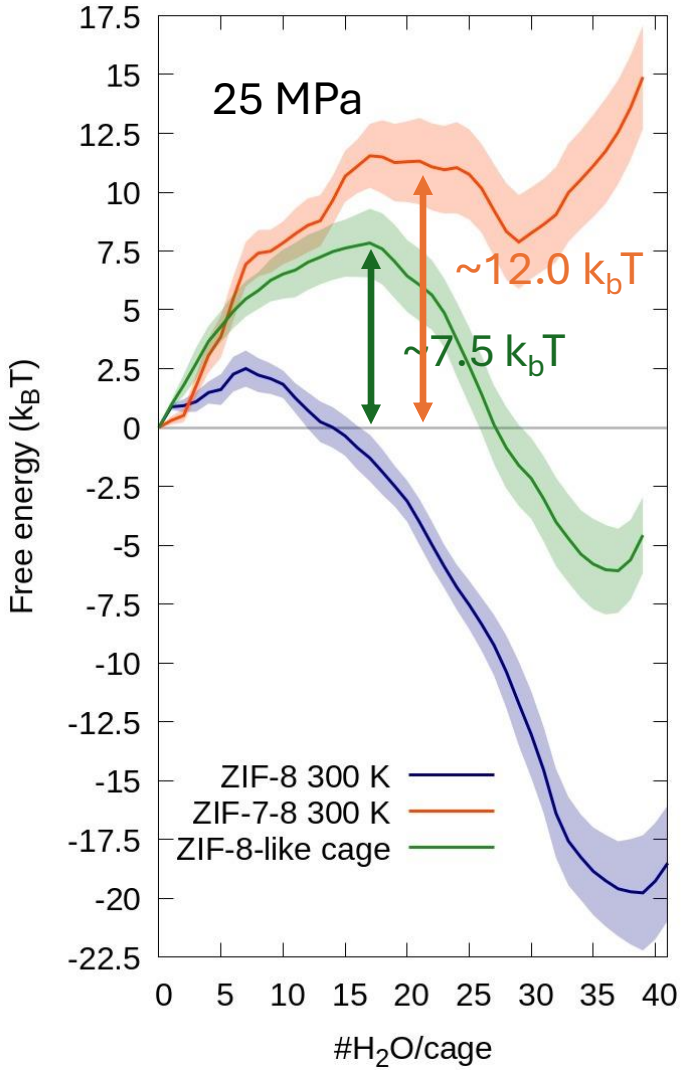
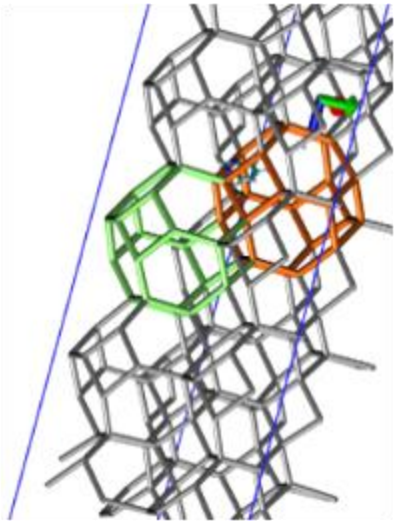
Tuning critical temperature by reducing the liquid density: the ZIF case



	$E^{\dagger}$ [k_BT]	at	E_{wet} [k_BT]	at	wet neigh.
ZIF-8	2.50	7	-19.78	39	5
ZIF-8-like-cage	7.84	17	-6.09	37	6
ZIF-7-8	11.55	17	7.88	29	5



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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.
- 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

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Acknowledgements

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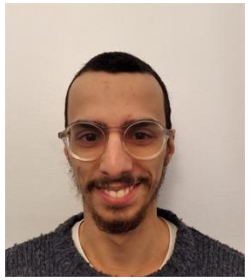
L. Johnson (CIC)



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Pawel Zajdel (USK)

E. Amayuelas (CIC)

M. Tortora (Sapienza)

M. Alvelli (UNIFE)

Alex Lowe(USK)

M. Chorazewski (USK)

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