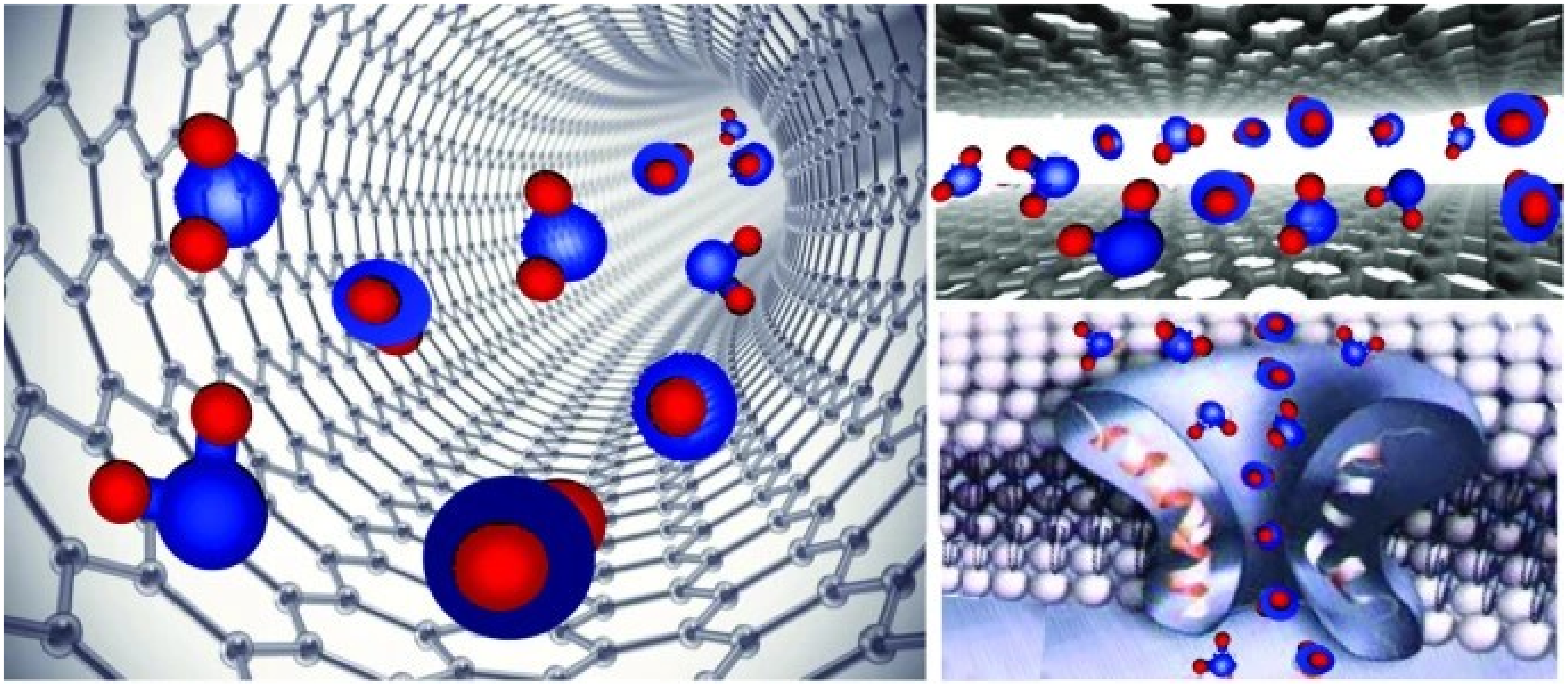
Nanoconfined Water



https://link.springer.com/article/10.1140/epje/s10189-021-00136-4

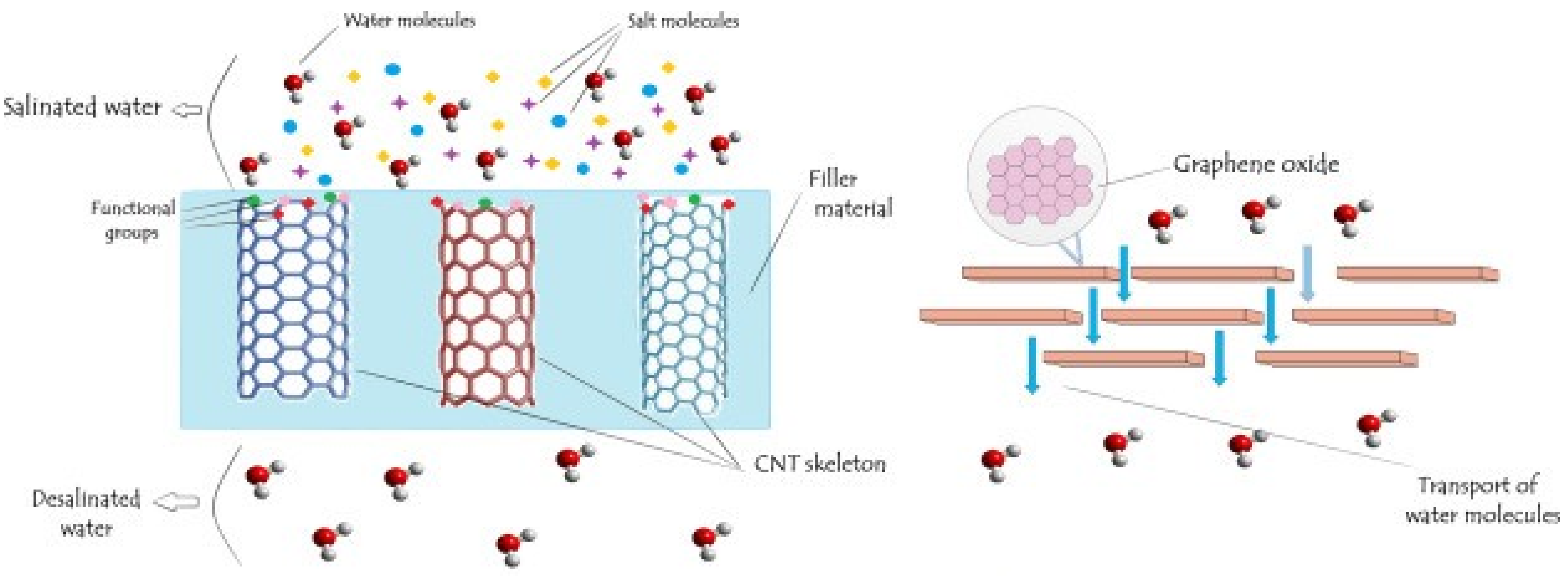
Summary

Phase Transitions-
Water Anomalies

Nanoconfined Water in
Solid State Materials

Nanoconfined Water in
Biology

Solid – Nanoconfined Water

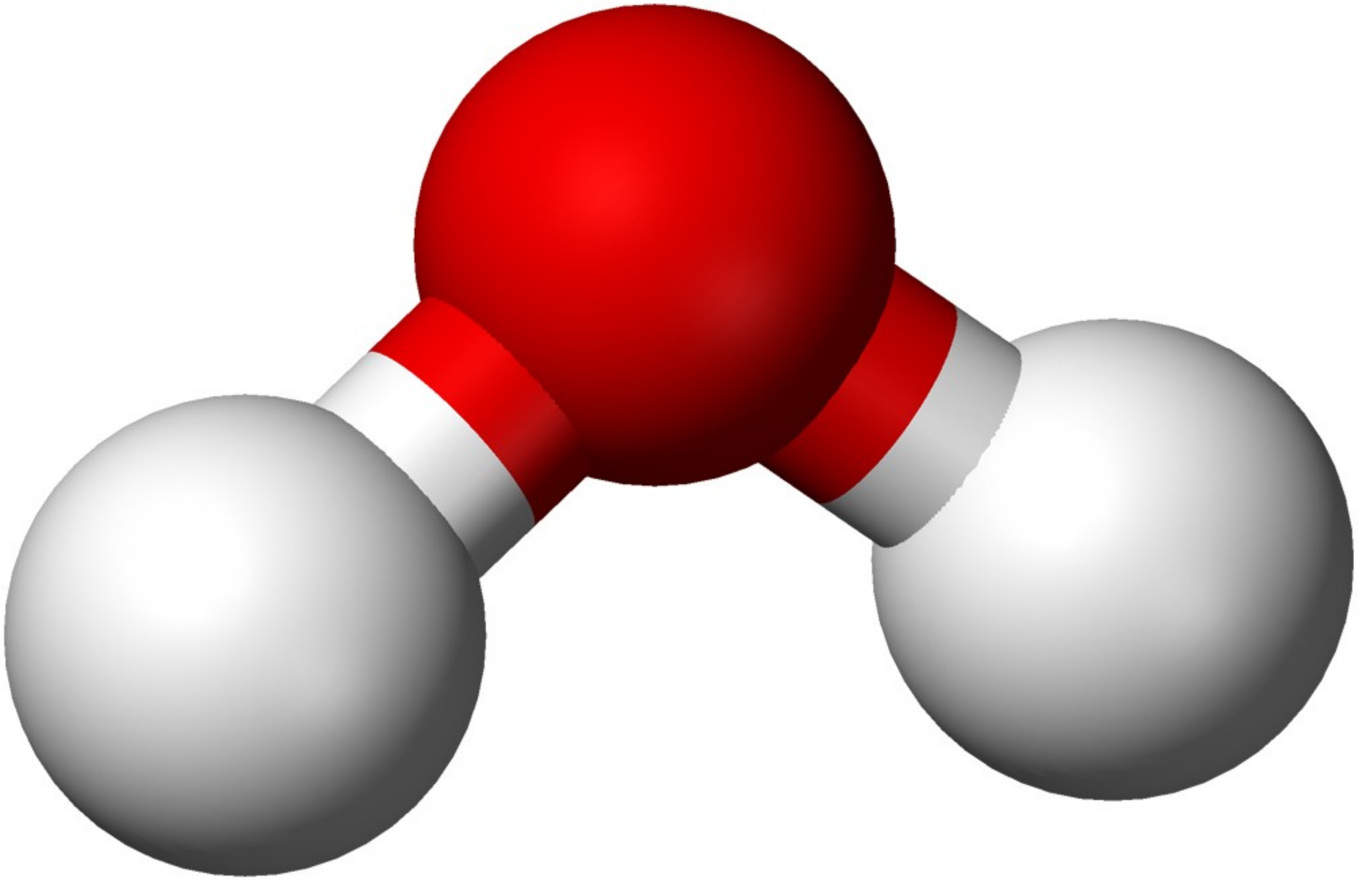


Transport of water molecules through CNT and graphene oxide

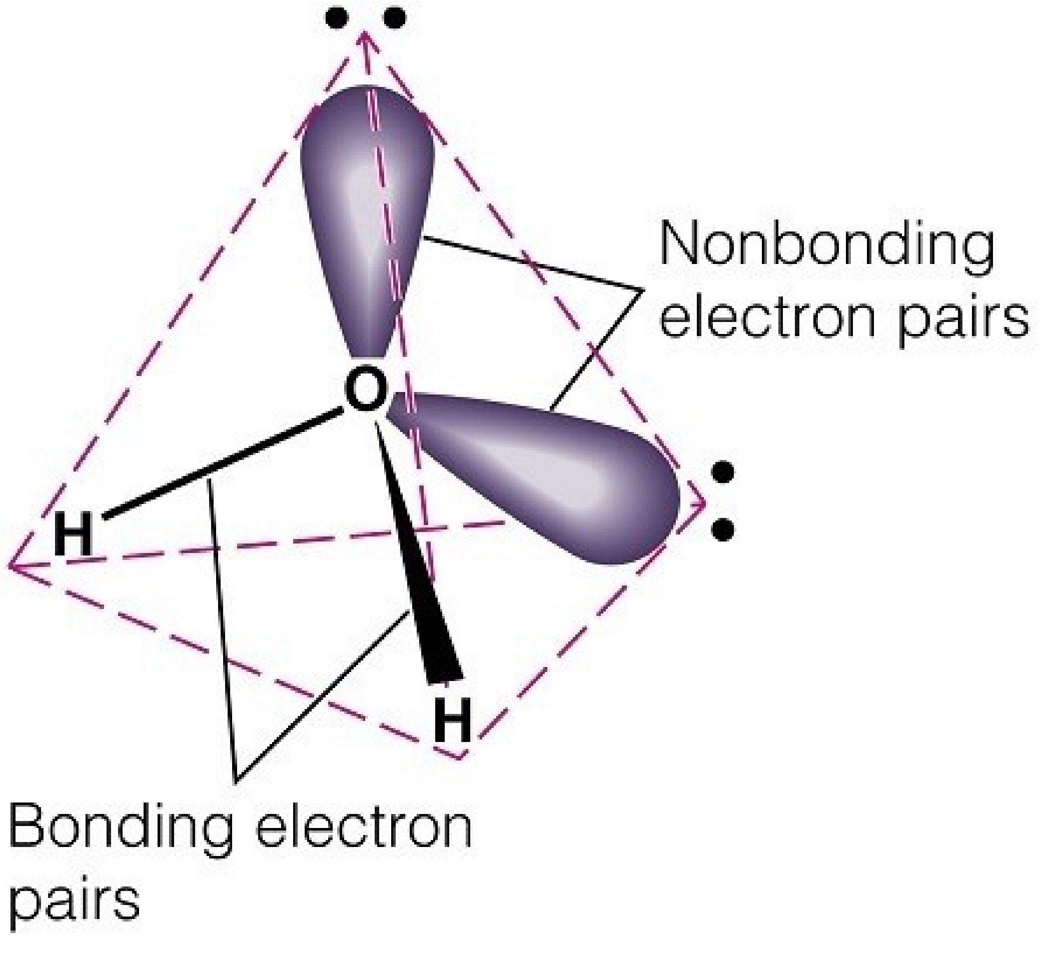
https://www.sciencedirect.com/science/article/abs/pii/B9780128139264000197

Review

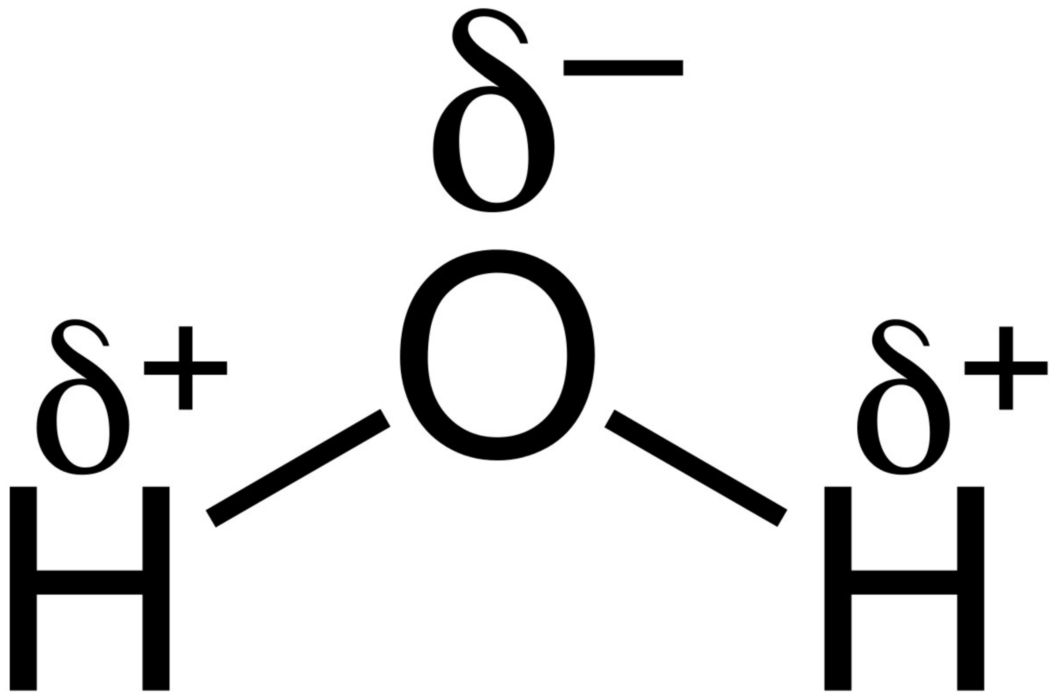
Water



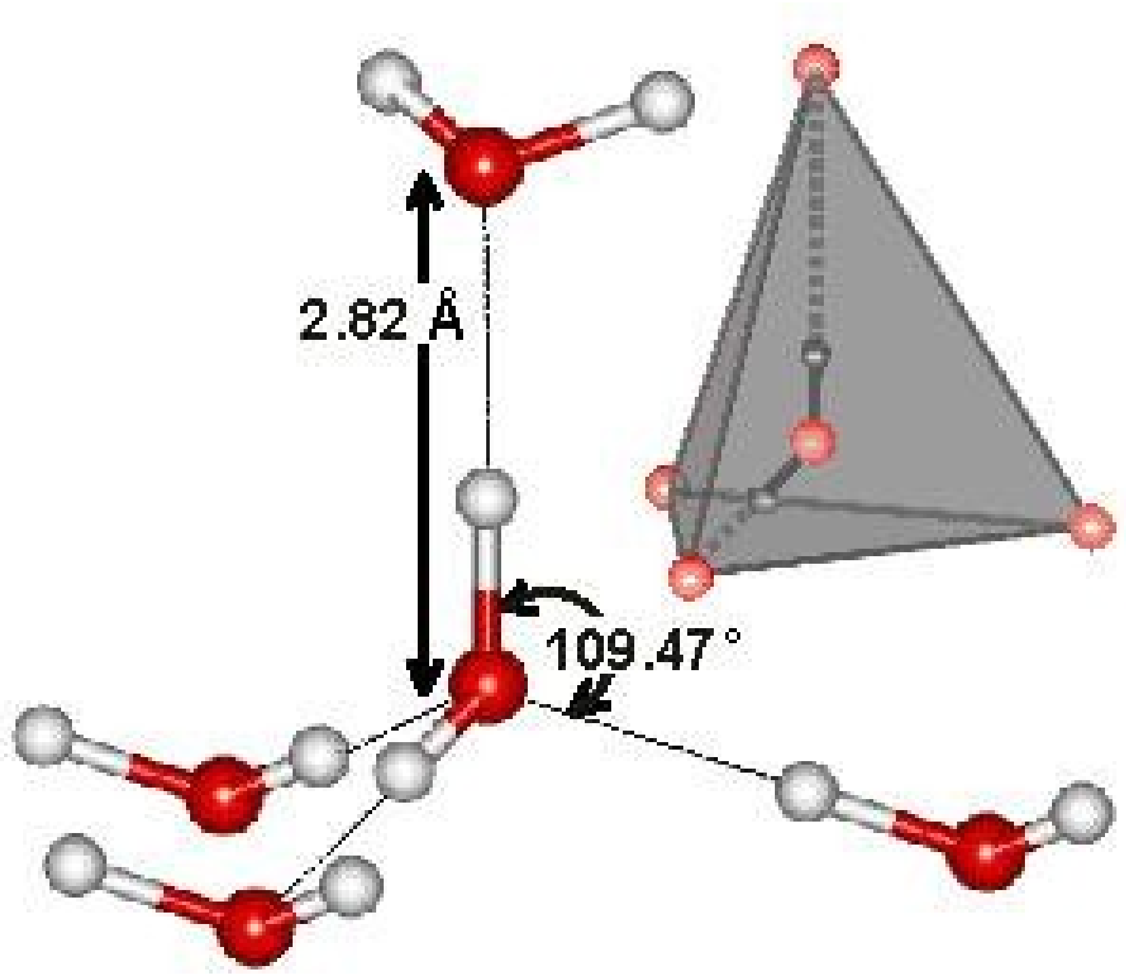
Water



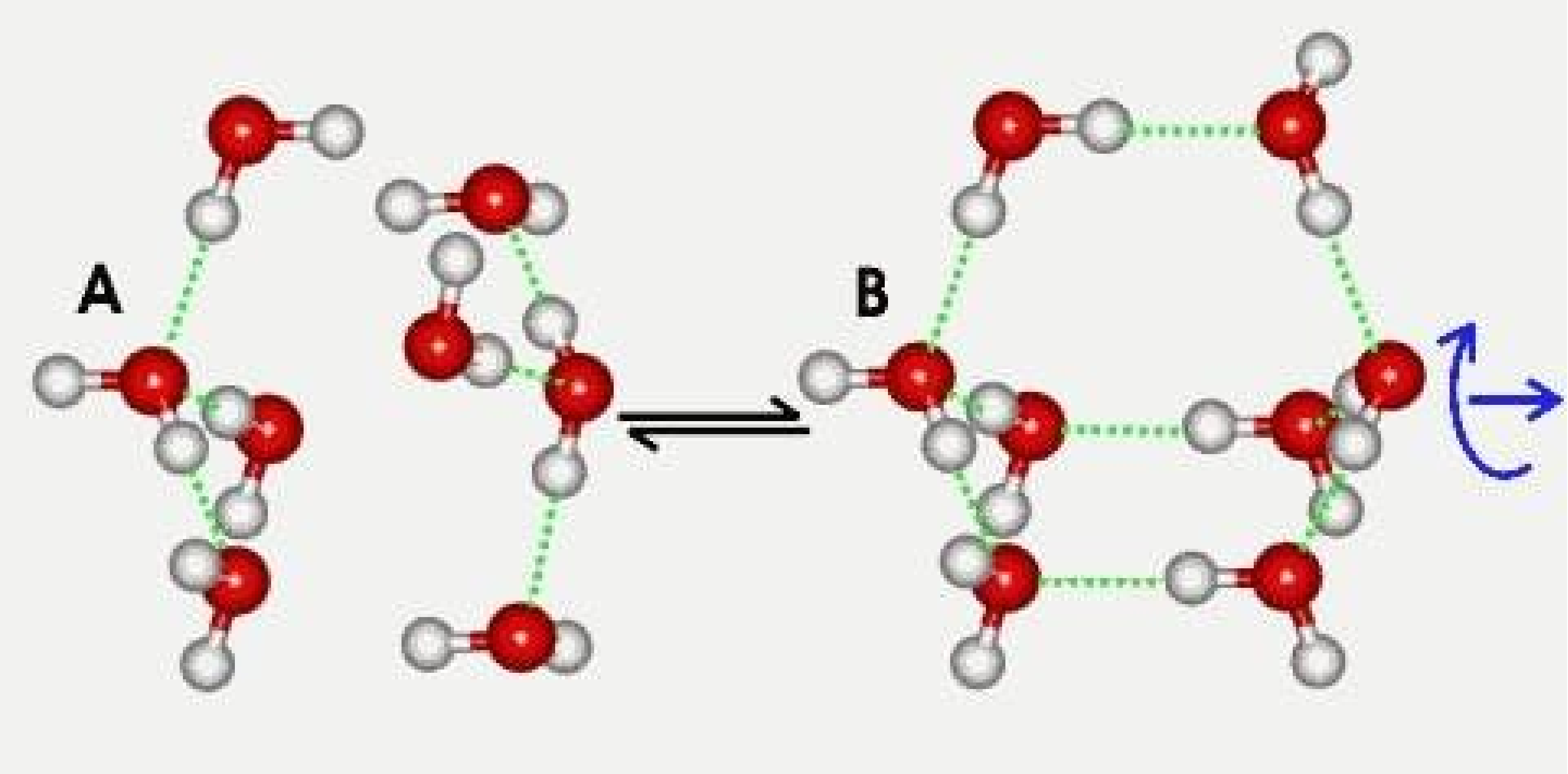
Water



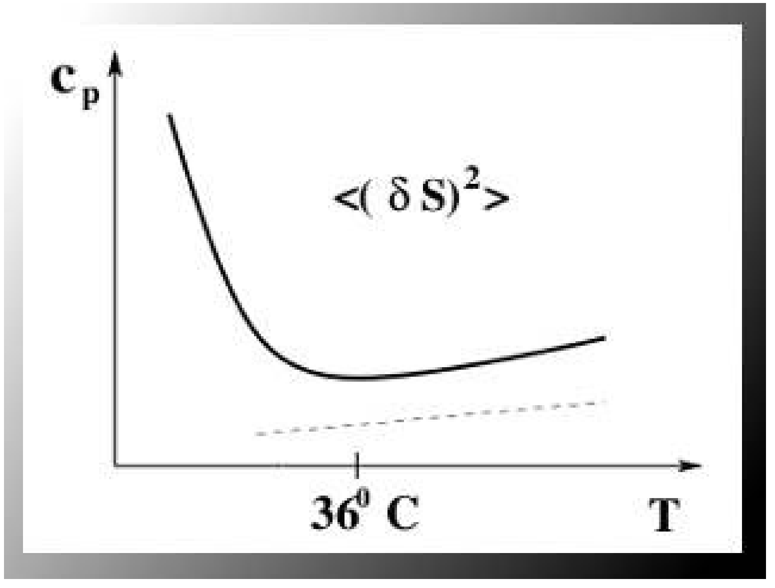
Hydrogen Bonds

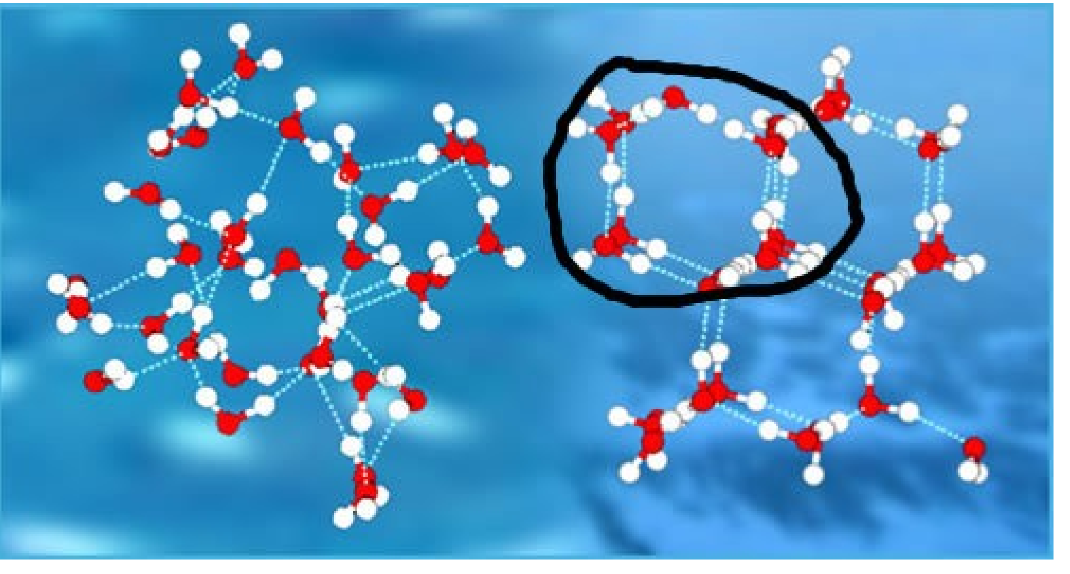


Tetramers Open and Closed

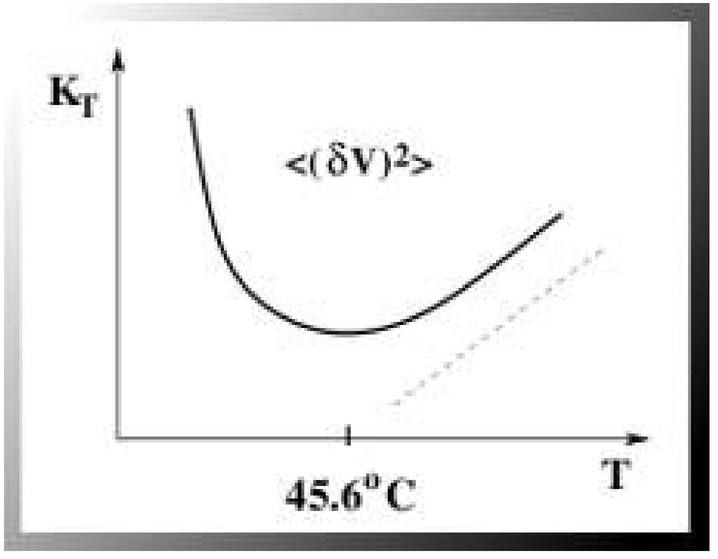


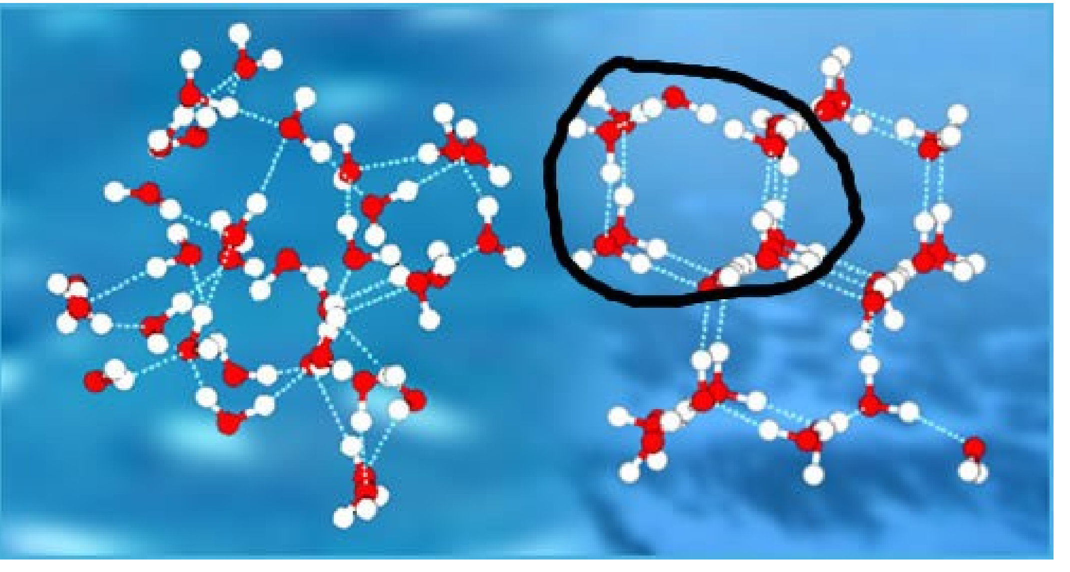
Specific Heat



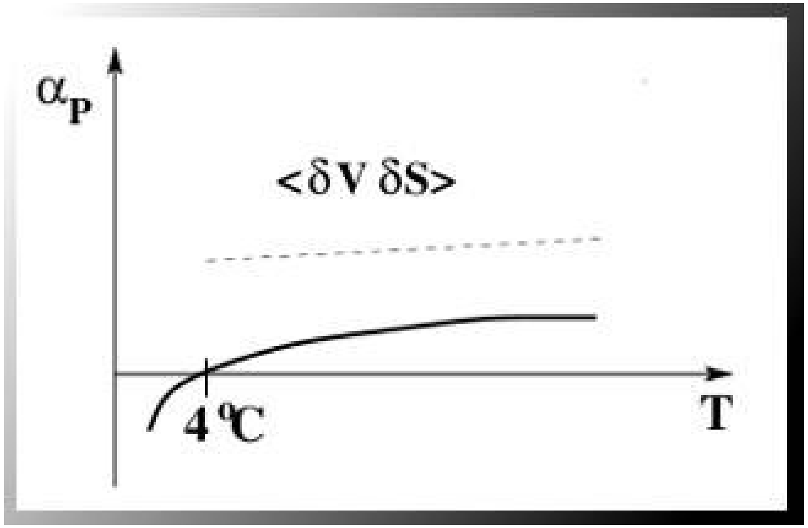


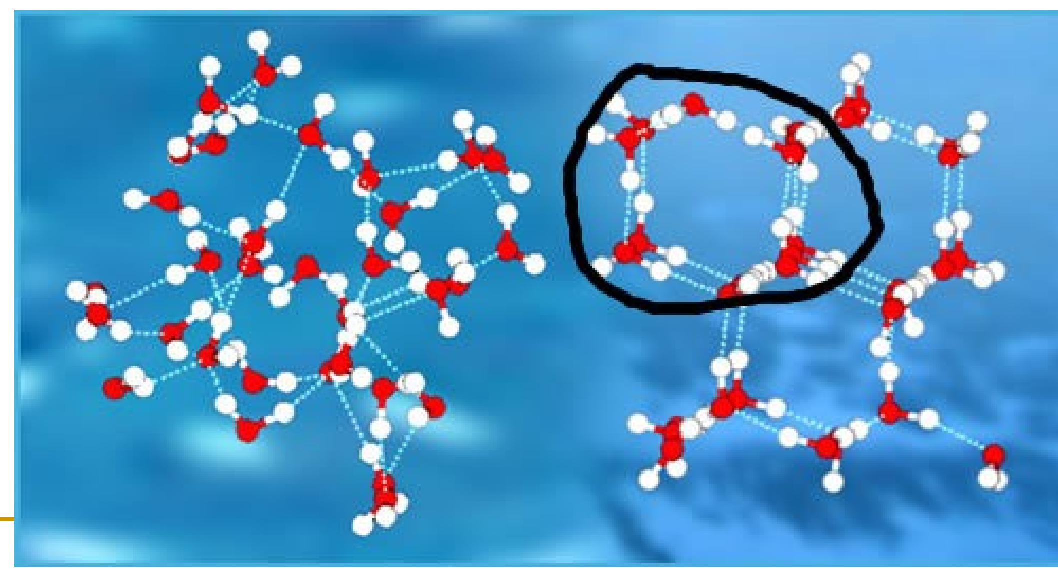
Compressibility



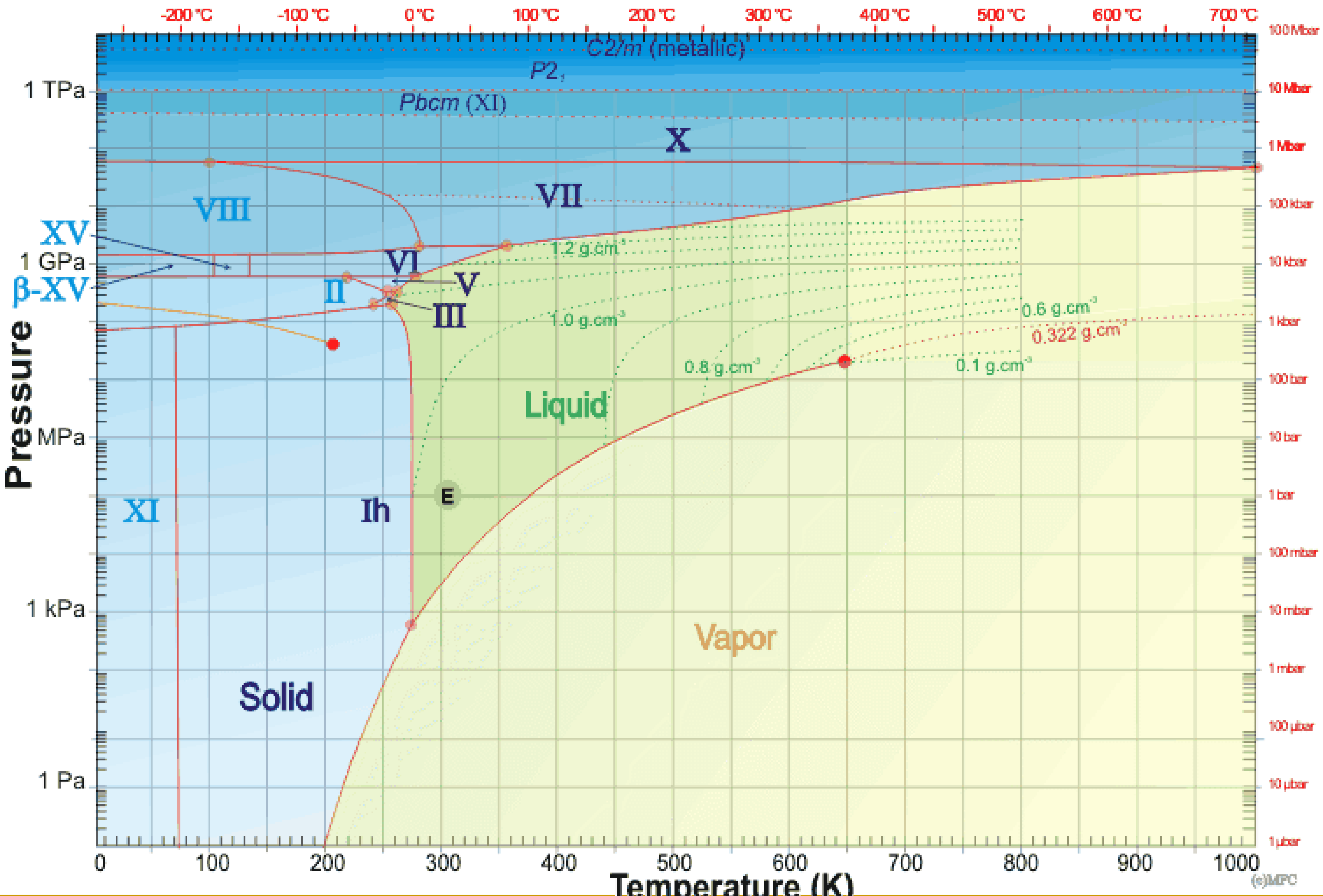


Thermal Expansion Coefficient





Water Phase Diagram



https://water.lsbu.ac.uk/water/water_phase_diagram.html

Diffusion

Diffusion

$$< \Delta^2 r(t) > = \frac{1}{N} \sum_{i=1}^{N} < [\underline{R}_i(t) - \underline{R}_i(0)]^2 >$$

$$< \Delta^2 r(t) > \sim 6Dt$$

$$C(\mathbf{e}) = \langle \mathbf{e}(t) \cdot \mathbf{e}(0) \rangle$$

Diffusion

$$\eta = \frac{V}{k_B T}\int_0^{\infty} \mathrm{d}t \langle P_{\alpha\beta}(t) P_{\alpha\beta}(0) \rangle,$$

$$P_{\alpha\beta} = \frac{1}{V}\left(\sum_{i=1}^{N} \frac{p_{i\alpha} p_{i\beta}}{m} + \sum_{i=1}^{N} \sum_{j>i}^{N} r_{ij\alpha} f_{ij\beta} \right), \qquad (2)$$

where $P_{\alpha\beta}$ is the stress tensor, $r_{ij} = |\vec{r}_i - \vec{r}_j|$, $f_{ij} = -\partial U(r_{ij})/\partial r_{ij}$ and $\alpha, \beta \in (x,y,z)$ denotes Cartesian components.

$$D = \frac{k_B T}{6\pi\eta\sigma^3};$$

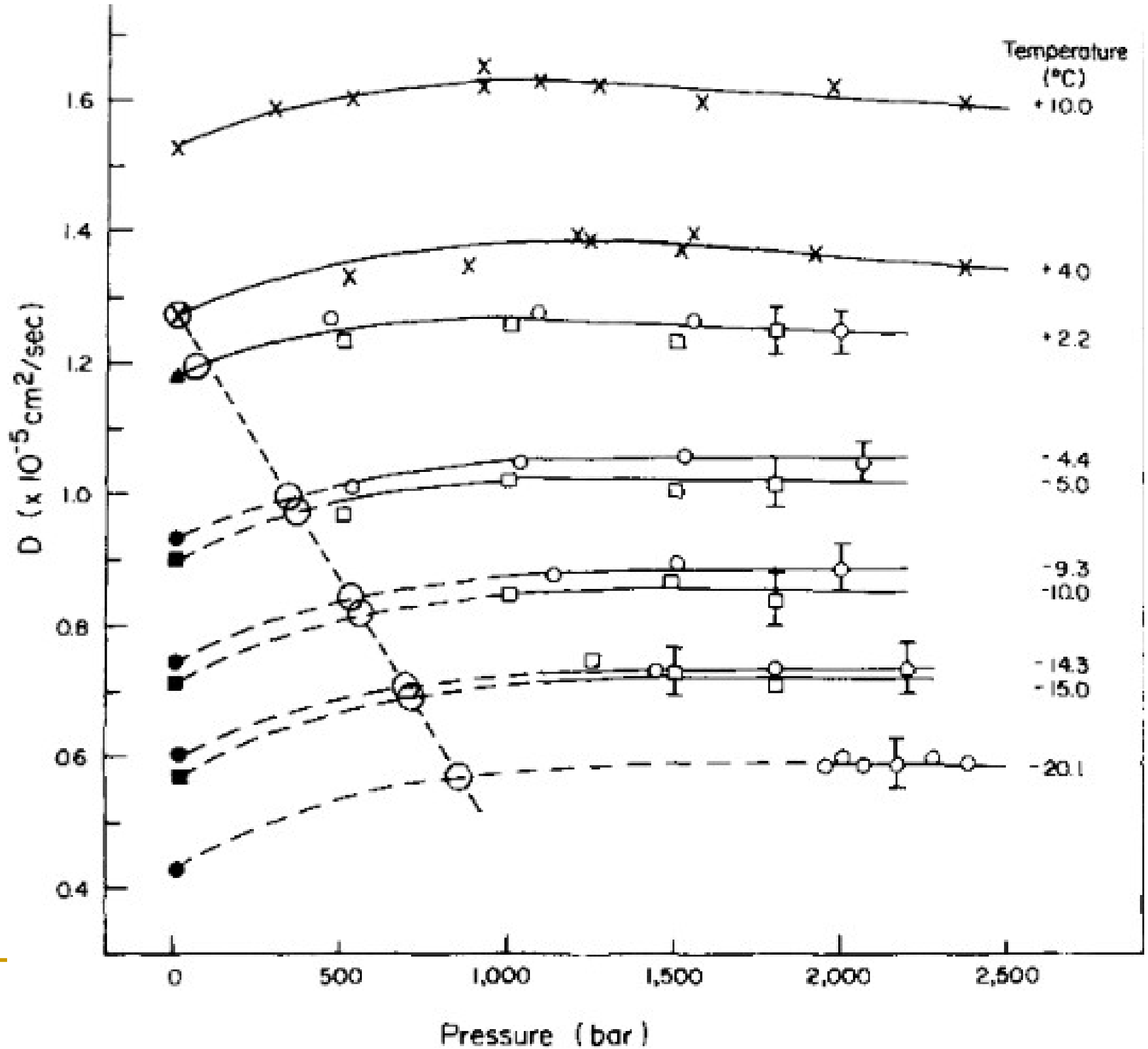
$$< \Delta^2 r(t) > \sim 6Dt$$

Diffusion Anomaly Water

Angell, Finch, Bach JCP 65, 3063 (76)

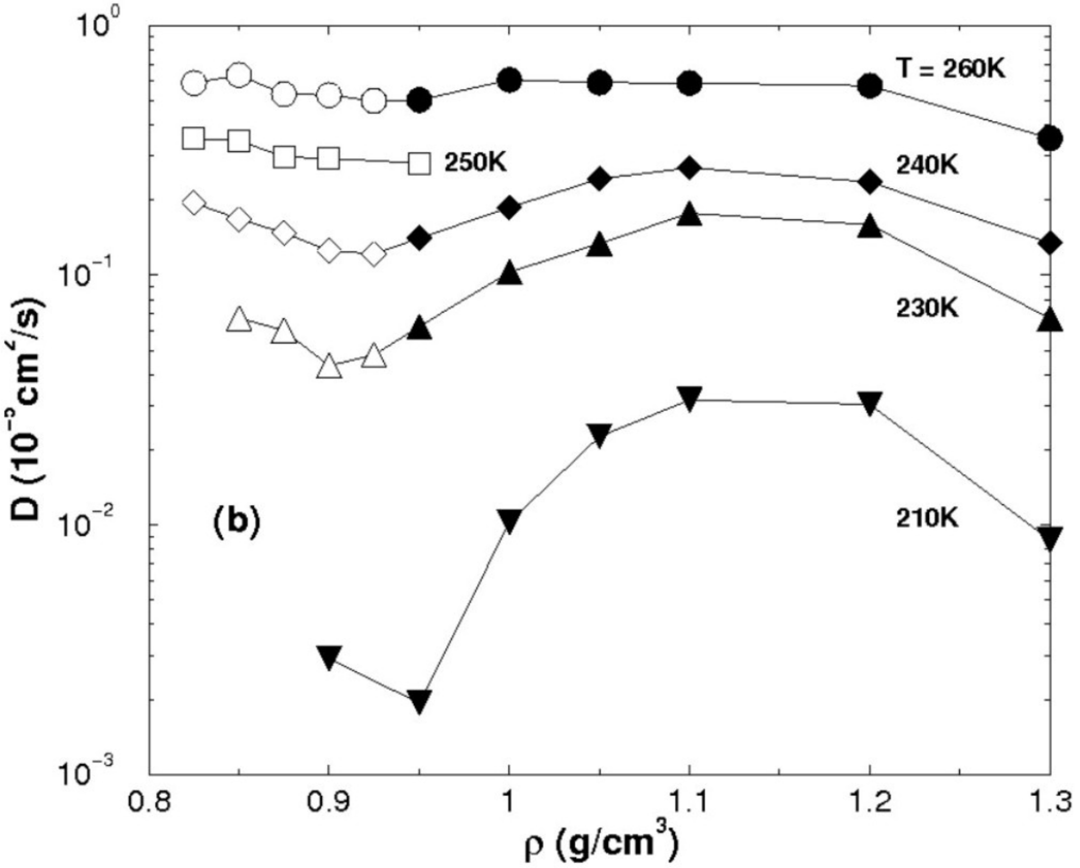
$$<\Delta^2 r(t)> = \frac{1}{N}\sum_{i=1}^{N} <[\underline{R}_i(t) - \underline{R}_i(0)]^2>$$

$$<\Delta^2 r(t)> \sim 6Dt$$



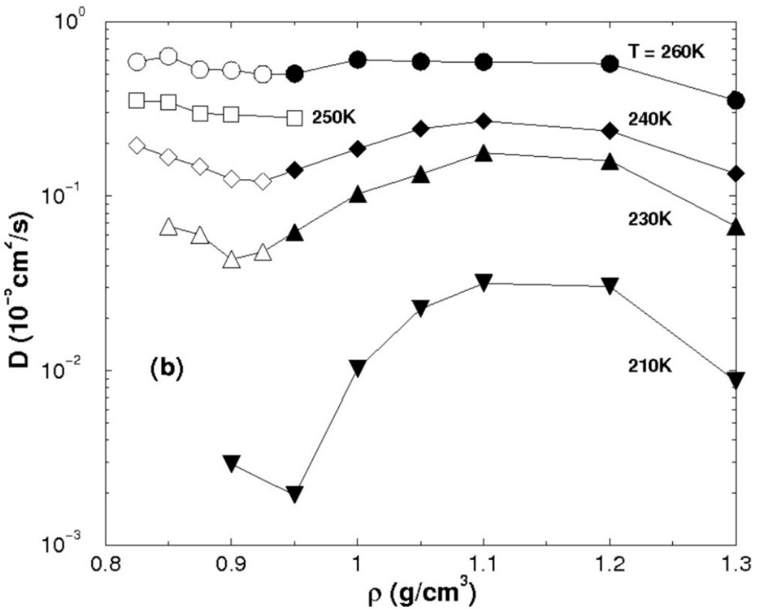
SPC/E Diffusion

Netz, Starr, Stanley, Barbosa JCP 115, 344 (01)



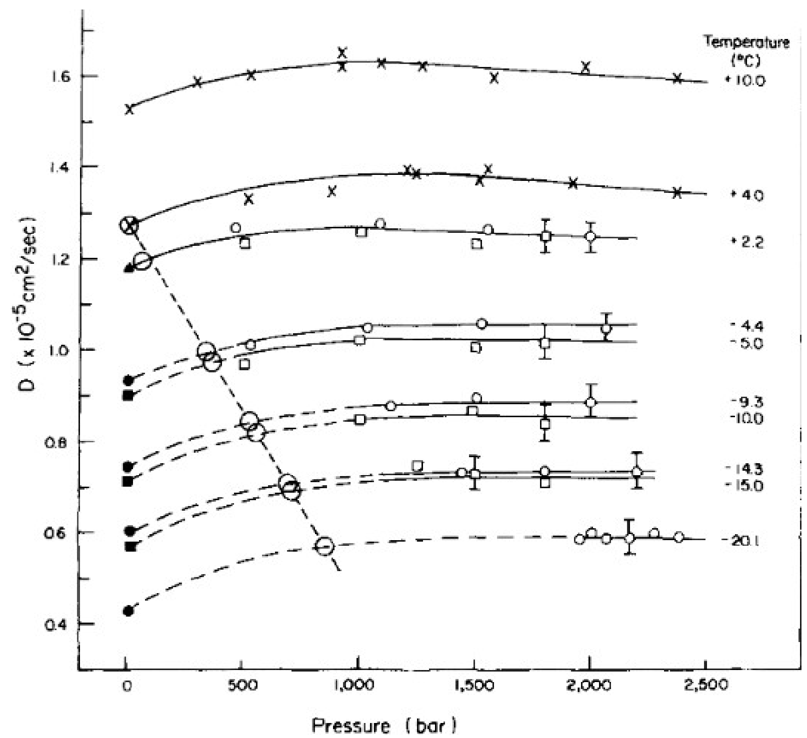
SPC/E Diffusion

Netz, Starr, Stanley, Barbosa JCP 115, 344 (01)



Atomistic Potential

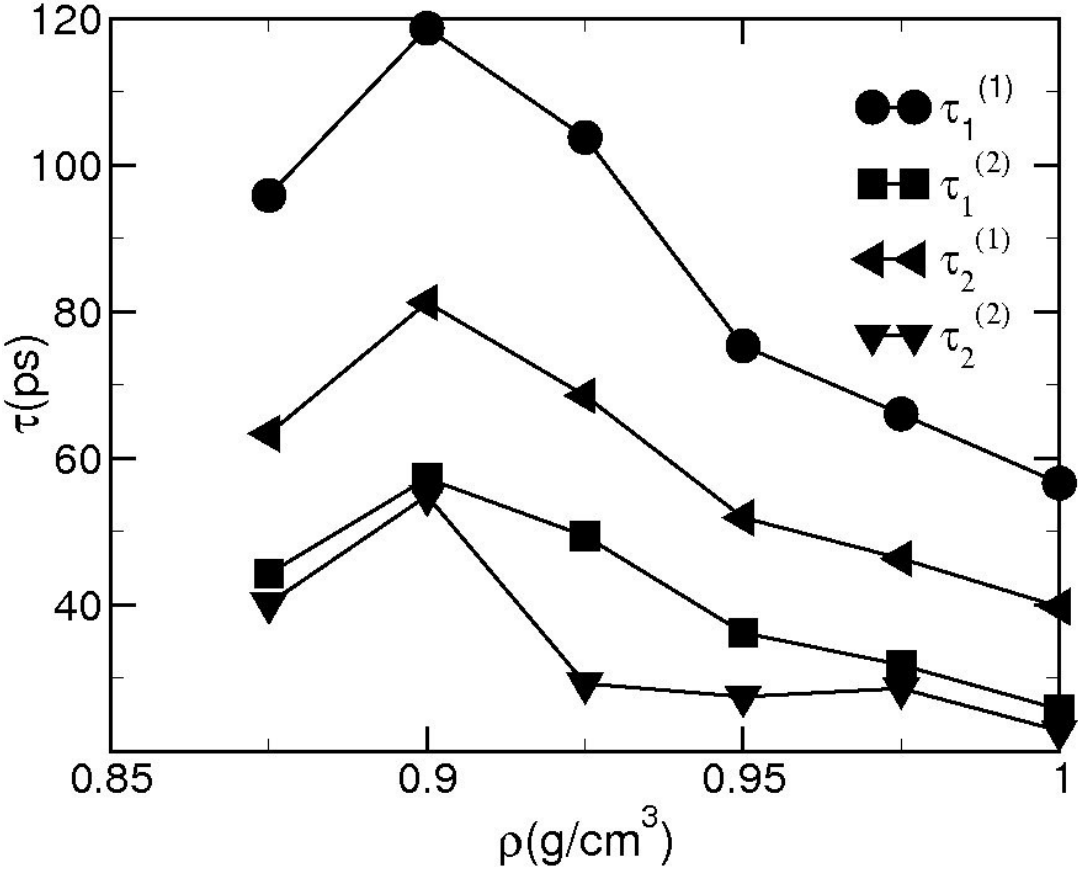
Experiment



SPC/E Rotational Diffusion

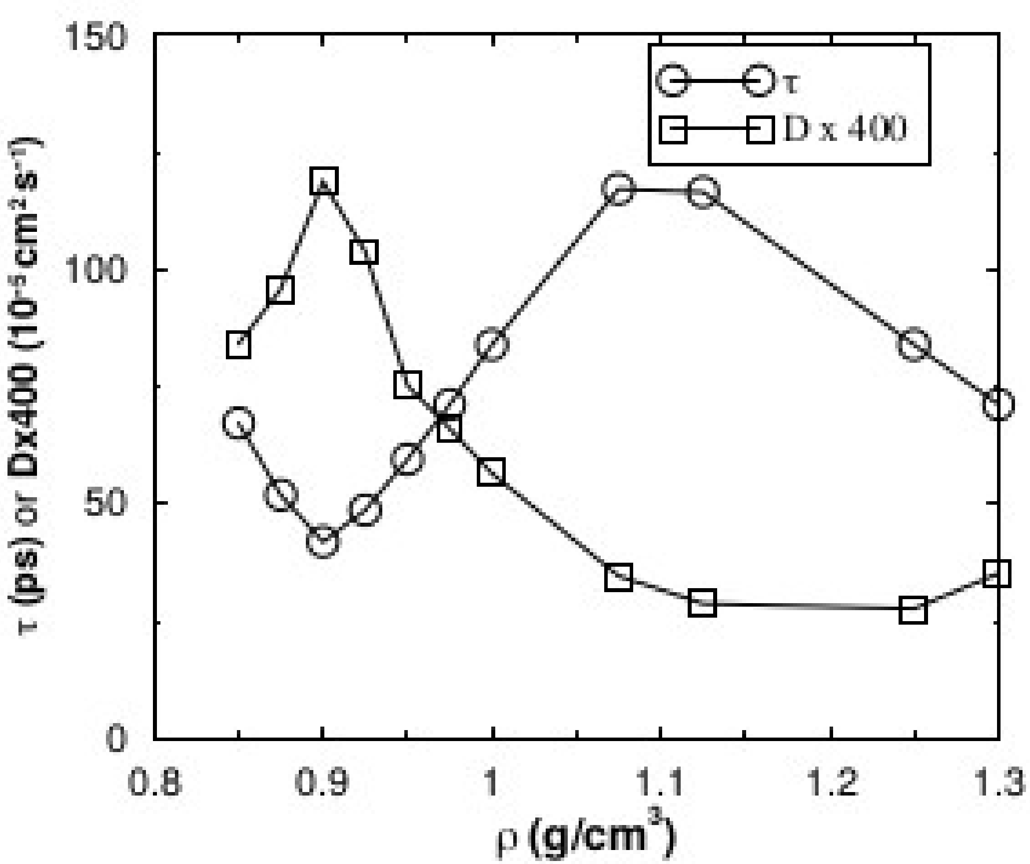
Netz, Starr, Barbosa, Stanley, JML 101, 159-168 (02)
Mazza,Giovanbaptista, Stanley, Starr, PRE 76, 31203 (07)

$$C(\mathbf{e}) = \langle \mathbf{e}(t) \cdot \mathbf{e}(0) \rangle$$



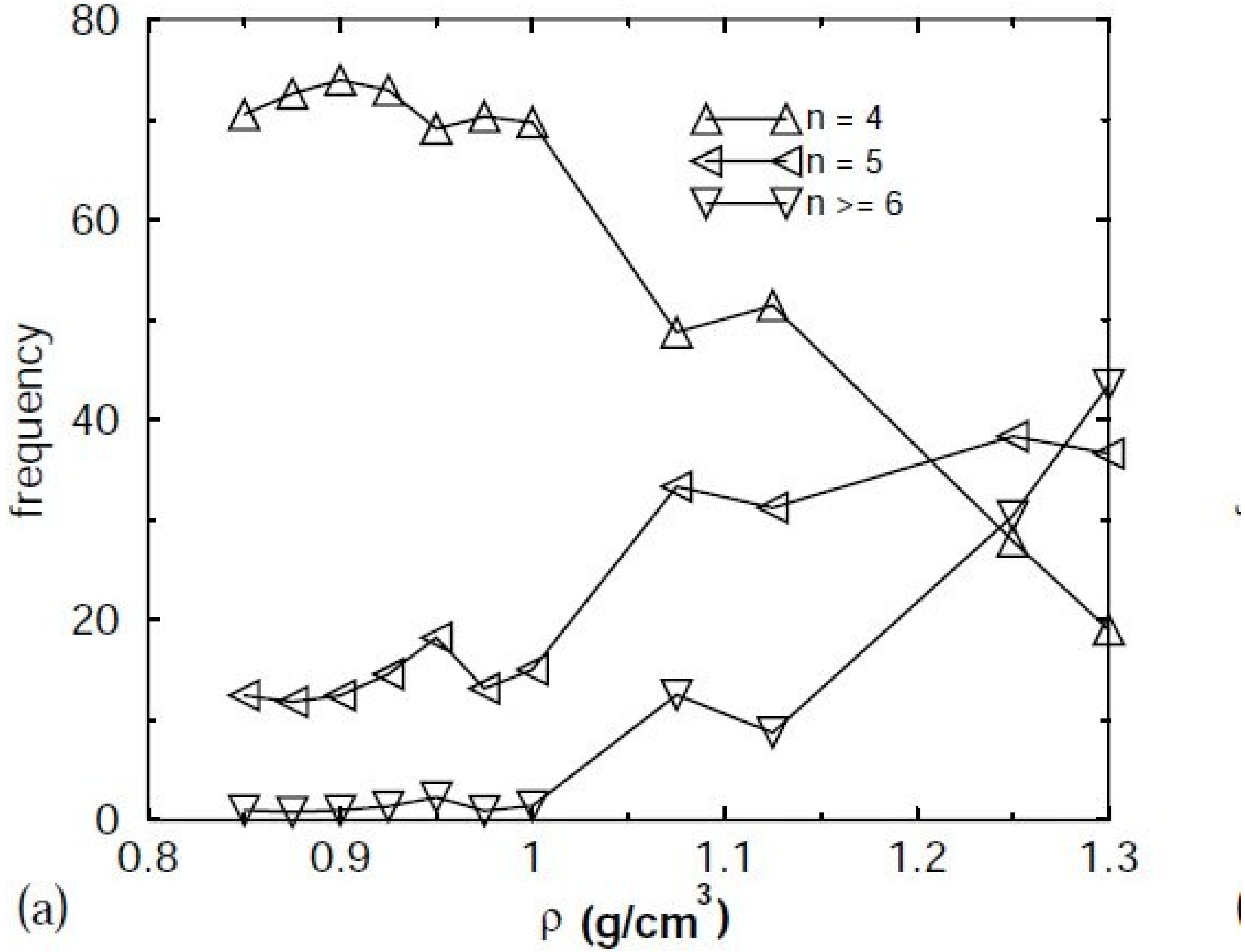
SPC/E Number of Neighbors

Netz, Starr, MCB and Stanley, Physica A 314, 470 (2002)

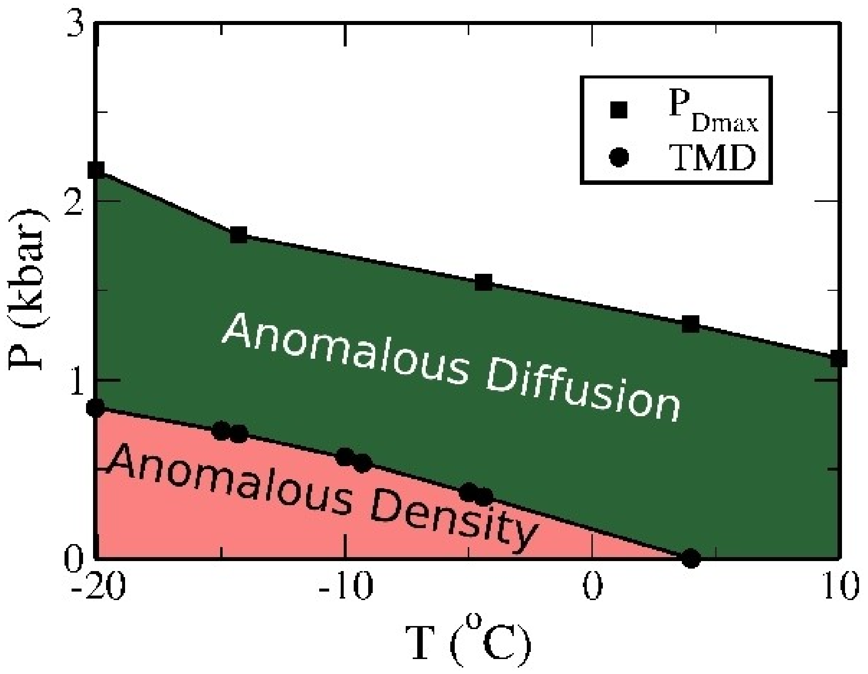


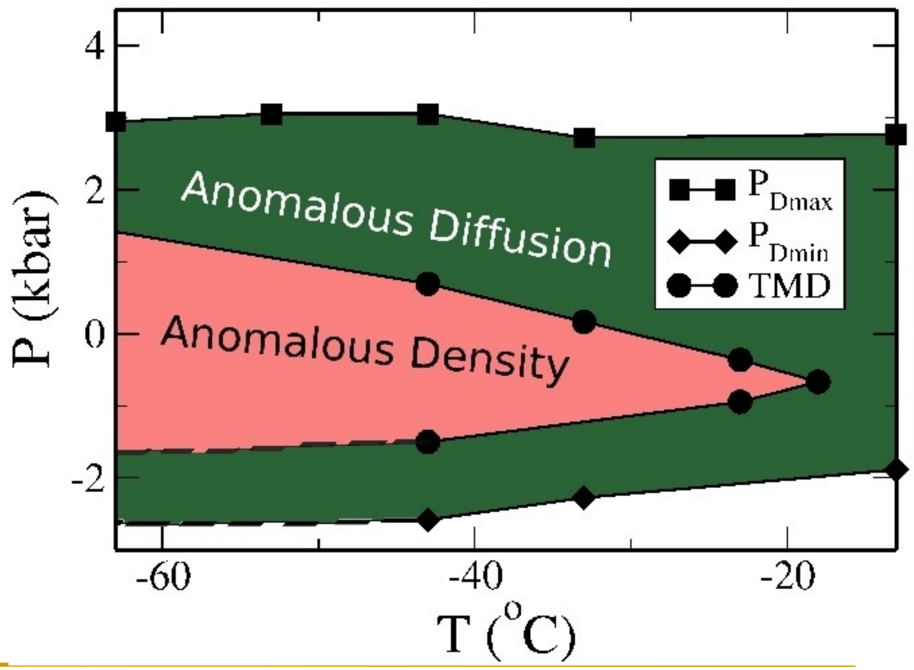
SPC/E Number of Neighbors

Netz, Starr, MCB and Stanley, Physica A 314, 470 (2002)

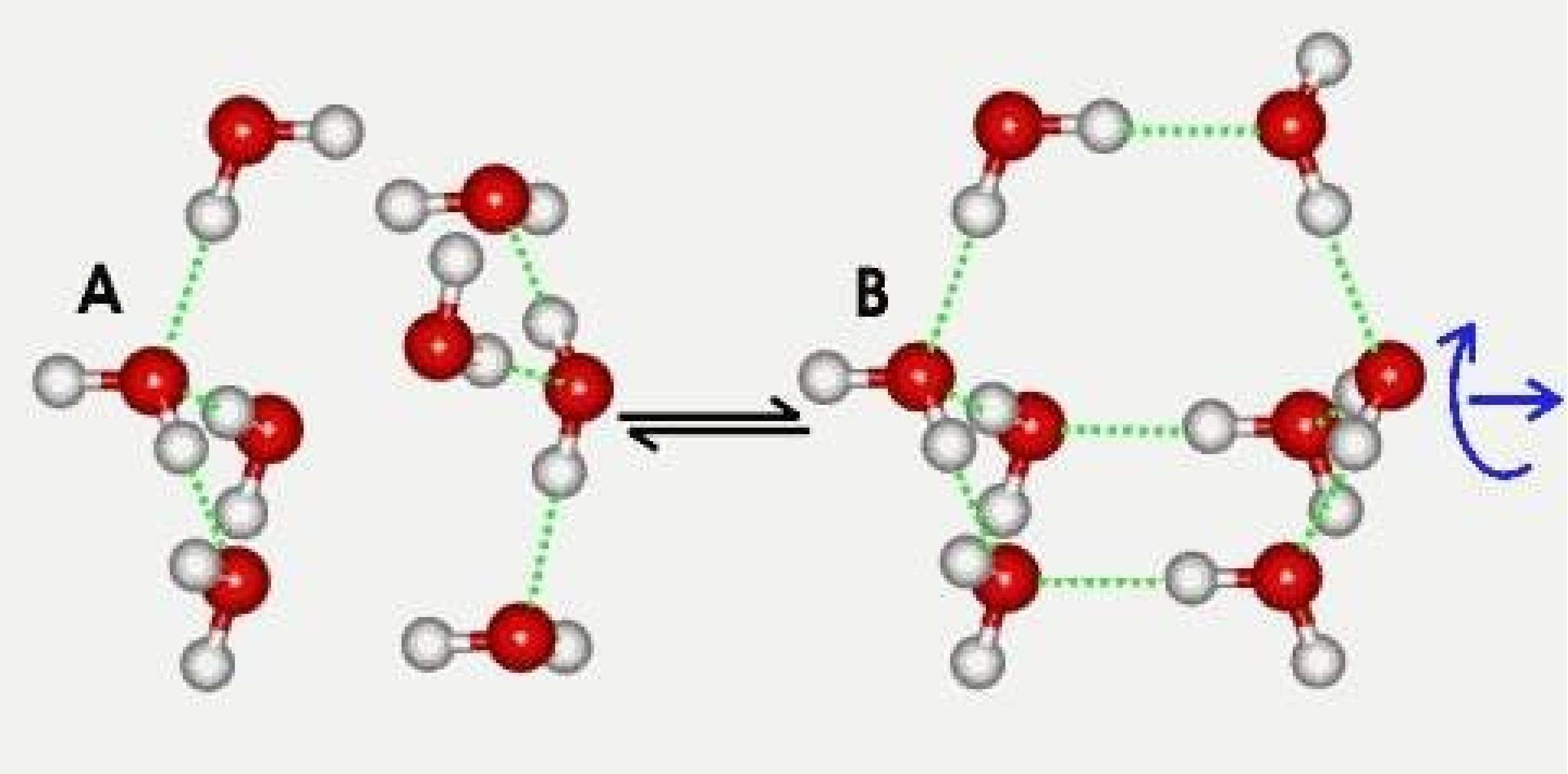


Experiments vs. Simulations

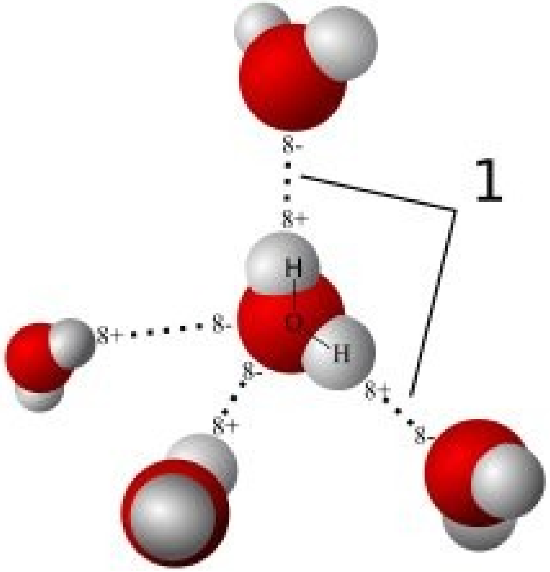


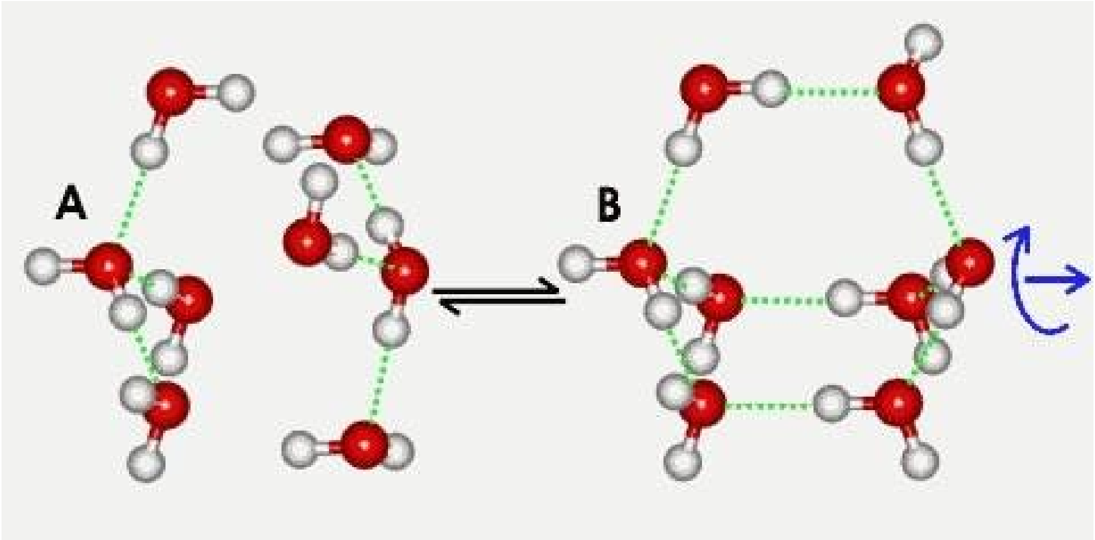


Two States: Open and Closed

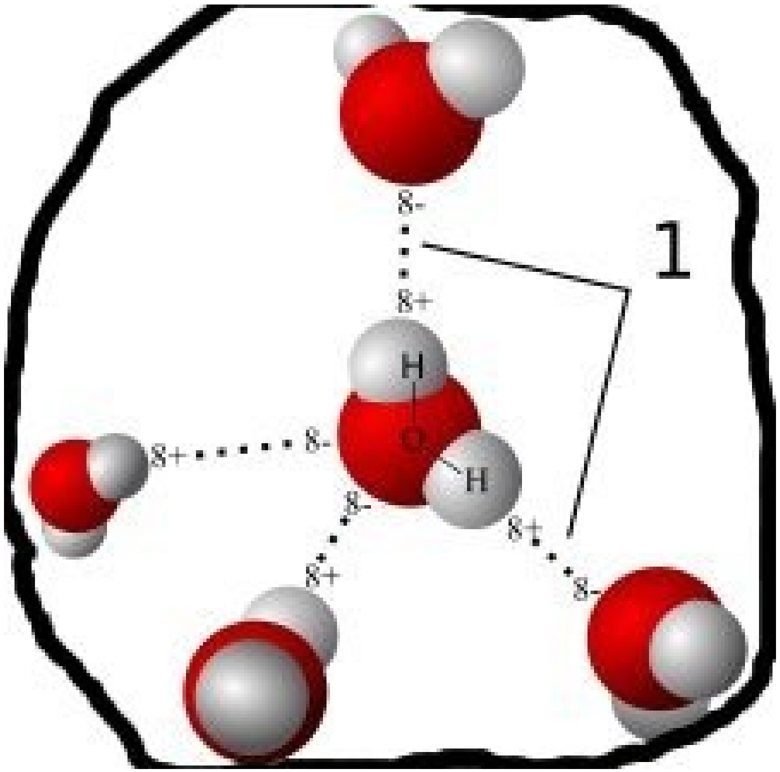


Two States



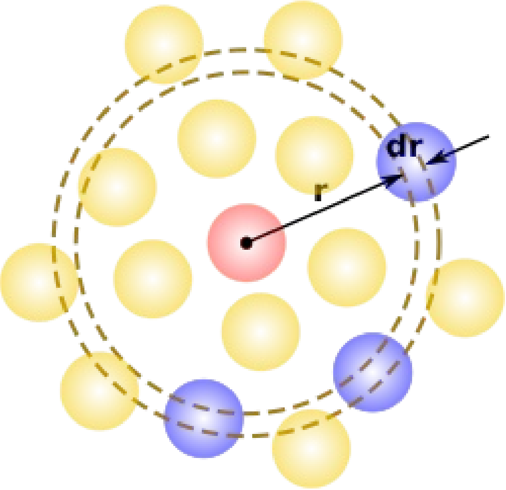


Effective Potential



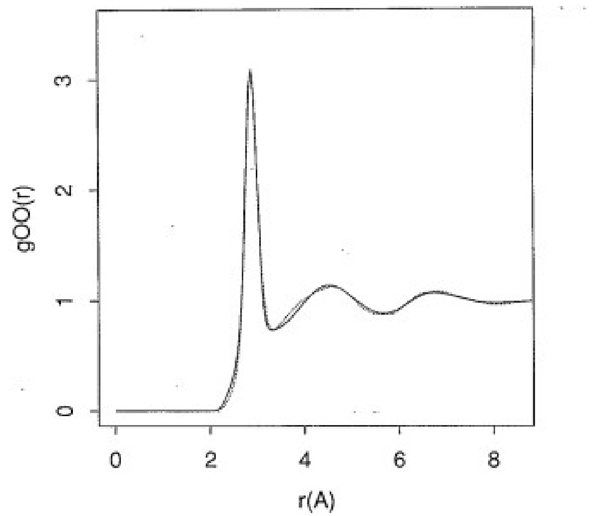
Effective Potential -HNC

$$h(r) = c(r) + \rho \int c(\mathbf{r}-\mathbf{r}')h(\mathbf{r}')d\mathbf{r}'$$



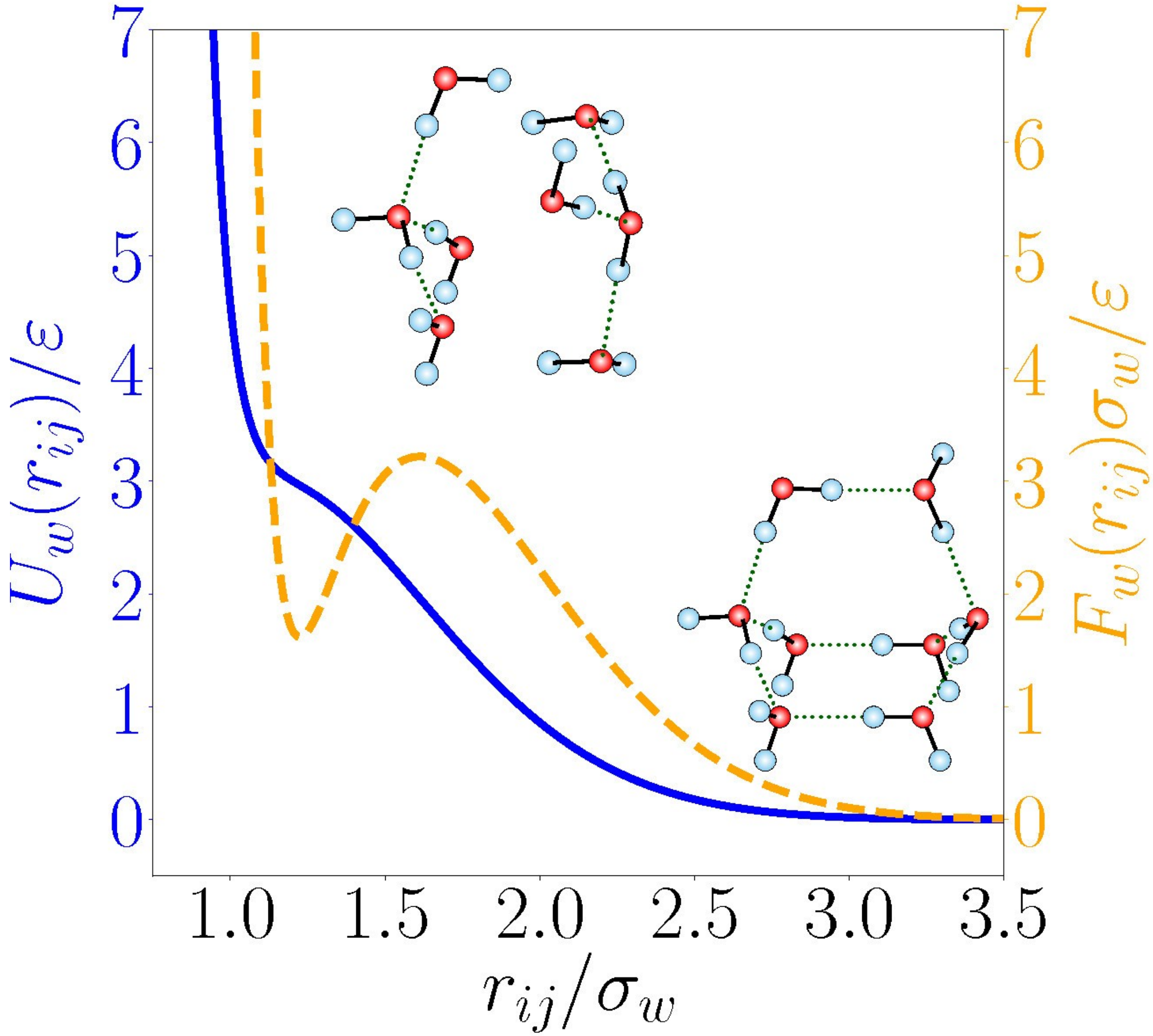
$$h(r) = g(r) - 1$$

$$\phi(r) = k_b T \ln[1 - c(r)/g(r)]$$



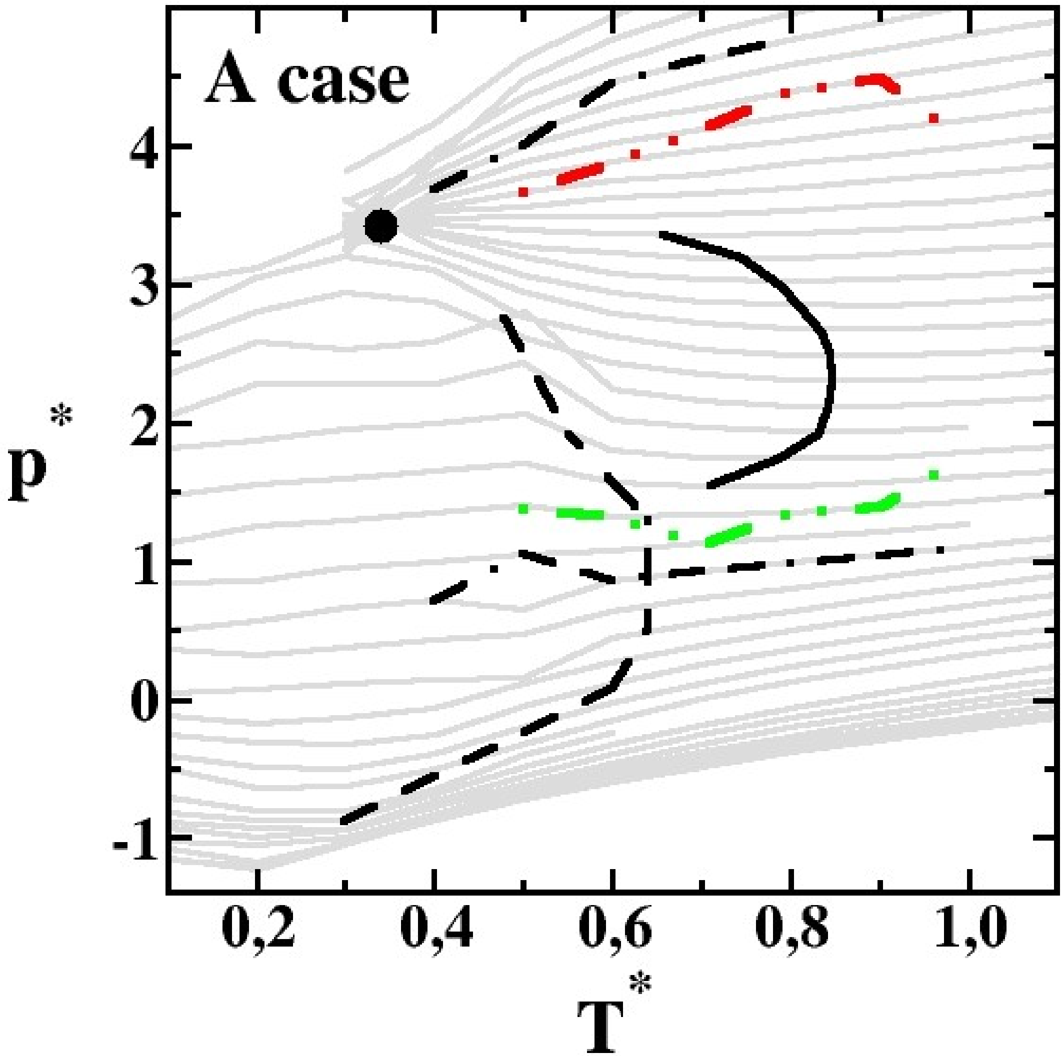
https://pubs.aip.org/aip/jcp/article-abstract/98/4/3313/980508/An-orientational-perturbation-theory-for-pure?redirectedFrom=fulltext

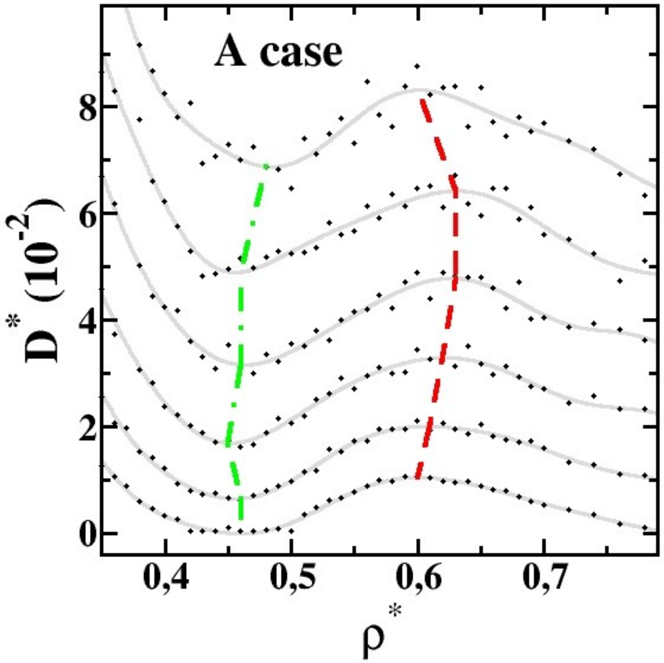
Effective Potential



Phase Diagram

Barraz, Salcedo, Barbosa, JCP 131, 094504 (09)

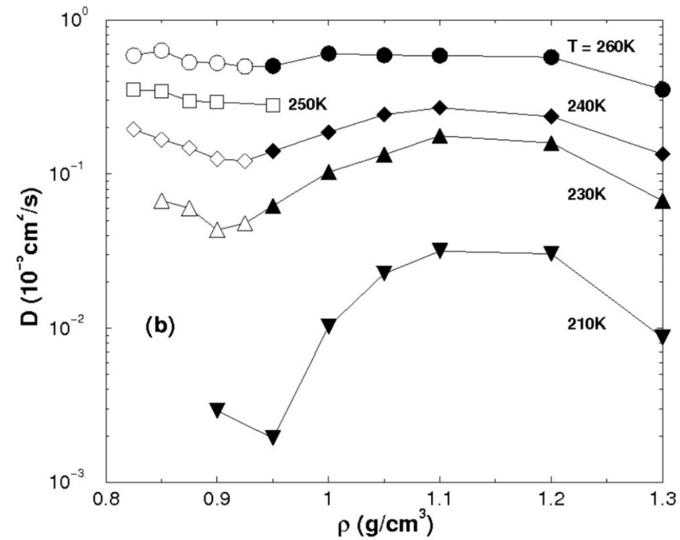


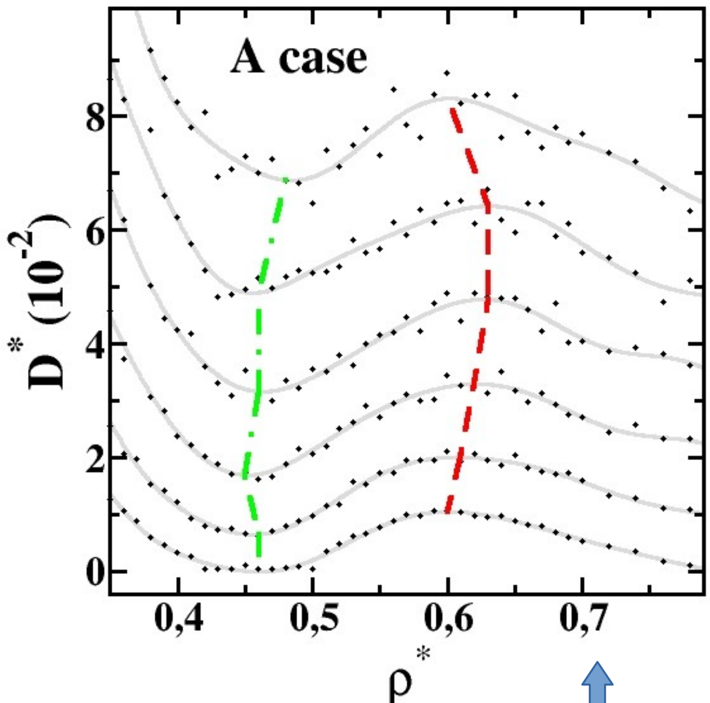


Phase Diagram

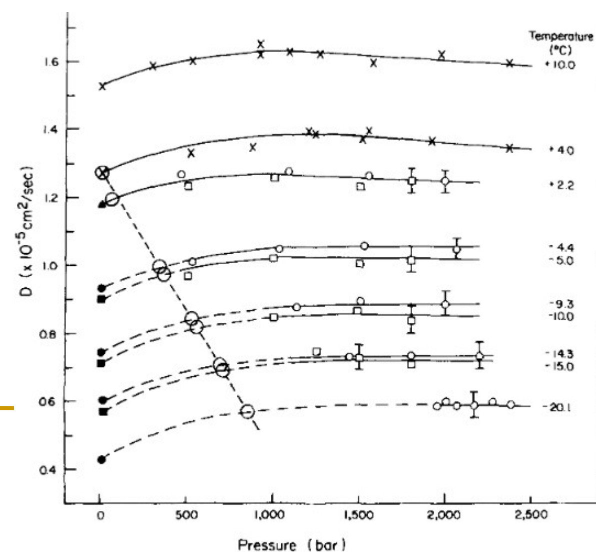
Barraz, Salcedo, Barbosa, JCP 131, 094504 (09)

Atomistic Potential





Effective Potential



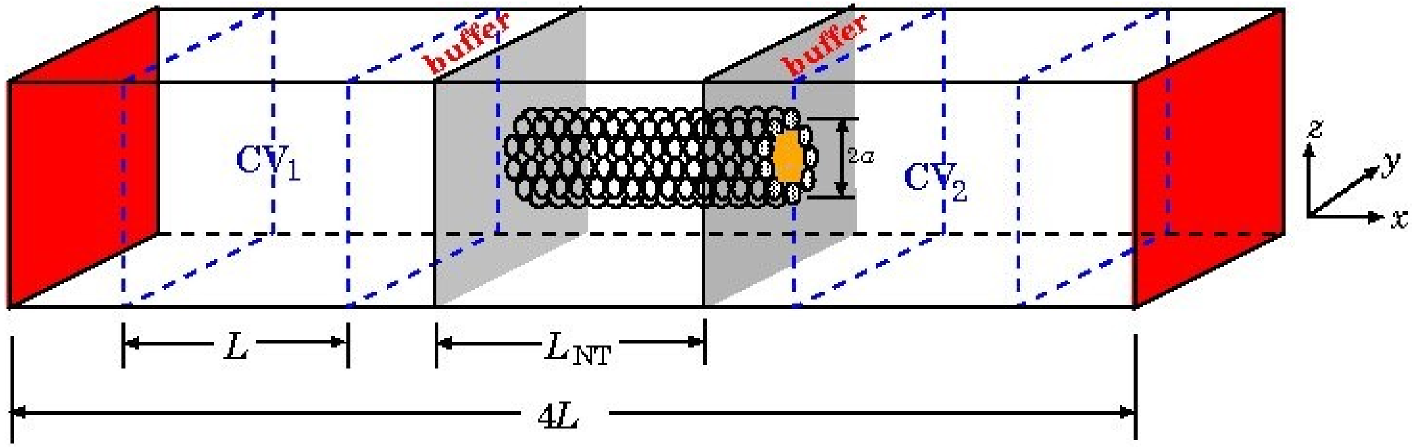
Experimental

Nanoconfined Water

Diffusion-Radius

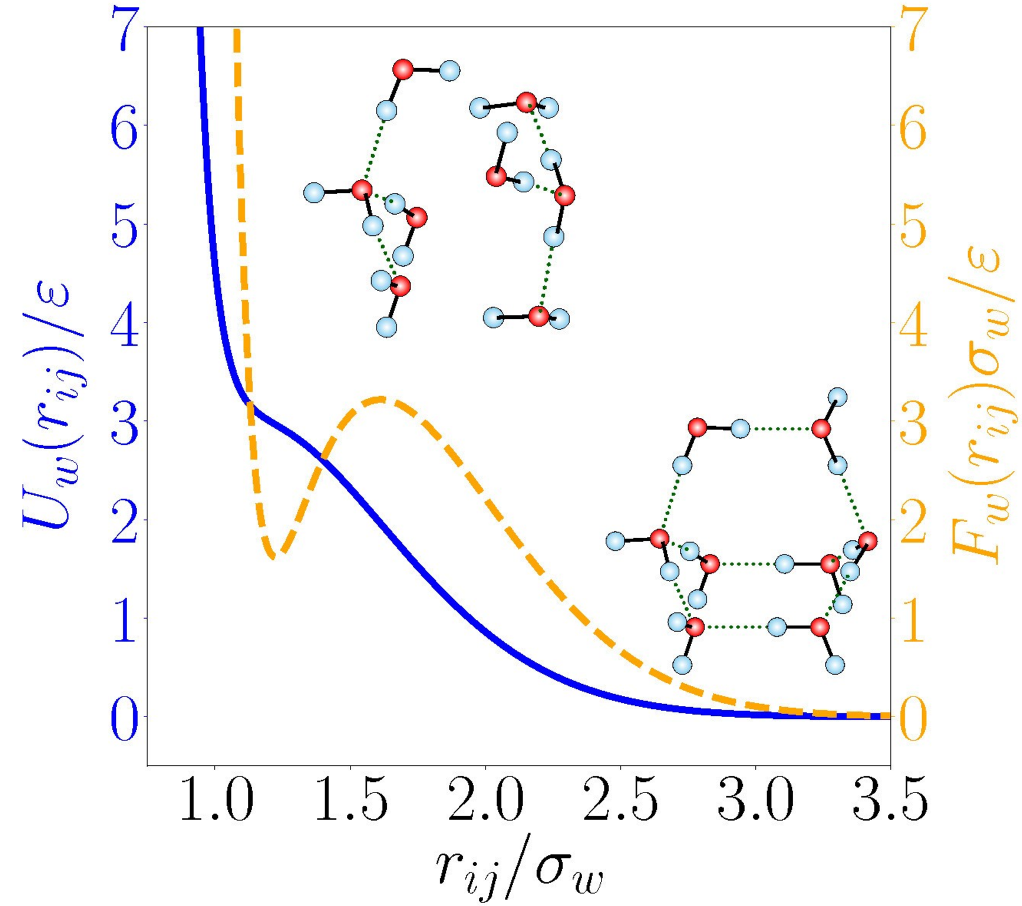
Confined Water Nanotube

J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)



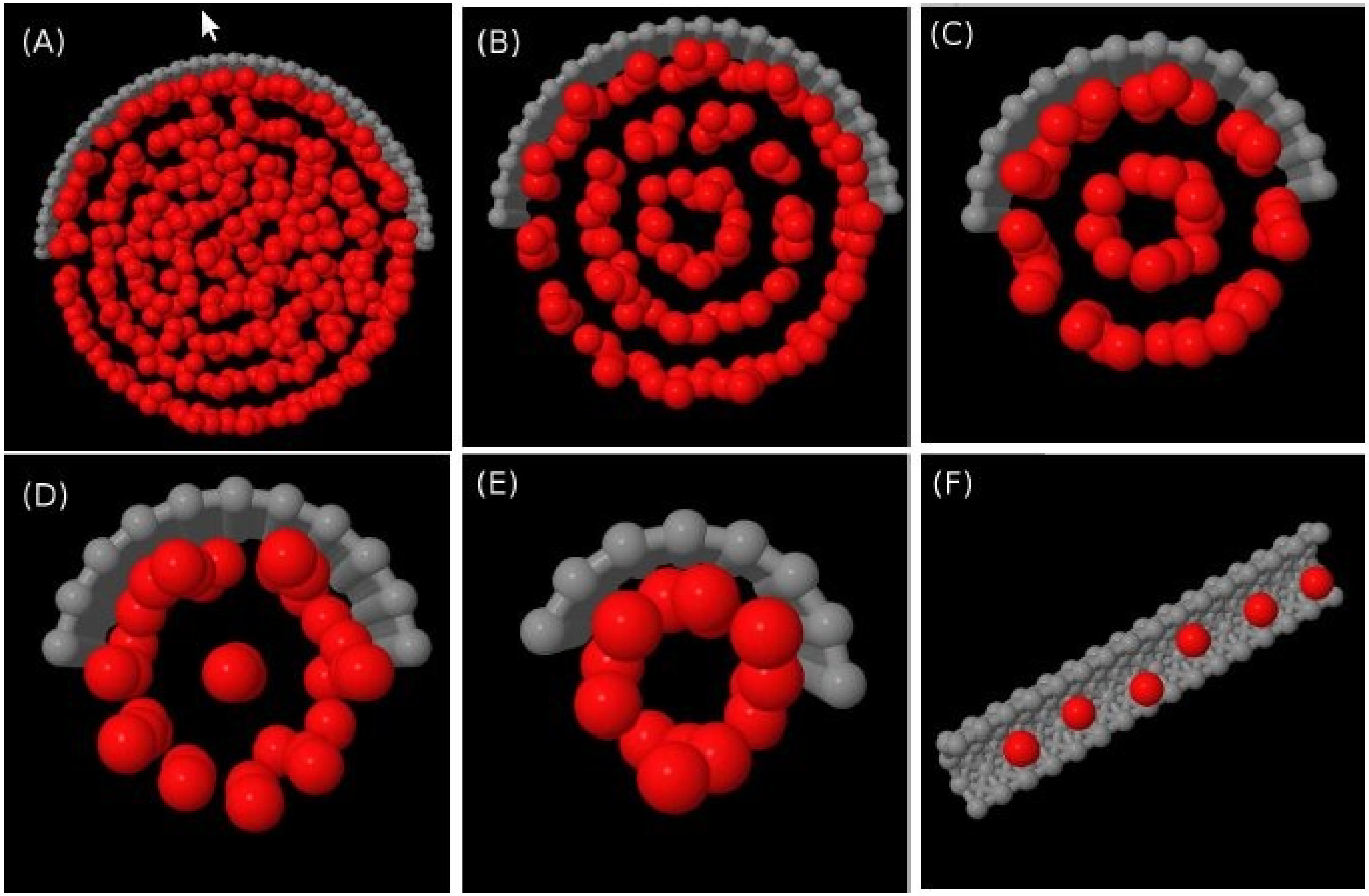
Effective Potential

J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)



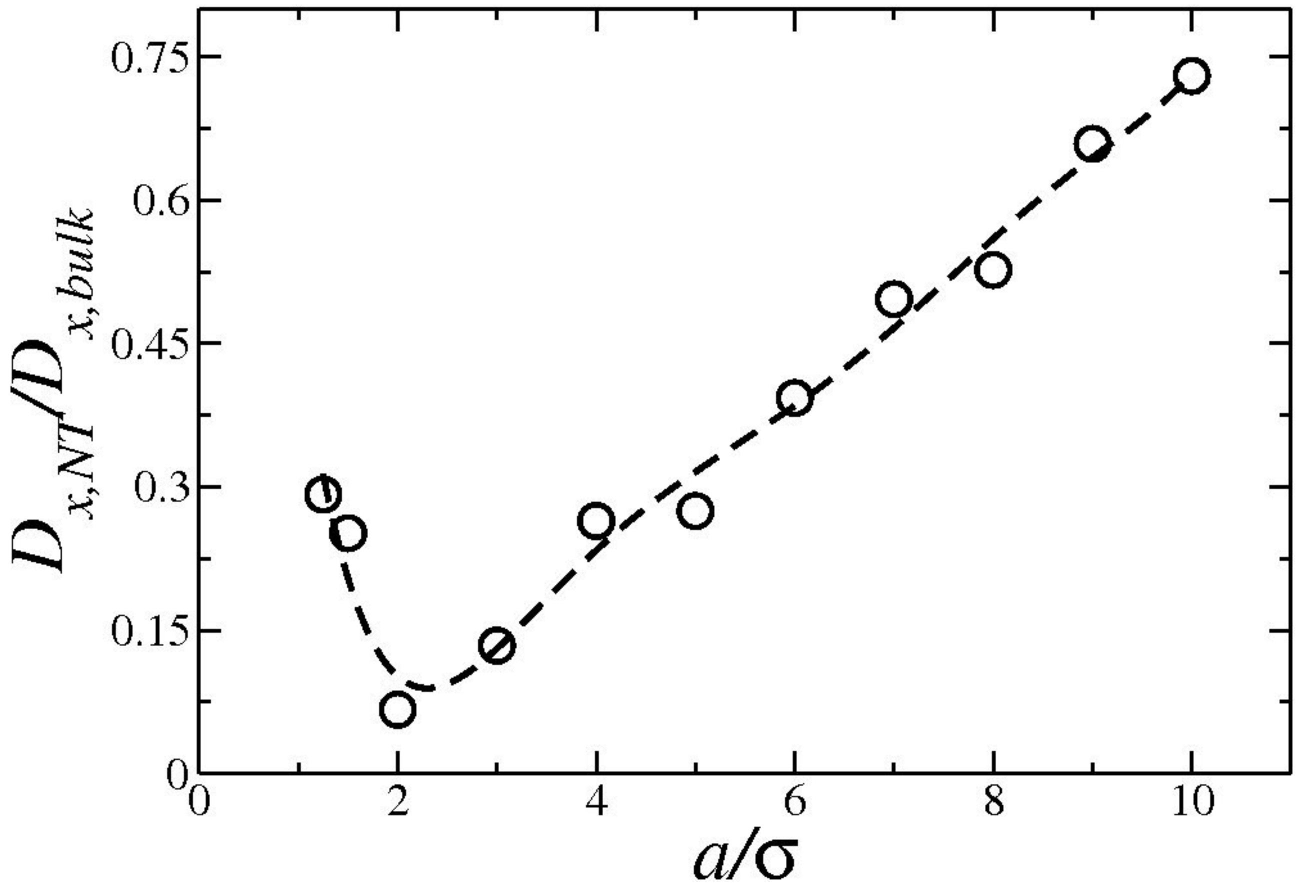
Water Layering

J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)



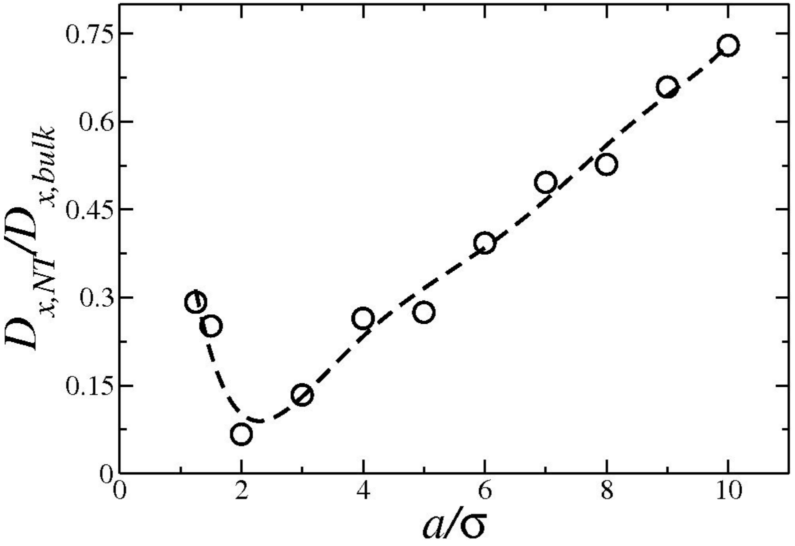
Diffusion

J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)



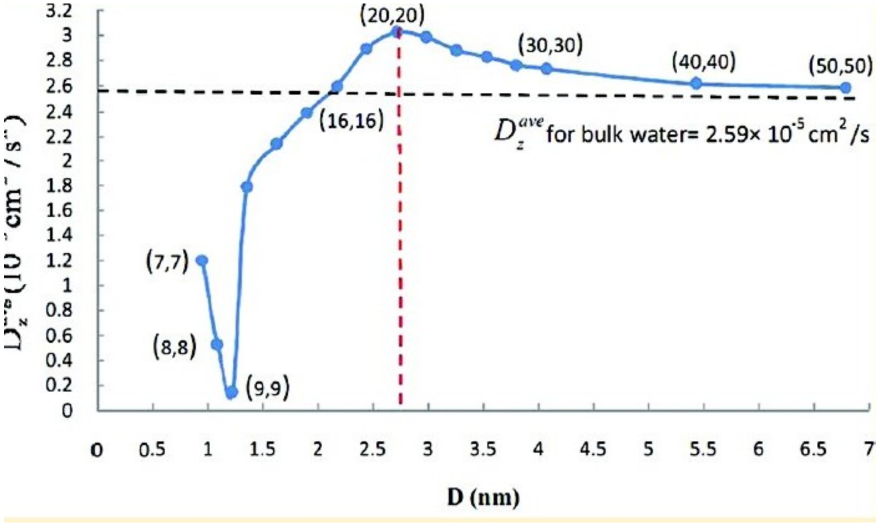
Diffusion

J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)
A.B. Farinami, JPCB 115, 12145 (2012)



Effective Potential

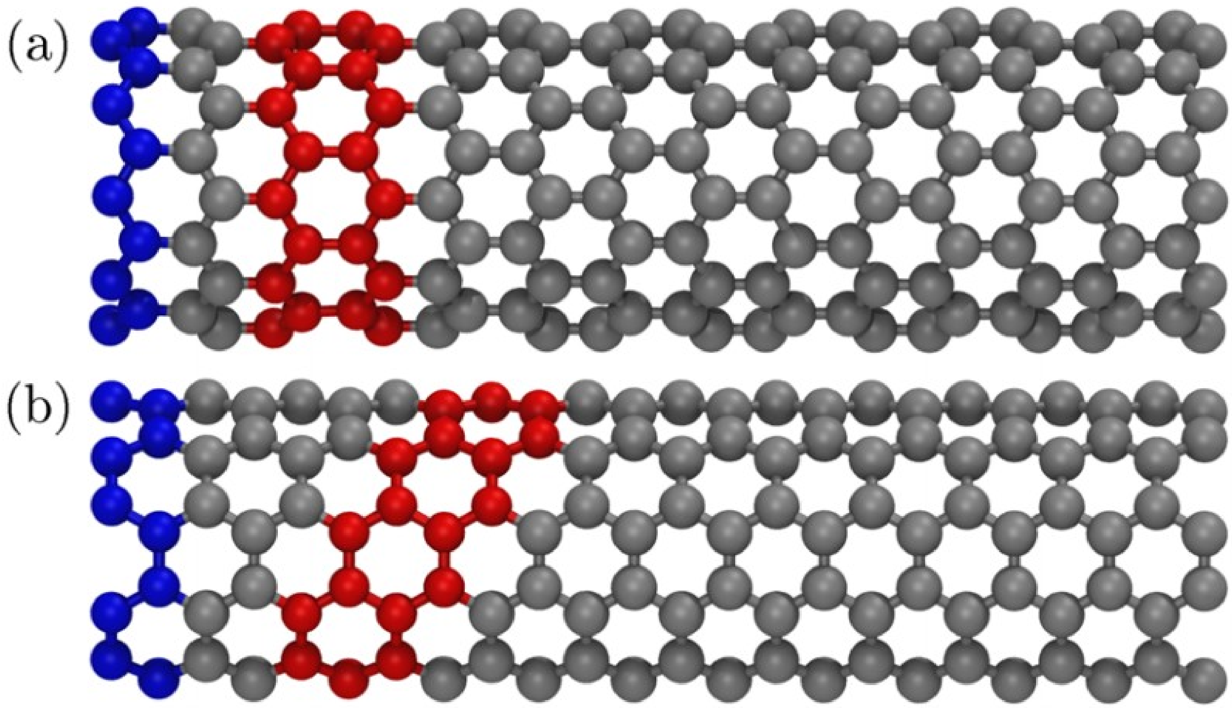
Atomistic Potential



Diffusion-Chirality

Chirality

Mendonça, Ternes, Salcedo, Oliveira and MCB
JCP 152 024708 (2020)



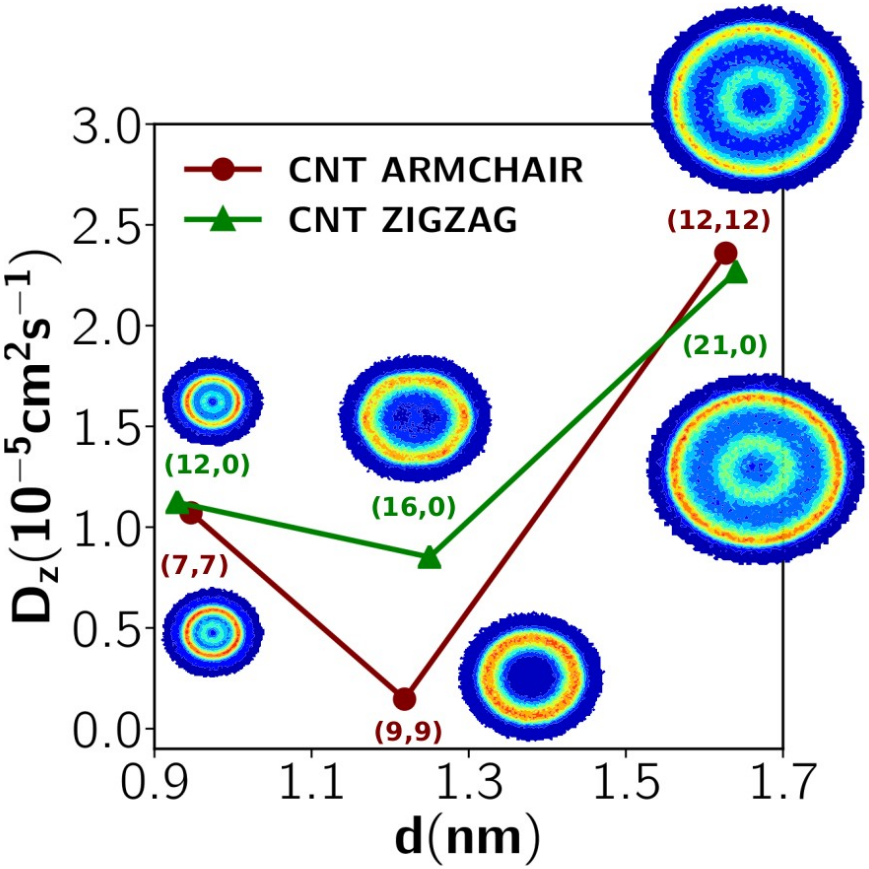
Chirality

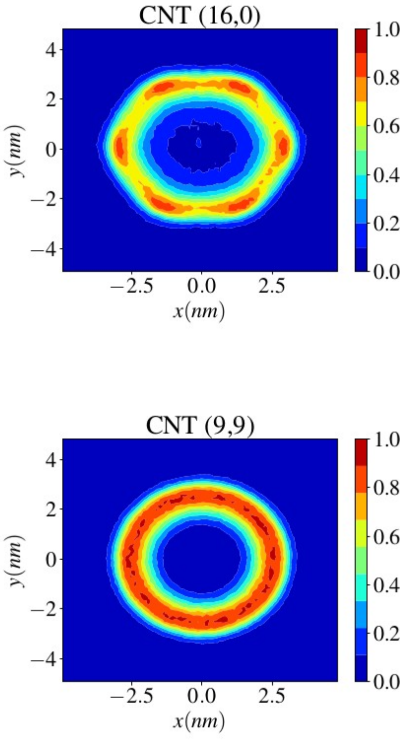
Mendonça, Ternes, Salcedo, Oliveira and MCB
JCP 152 024708 (2020)

CNT	d (nm)	L_z (nm)	H_2O	ρ (g/cm^3)
(9, 9)	1.22	50.5	908	0.92
(12, 12)	1.63	22.5	901	0.94
(16, 0)	1.25	50.5	908	0.80
(21, 0)	1.64	22.9	901	0.86

Chirality

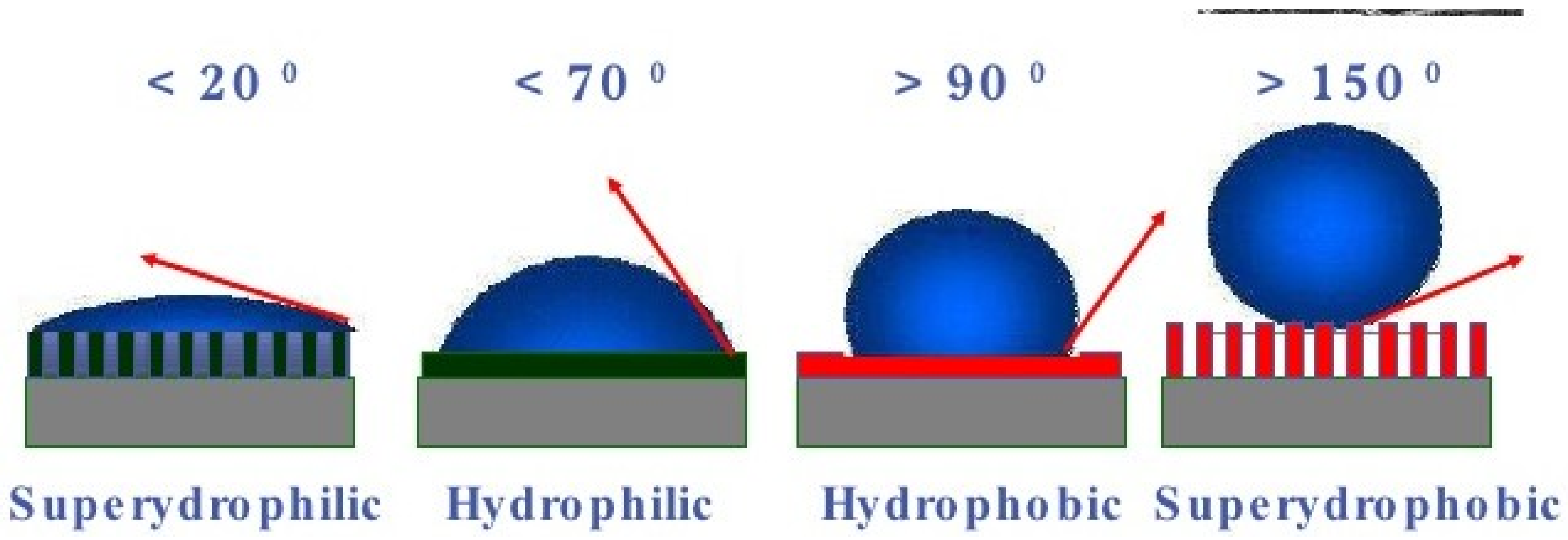
Mendonça, Ternes, Salcedo, Oliveira and MCB
JCP 152 024708 (2020)
JCP 153, 244504 (2020)





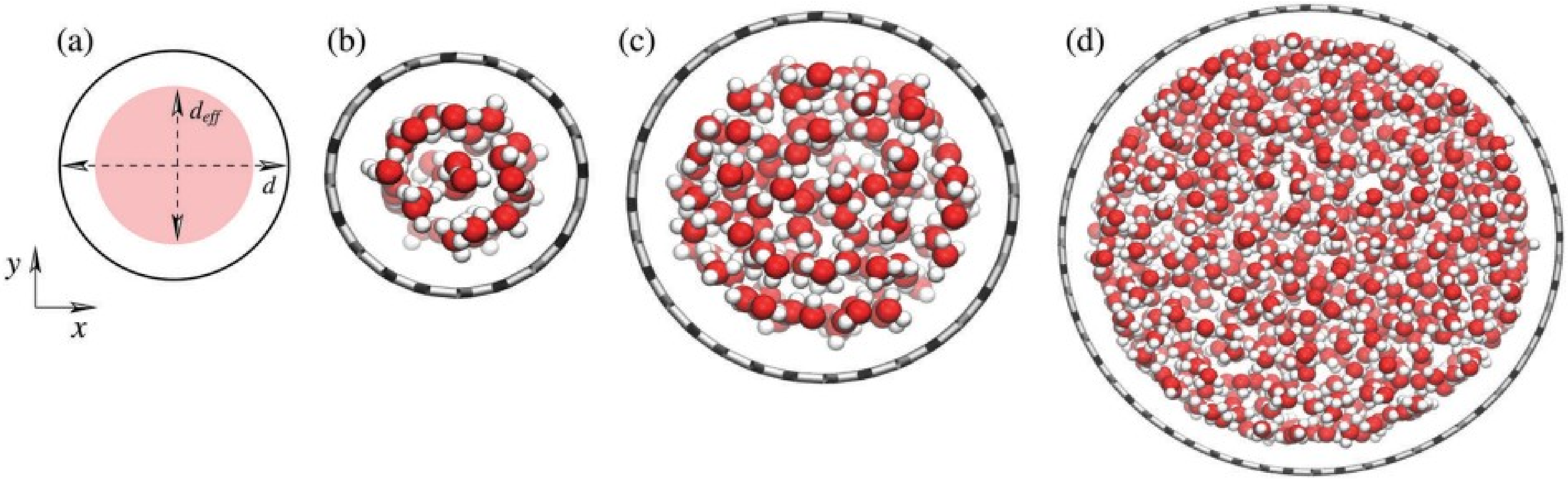
Diffusion-Viscosity

Hydrophobic and Hydrophilic



Hydrophobicity

Kohler, Bordin, da Silva and MCB
PCCP 19 12921 (2017).



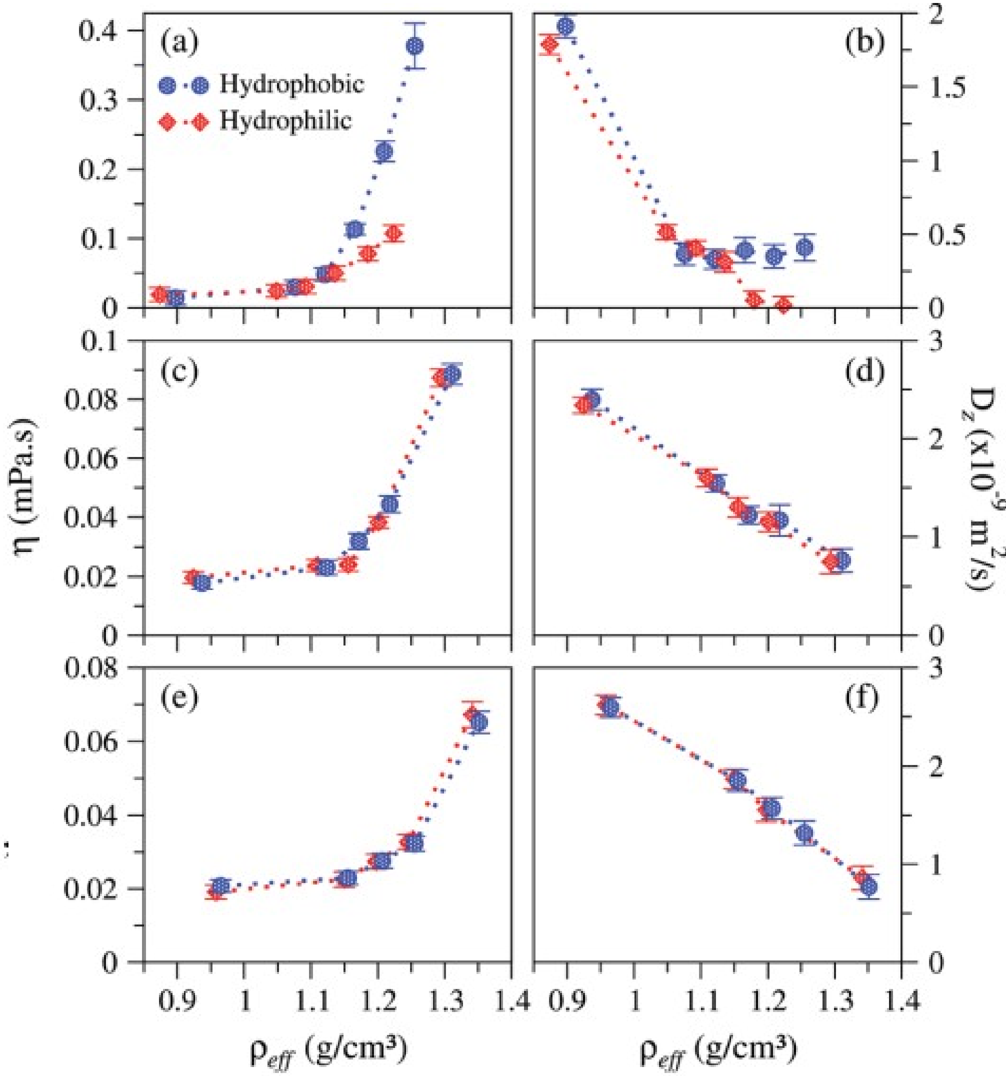
Chirality	d (nm)	ℓ (nm)	N	ρ_{eff} (g cm^{-3})
(10,10)	1.35	37.14	900–1260	0.87–1.25
(16,16)	2.17	11.07	911–1275	0.92–1.30
(30,30)	4.07	8.85	3115–4360	0.95–1.35

Hydrophobicity

Kohler, Bordin, da Silva and MCB
PCCP 19 12921 (2017).

$$D = \frac{k_B T}{6\pi\eta\sigma^3}$$

$$\eta = \frac{V}{k_B T}\int_0^\infty \mathrm{d}t\langle P_{\alpha\beta}(t)P_{\alpha\beta}(0)\rangle$$



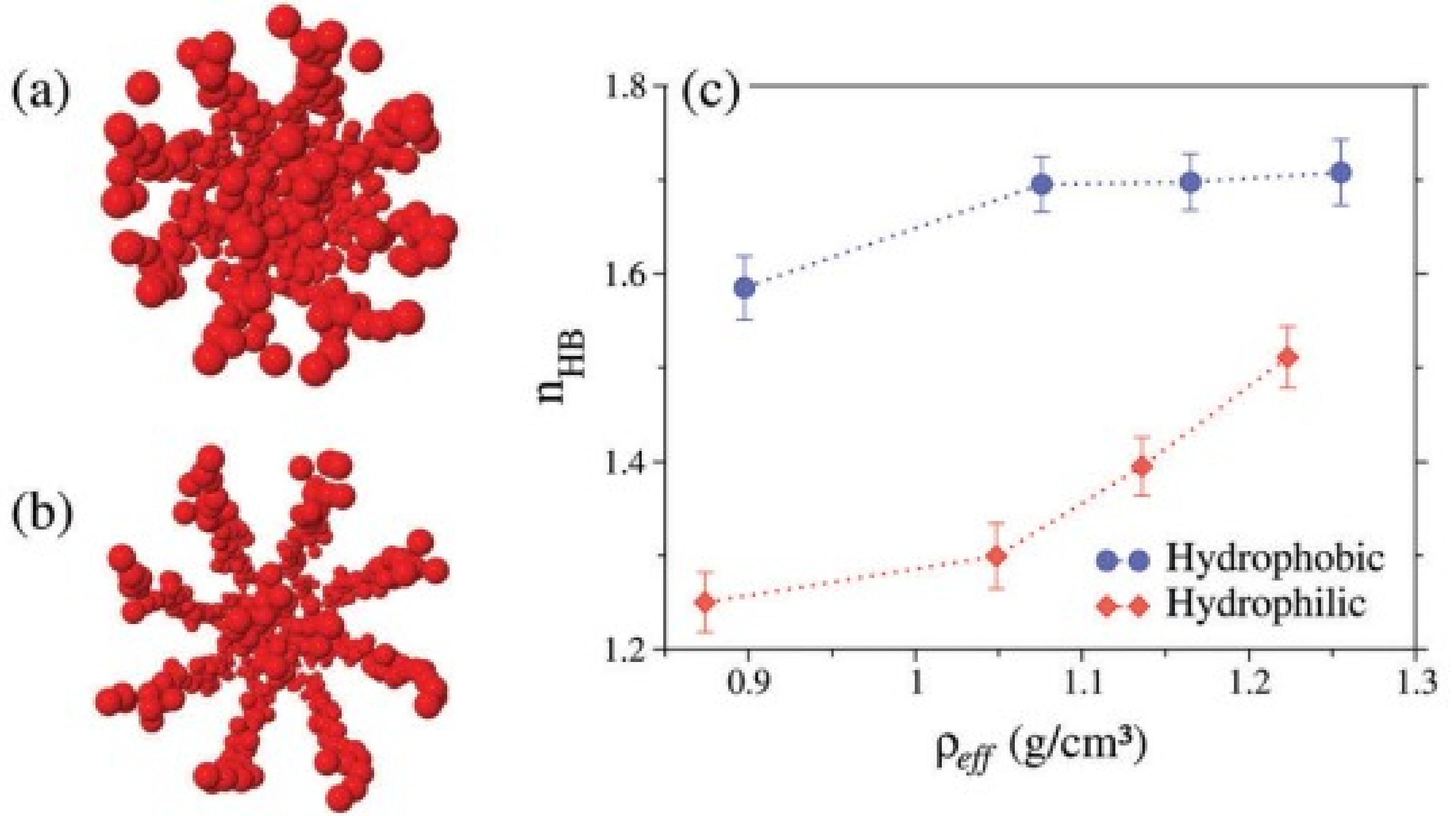
(10,10)

(16,16)

(30,30)

Hydrophobicity

Kohler, Bordin, da Silva and MCB
PCCP 19 12921 (2017).



10,10)

FLUX - Nanotubes

Enhancement Factor

J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)

$$D_x = \frac{1}{N}\sum_{i=1}^{N}\int_0^\infty \langle v_{x,i}(t)\cdot v_{x,i}(0)\rangle \, \mathrm{d}t$$

$$\eta = \frac{k_B T}{3\pi\sigma D_x}$$

$$\langle v_x \rangle = \gamma_{HP}\frac{\Delta p}{L_{NT}}$$

$$\gamma_{HP} = \frac{a^2}{8\eta}$$

$$\langle v_x \rangle = \gamma_{MD}\frac{\Delta p}{L_{NT}}$$

$$\varepsilon = \frac{\gamma_{MD}}{\gamma_{HP}}$$

Enhancement Factor

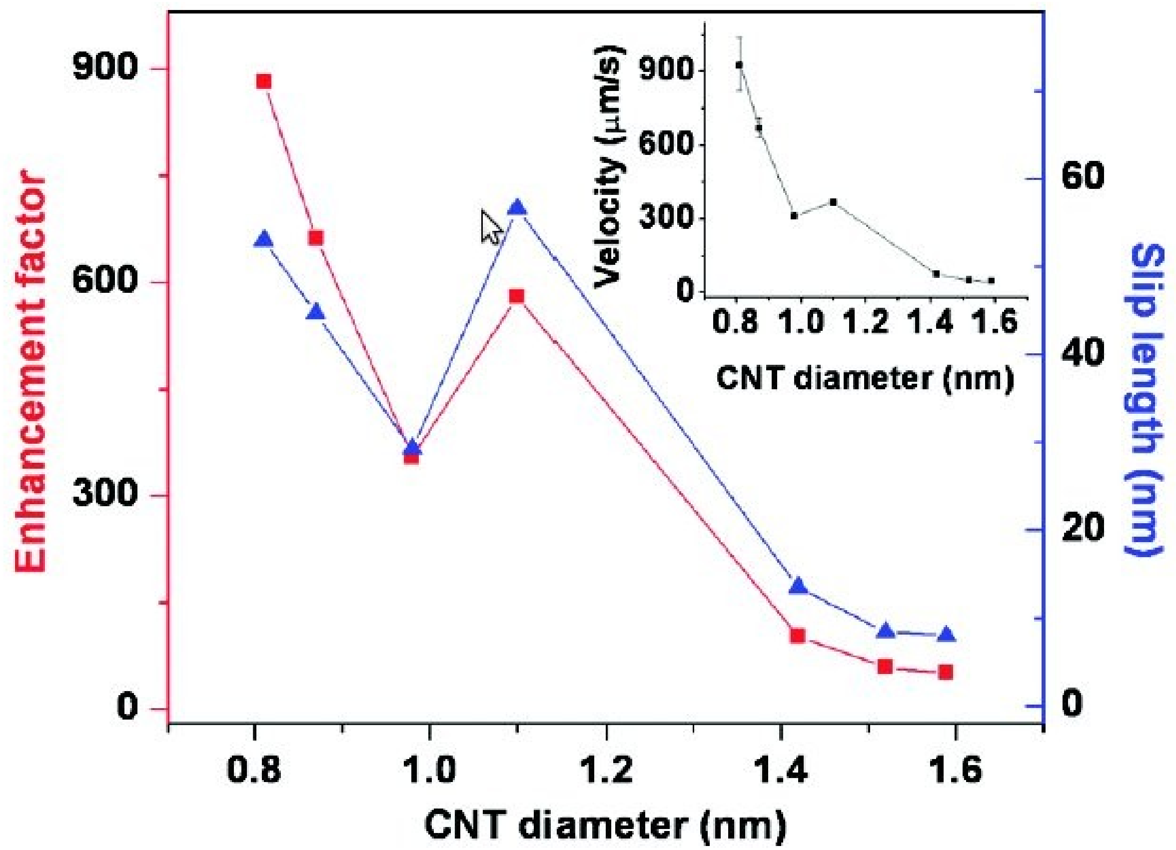
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)

$$\varepsilon = \frac{\gamma_{\mathrm{MD}}}{\gamma_{\mathrm{HP}}}$$

Enhancement Factor

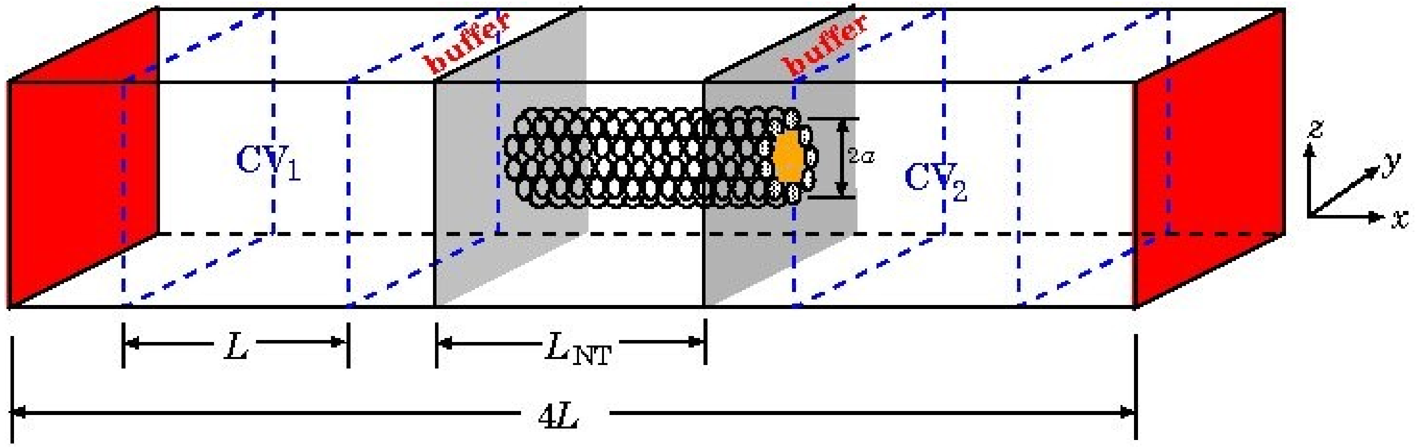
X. Qin et al, Nanoletters 11, 2173 (2011) - experimental

$$\varepsilon = \frac{\gamma_{MD}}{\gamma_{HP}}$$

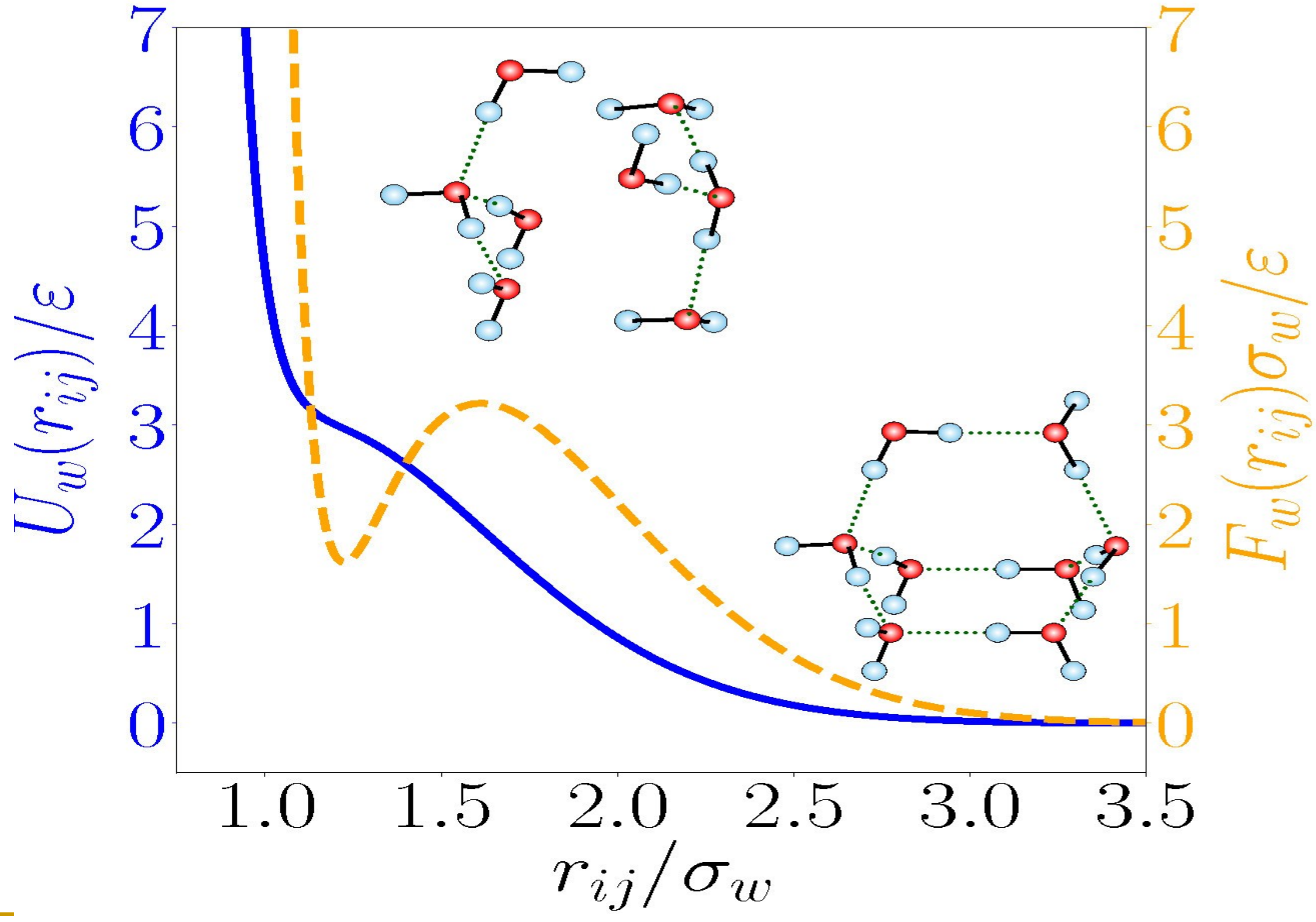


System

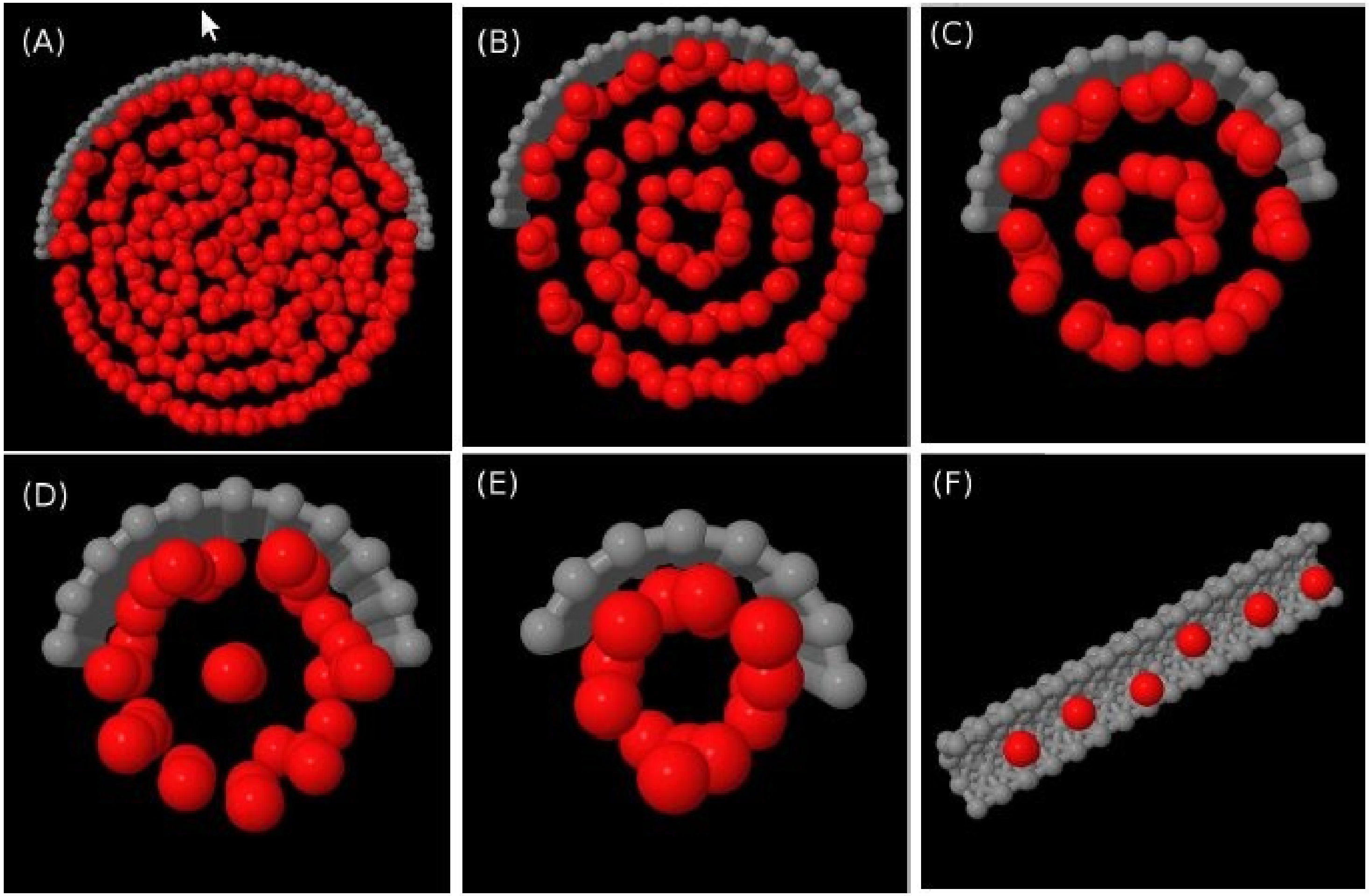
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)



Effective Potential

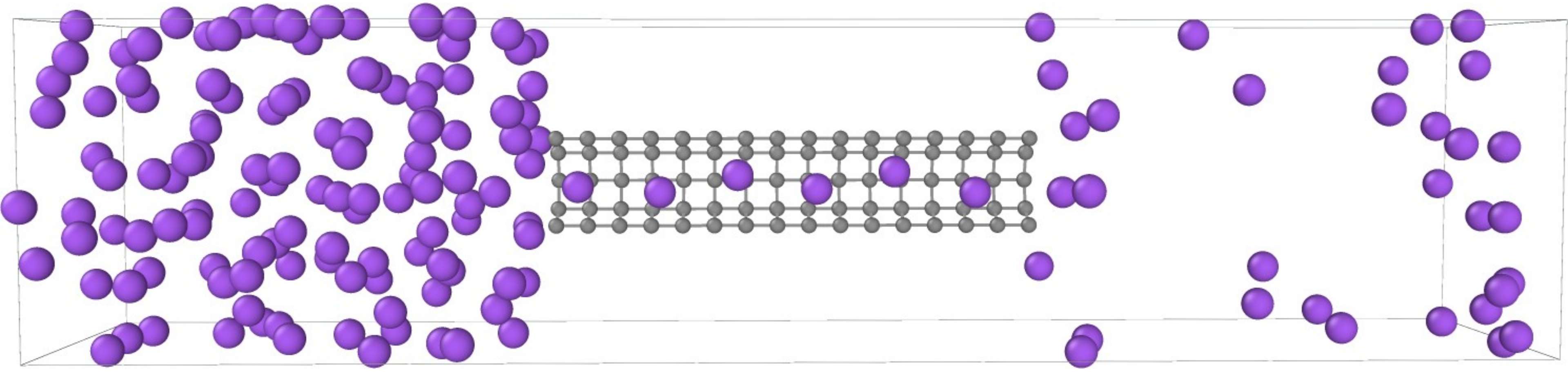


Water Layering



Flow

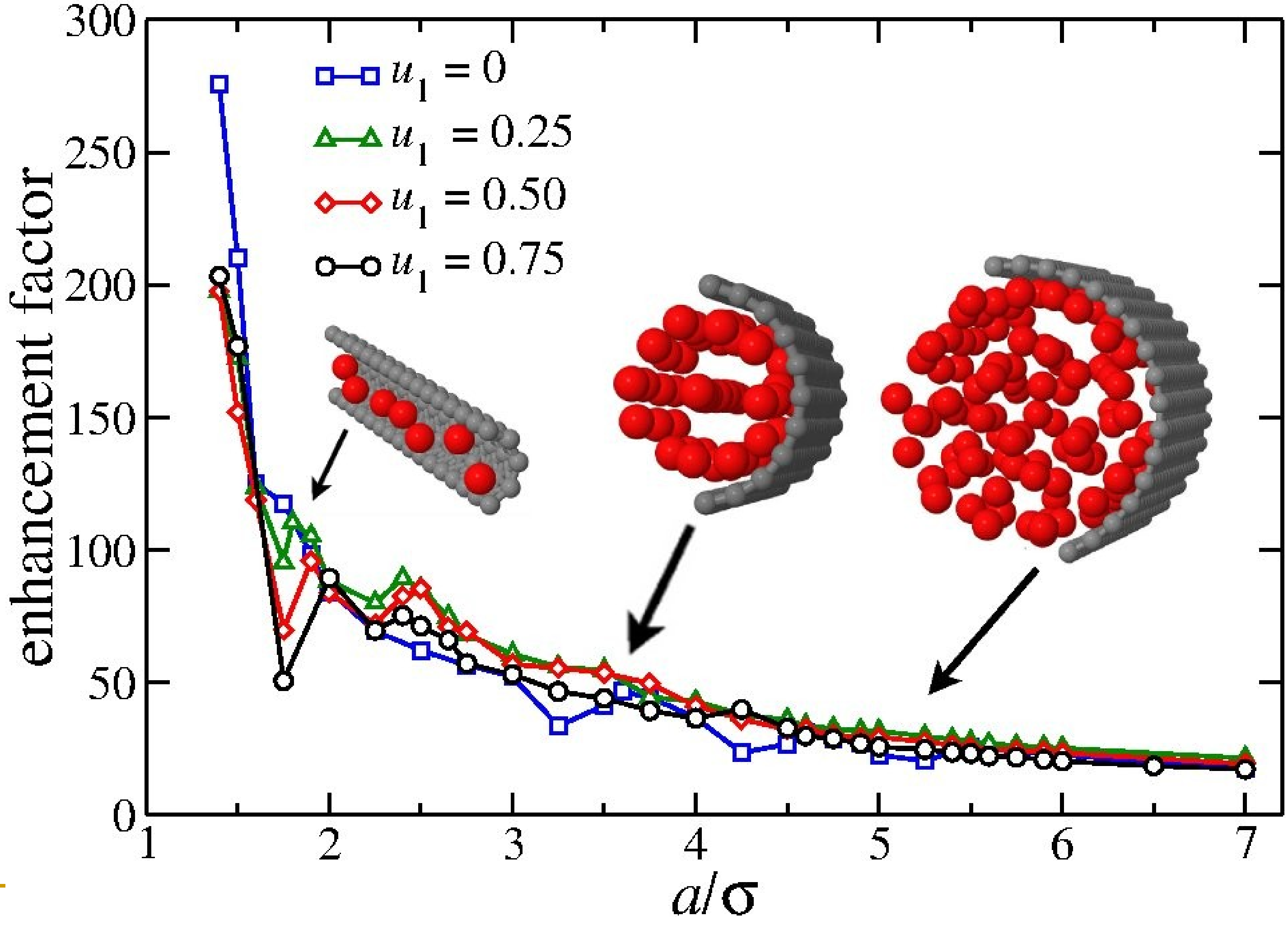
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)



Enhancement Factor

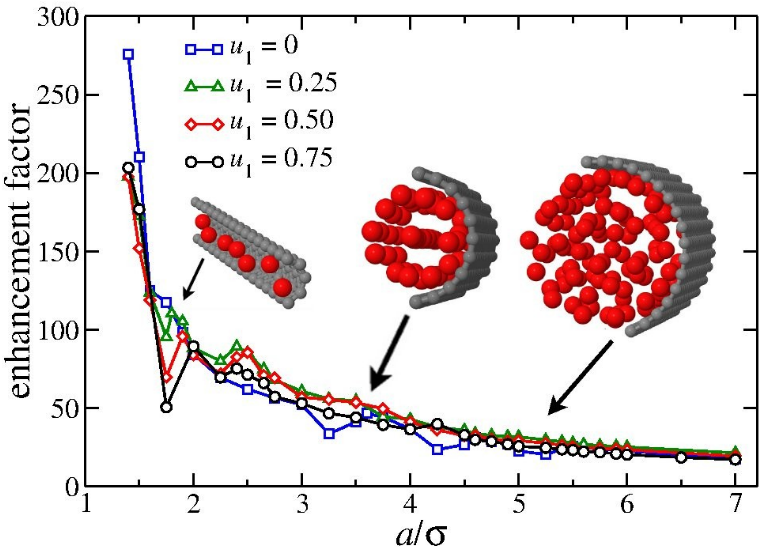
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)

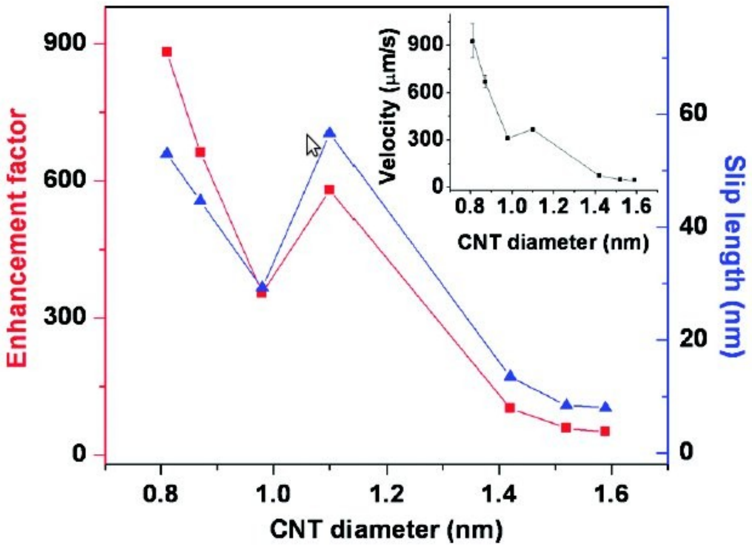
$$\varepsilon = \frac{\gamma_{MD}}{\gamma_{HP}}$$



Enhancement Factor

J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)
X. Qin et al, Nanoletters 11, 2173 (2011) - experimental

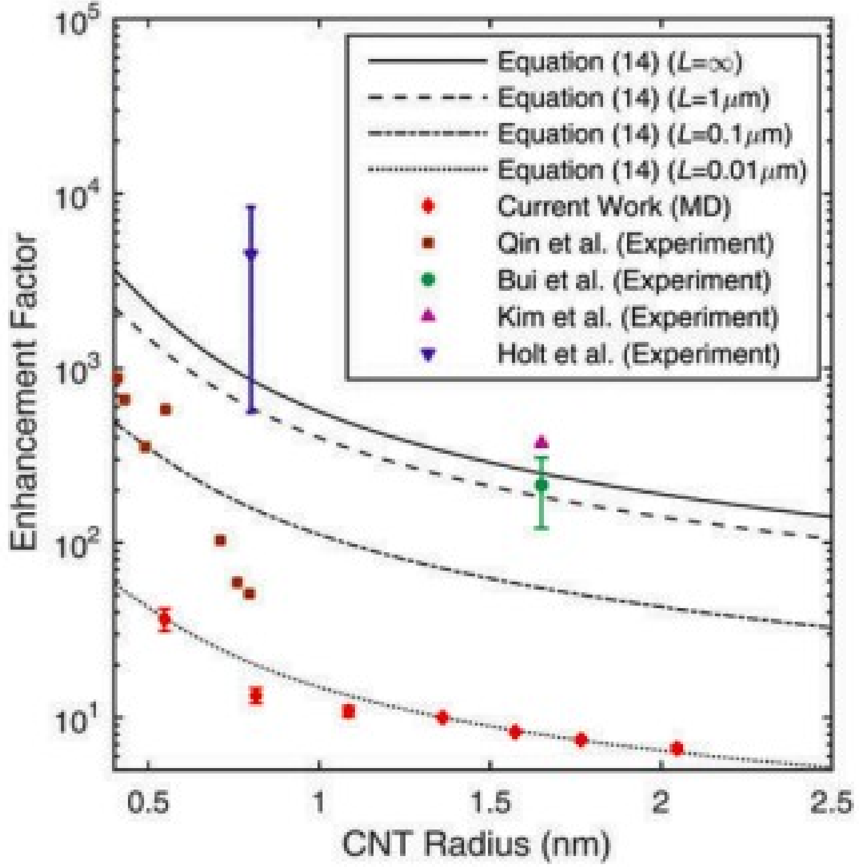




Enhancement Factor

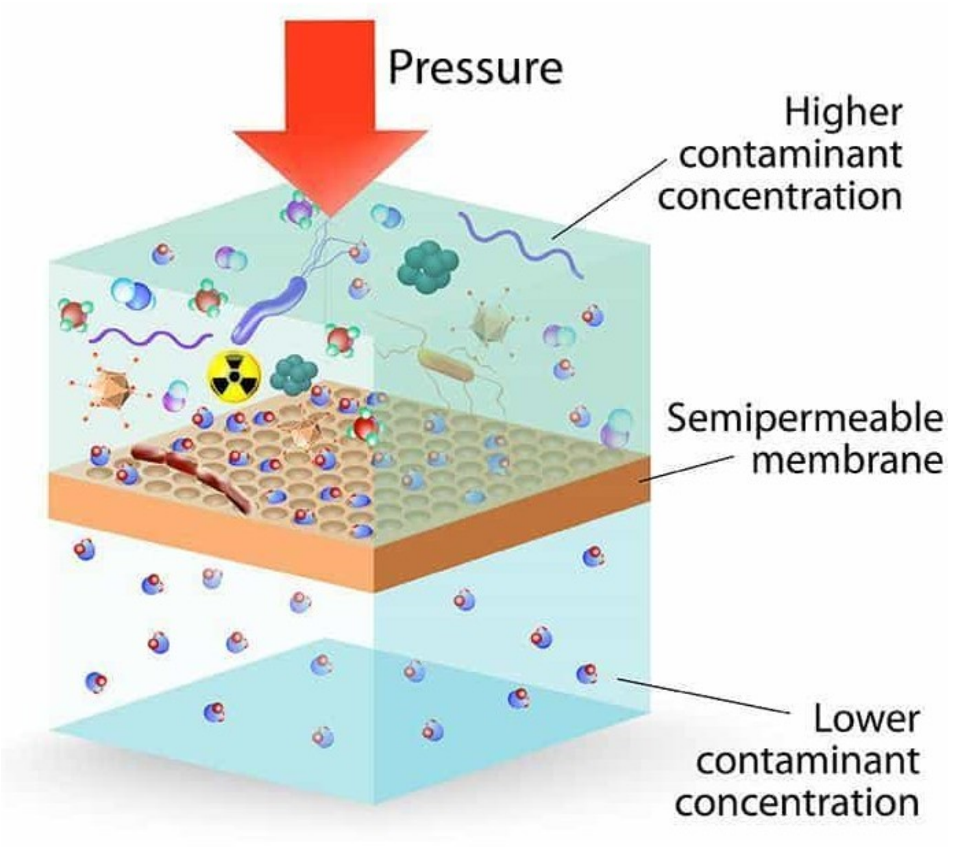
Suk and Aluru

2017, VOL. 21, NO. 4, 247–262



FLUX - Nanomembranes

Osmose Reversa

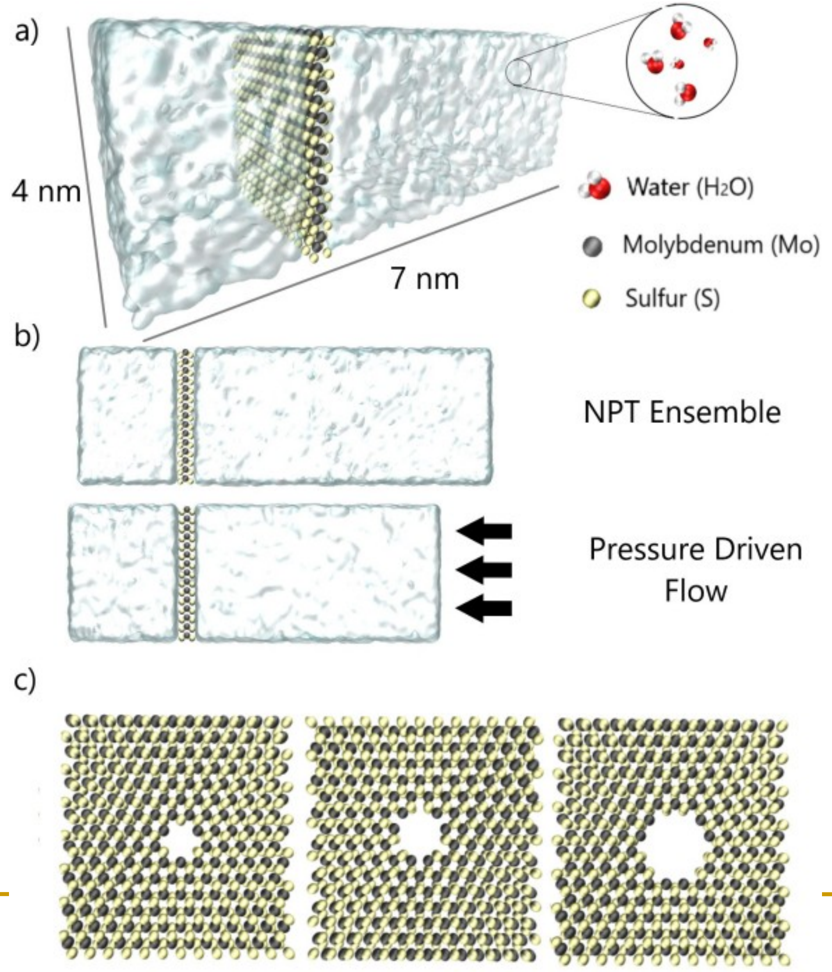


Reverse Osmosis

Charges and Sizes

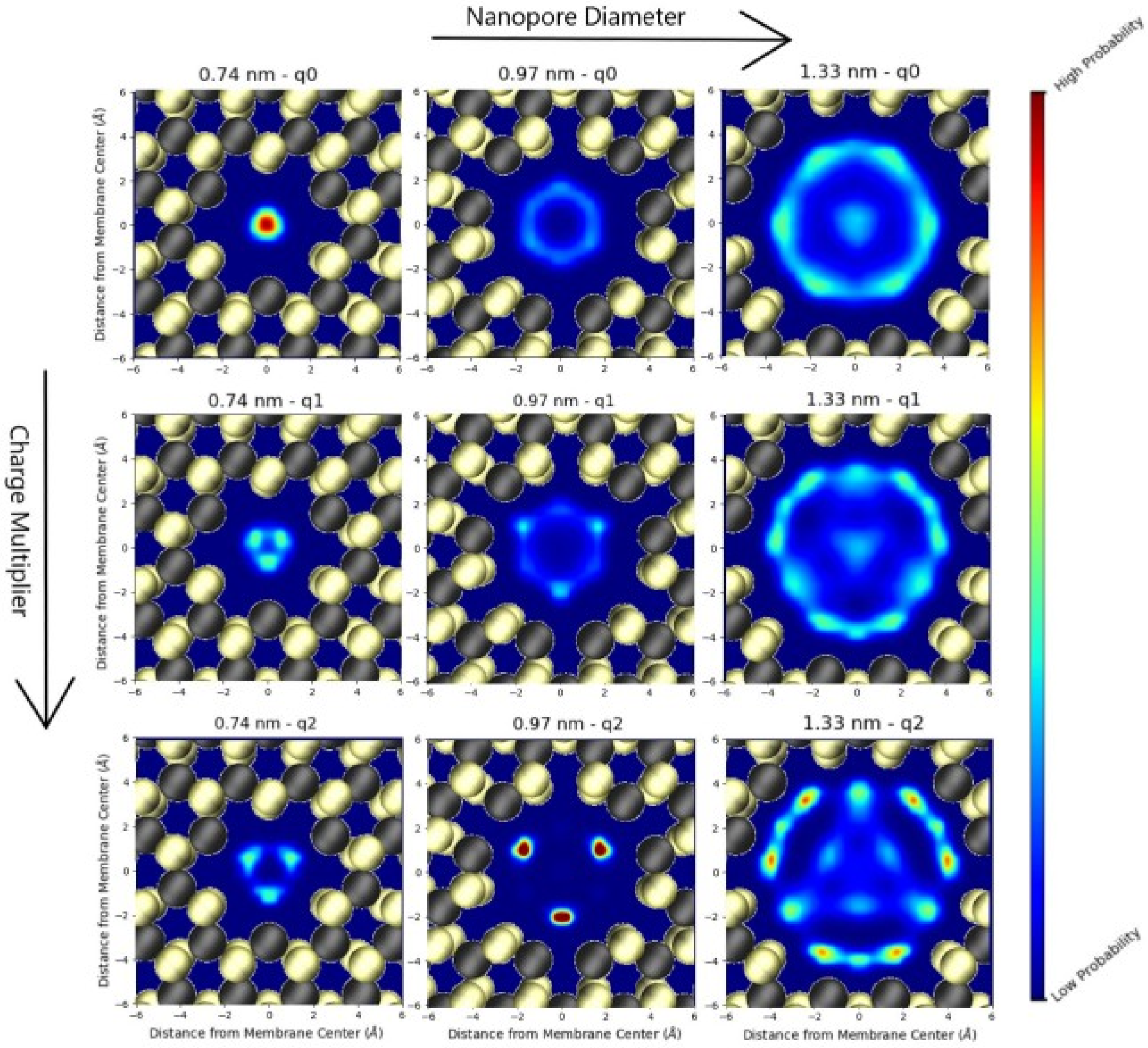
Abal, Barbosa

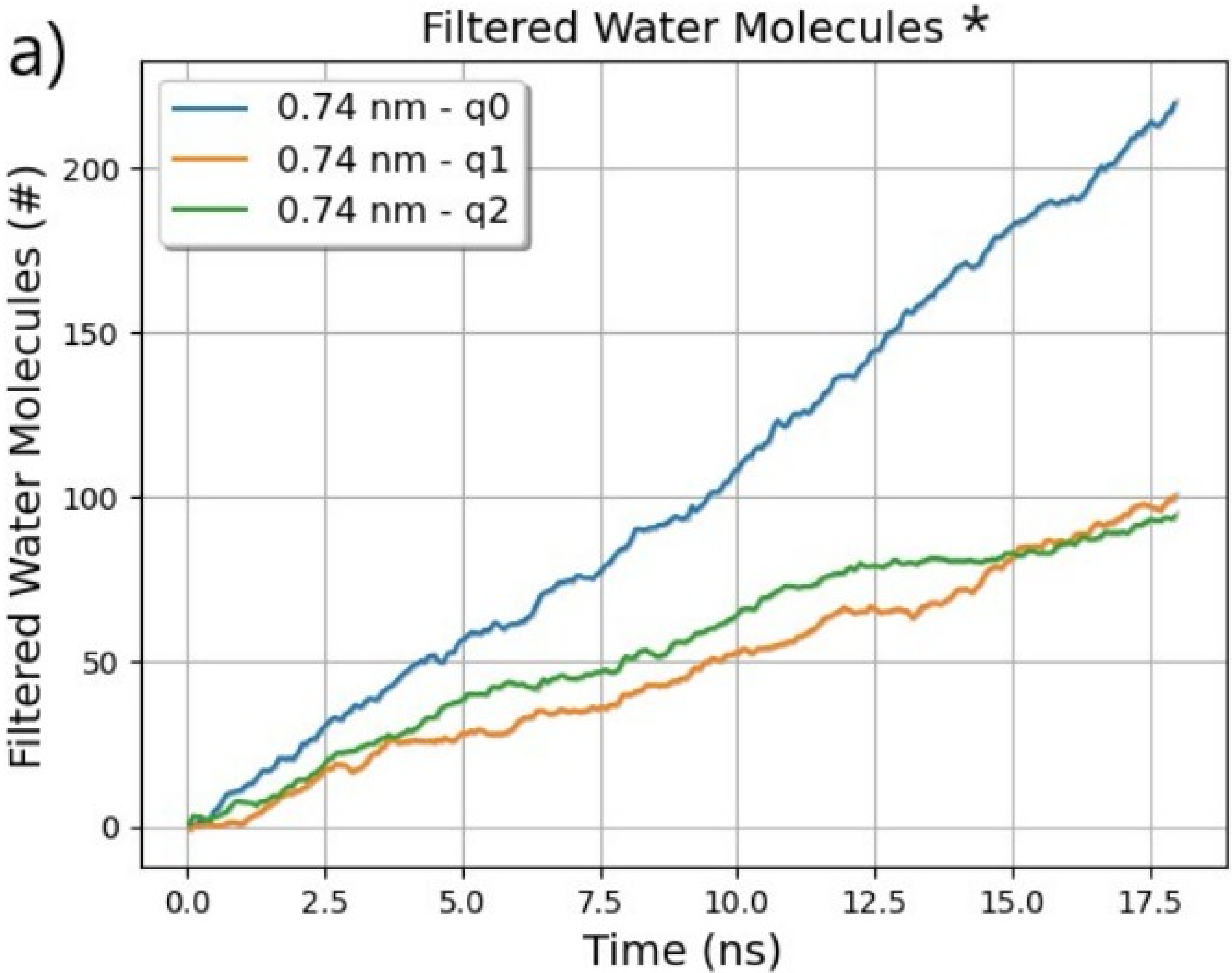
Phys. Chem. Chem. Phys. 23, 12075 (2021)

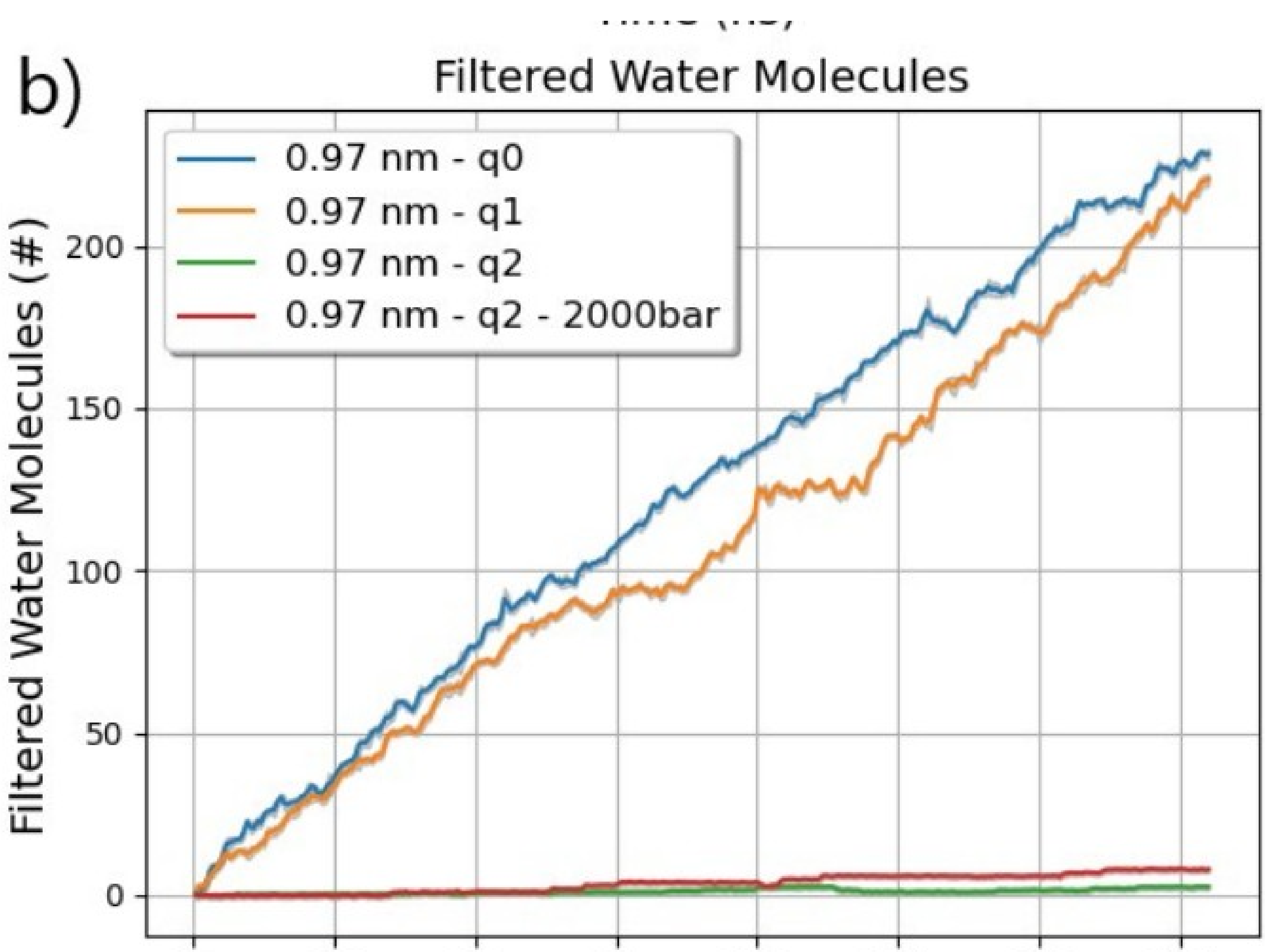


Charges and Sizes

DOI: 10.1039/D1CP00613D



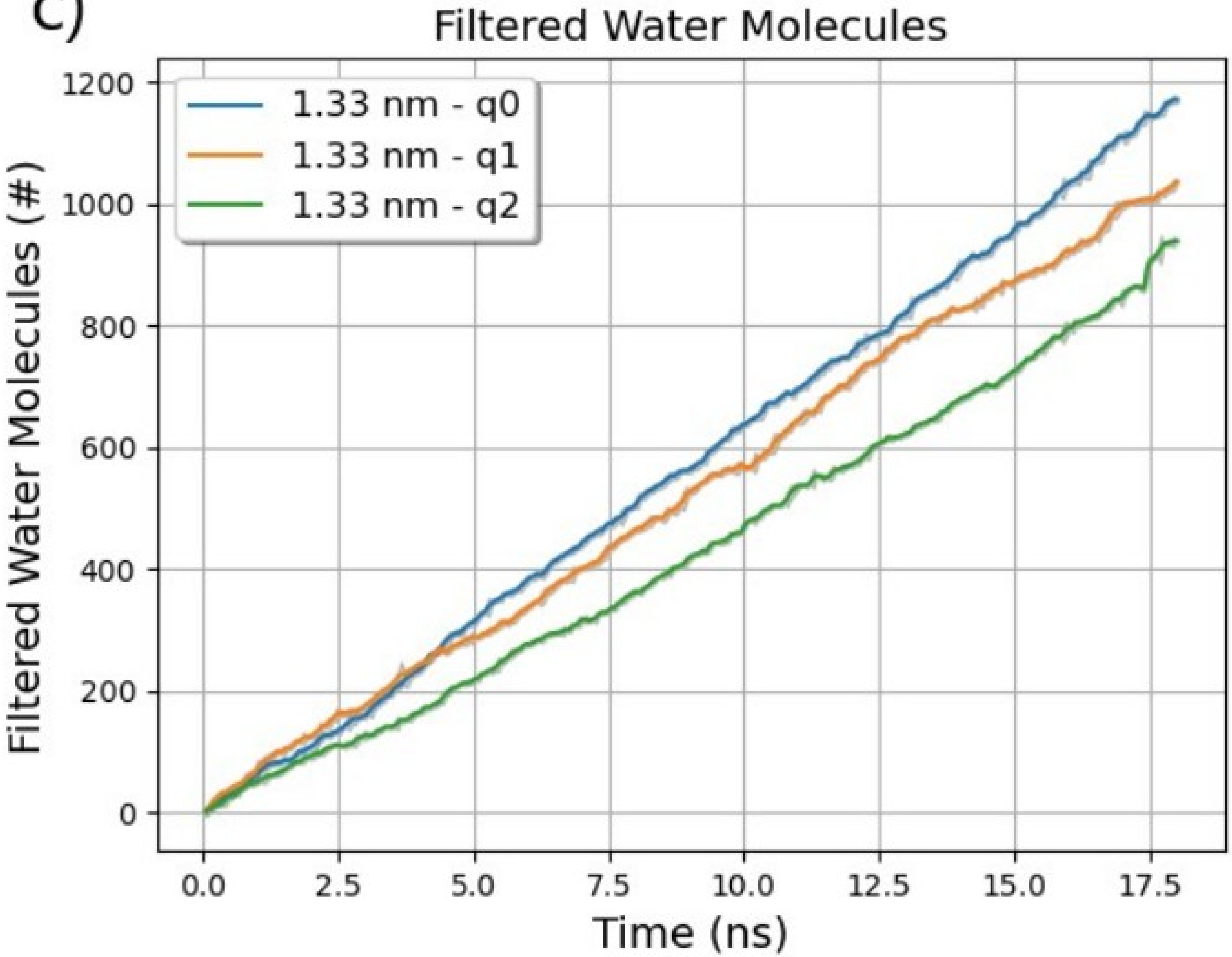

a)
Filtered Water Molecules *
0.74 nm - q0
0.74 nm - q1
0.74 nm - q2
Filtered Water Molecules (#)
Time (ns)
0
50
100
150
200
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5



b)
Filtered Water Molecules
0.97 nm - q0
0.97 nm - q1
0.97 nm - q2
0.97 nm - q2 - 2000bar
Filtered Water Molecules (#)
200
150
100
50
0

Time (ns)

c)

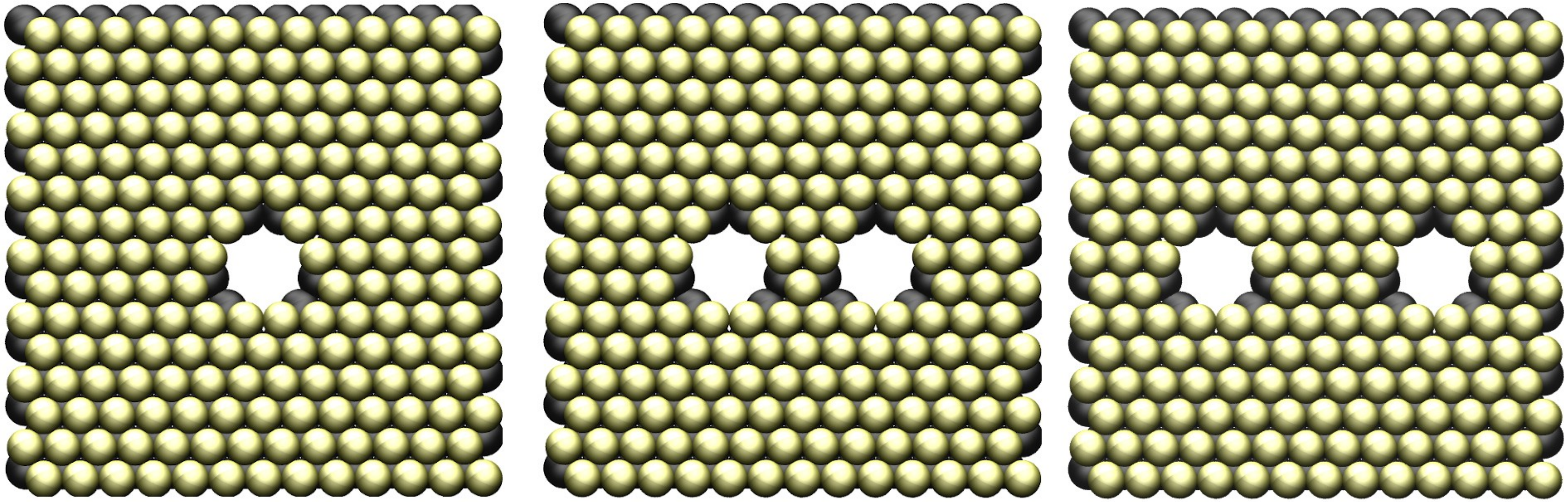

Filtered Water Molecules
1.33 nm - q0
1.33 nm - q1
1.33 nm - q2
Filtered Water Molecules (#)
1200
1000
800
600
400
200
0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Time (ns)

Turbulence?

Abal, Barbosa

Phys. Chem. Chem. Phys. 23, 12075 (2021)

J. Chem. Phys. 154, 134506 (2021)

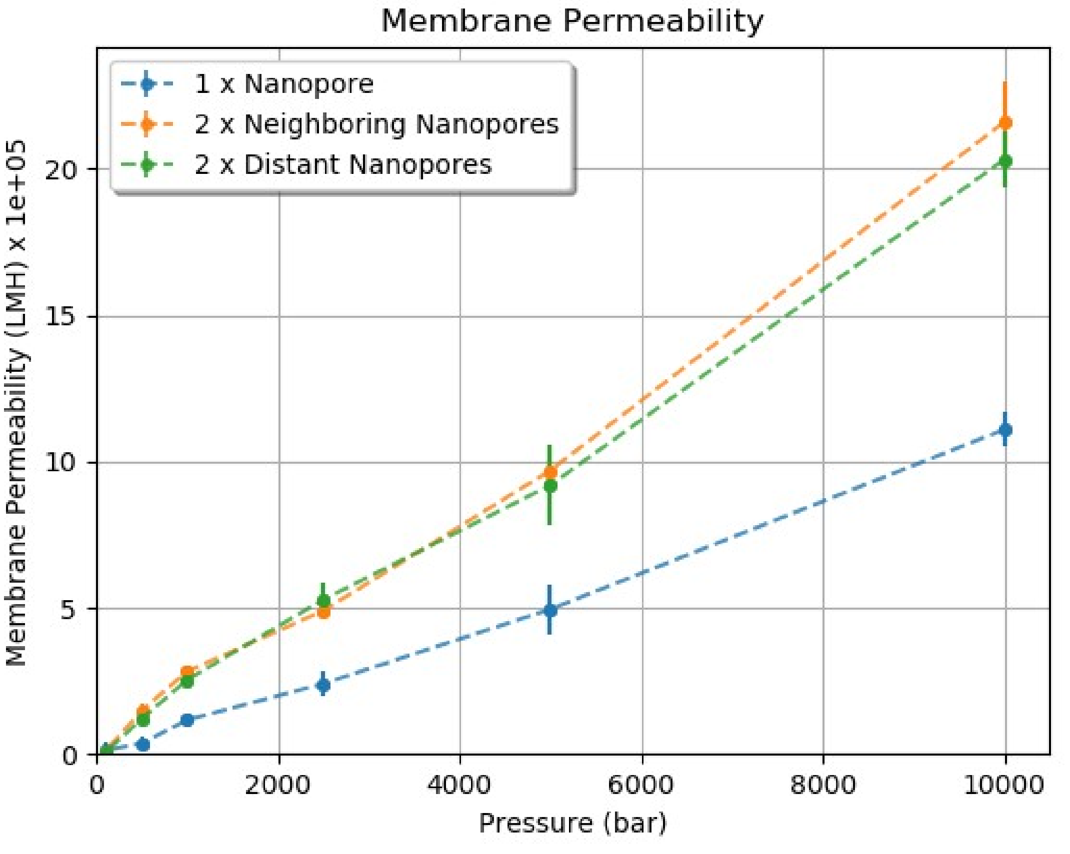


Permeability

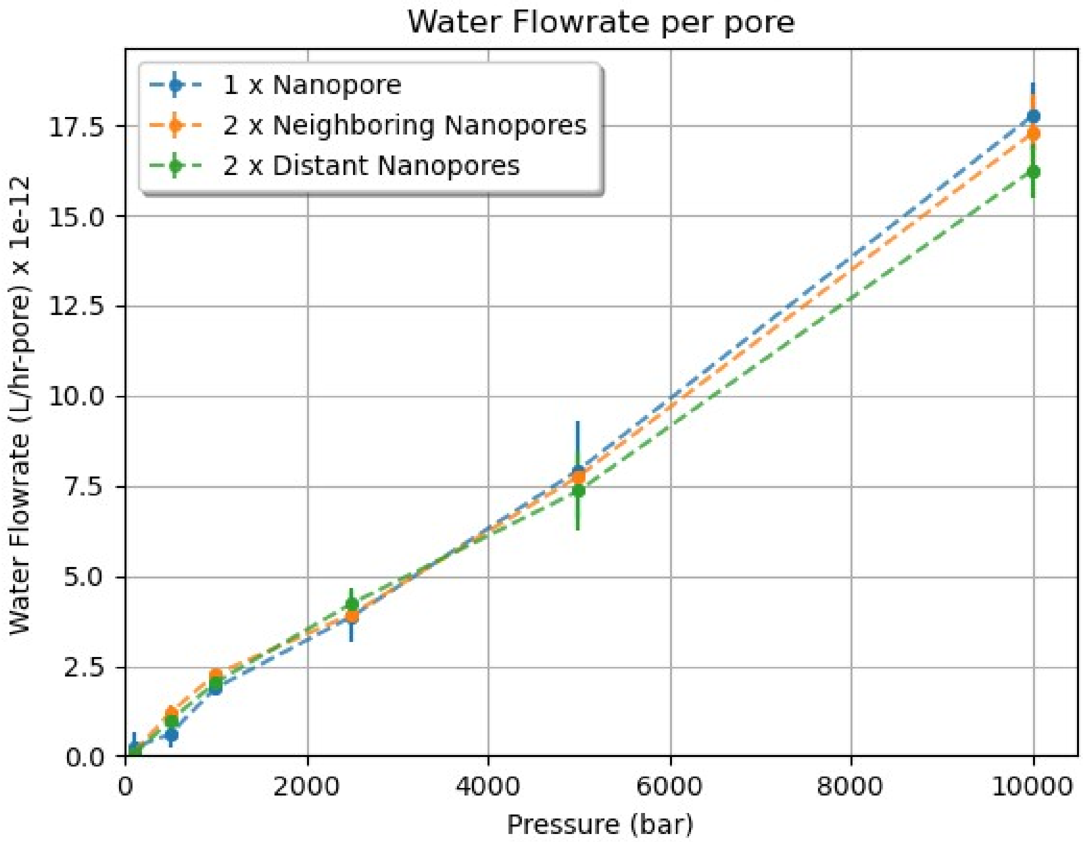
J = volume / Area /time (LMH)

Permeability=J/pressure

Permeability



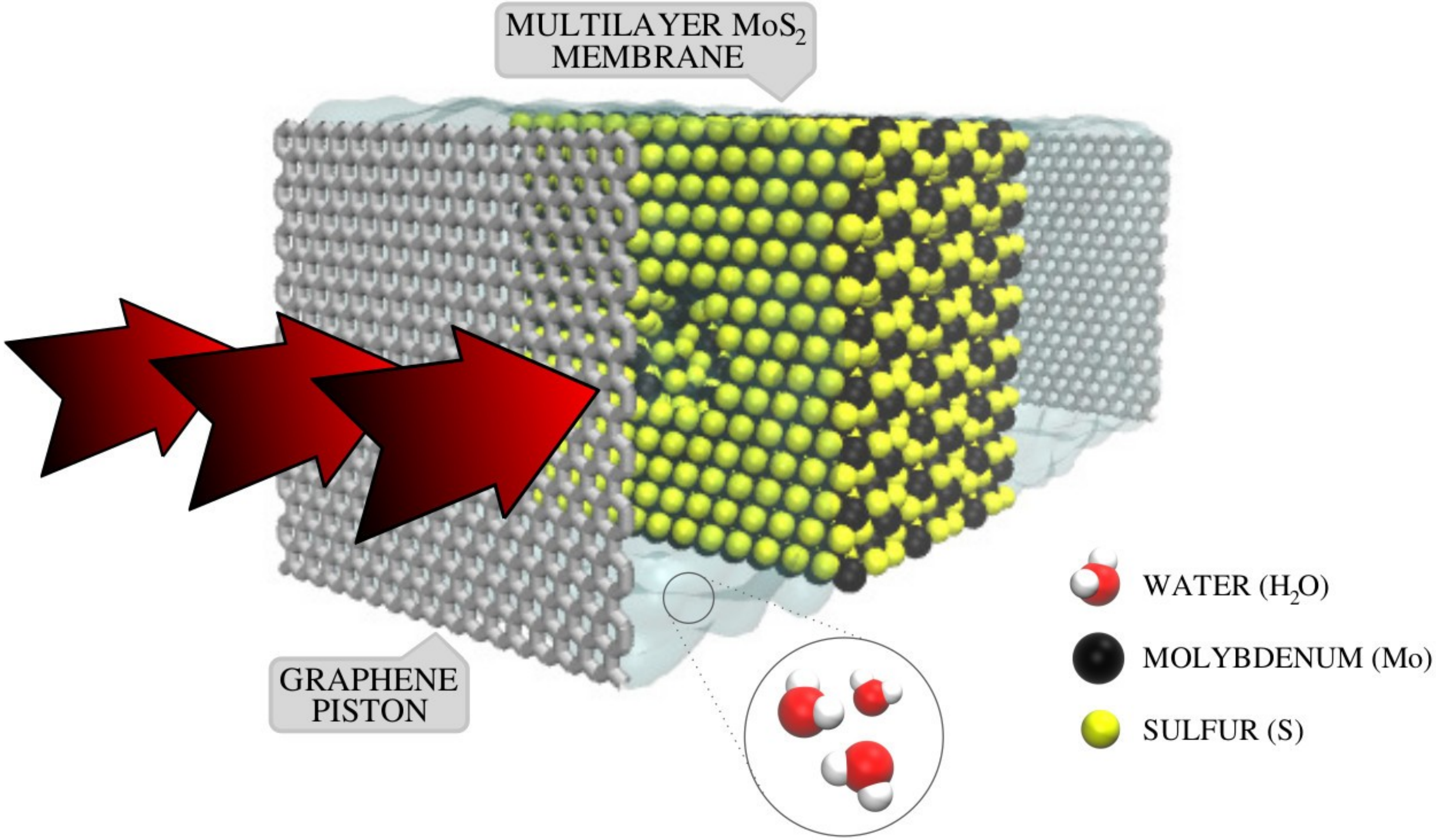
Rejeição de Sal



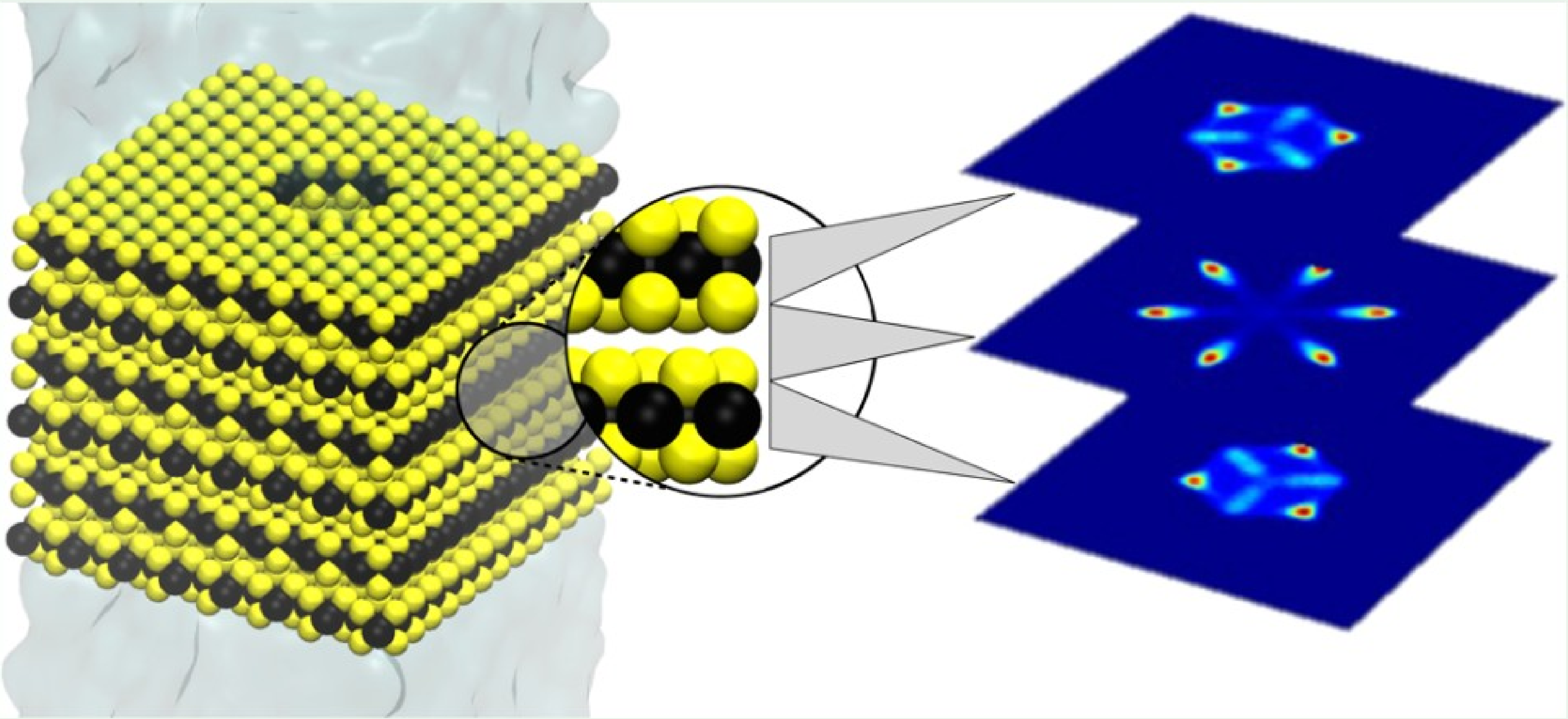
Nanopore to Nanotubes?

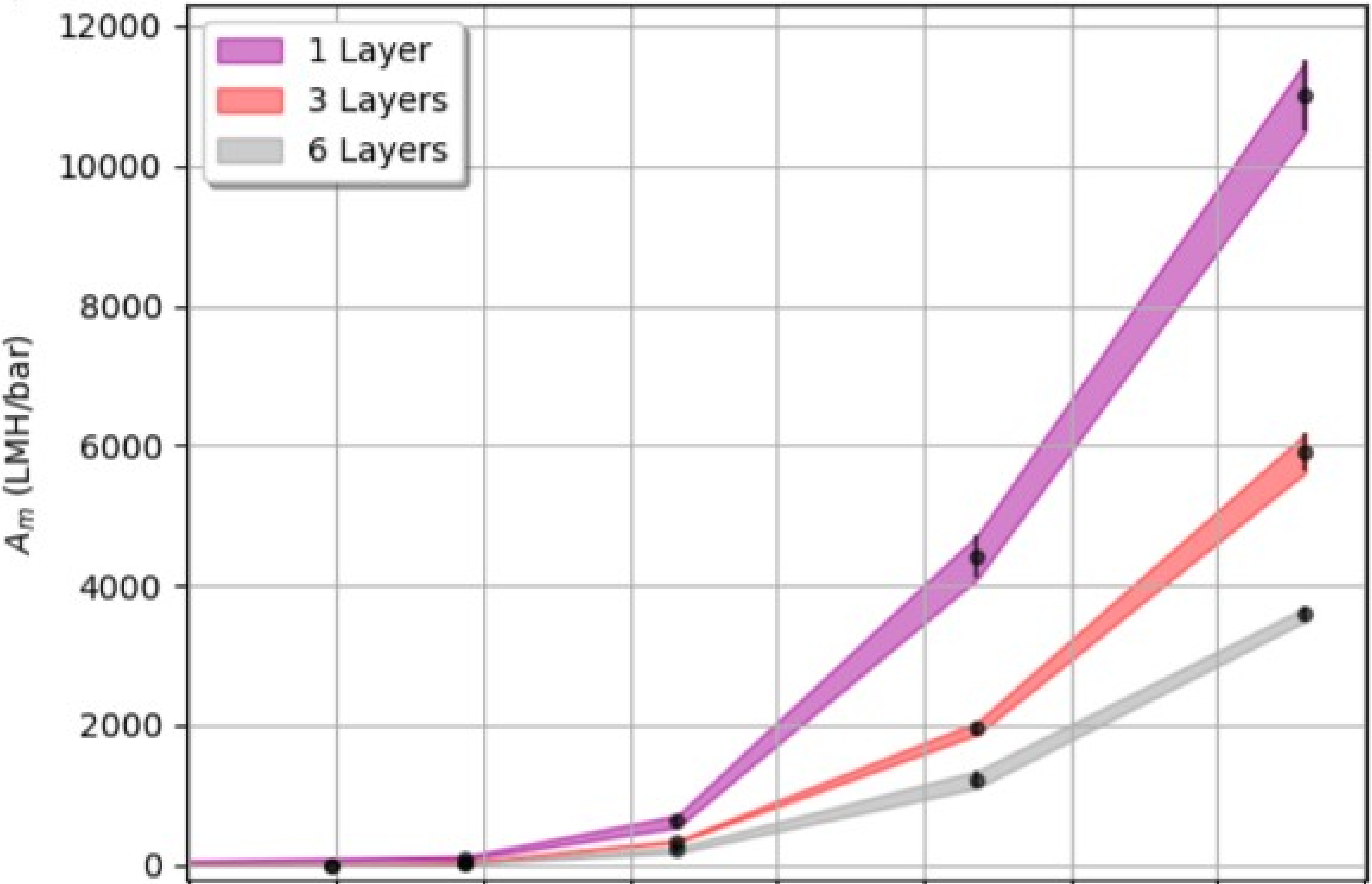
Multilayers

Abal, Dillenburg, Kohler, Barbosa
Applied Nano Materials 4, 10467 (2021)



Multilayers





1 Layer
3 Layers
6 Layers
12000
10000
8000
6000
4000
2000
0
A_m (LMH/bar)