Água

da Era do Gelo à Nanociência

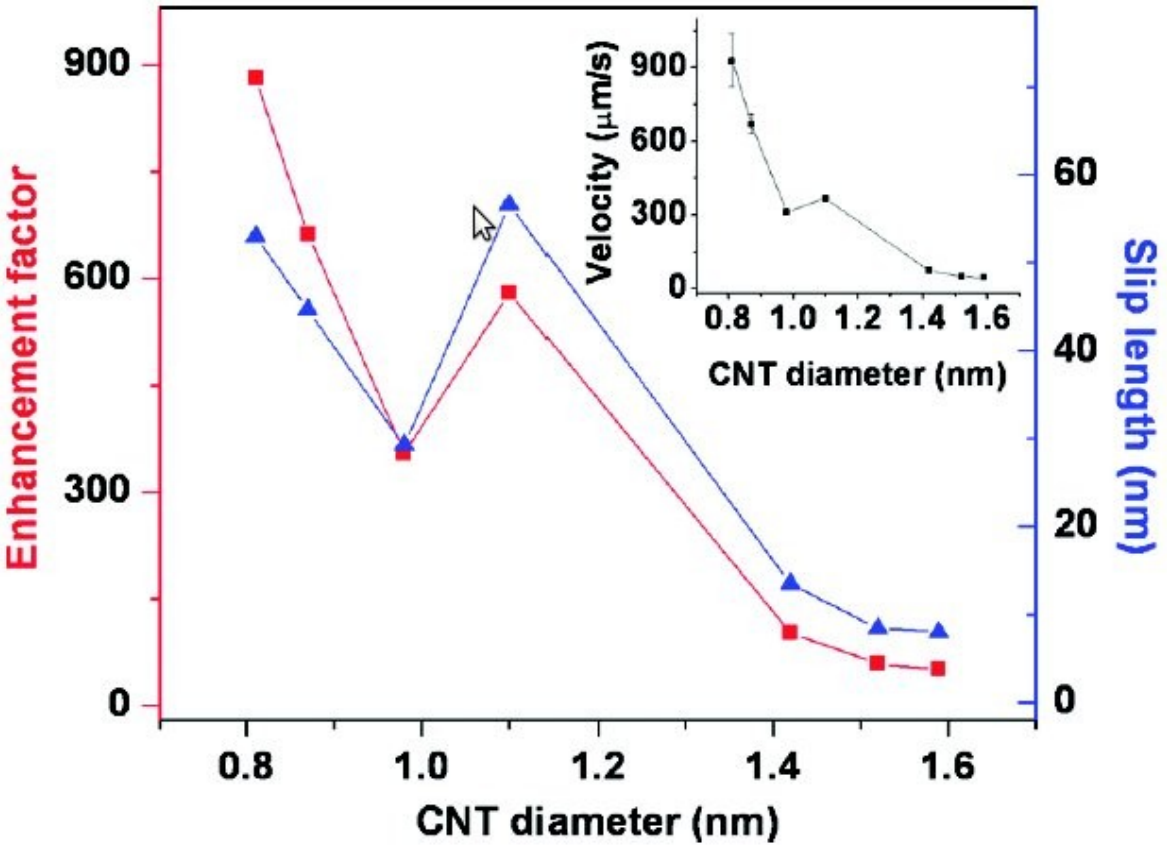


photo by Clóvis Jardim

QUAL É O PROBLEMA?

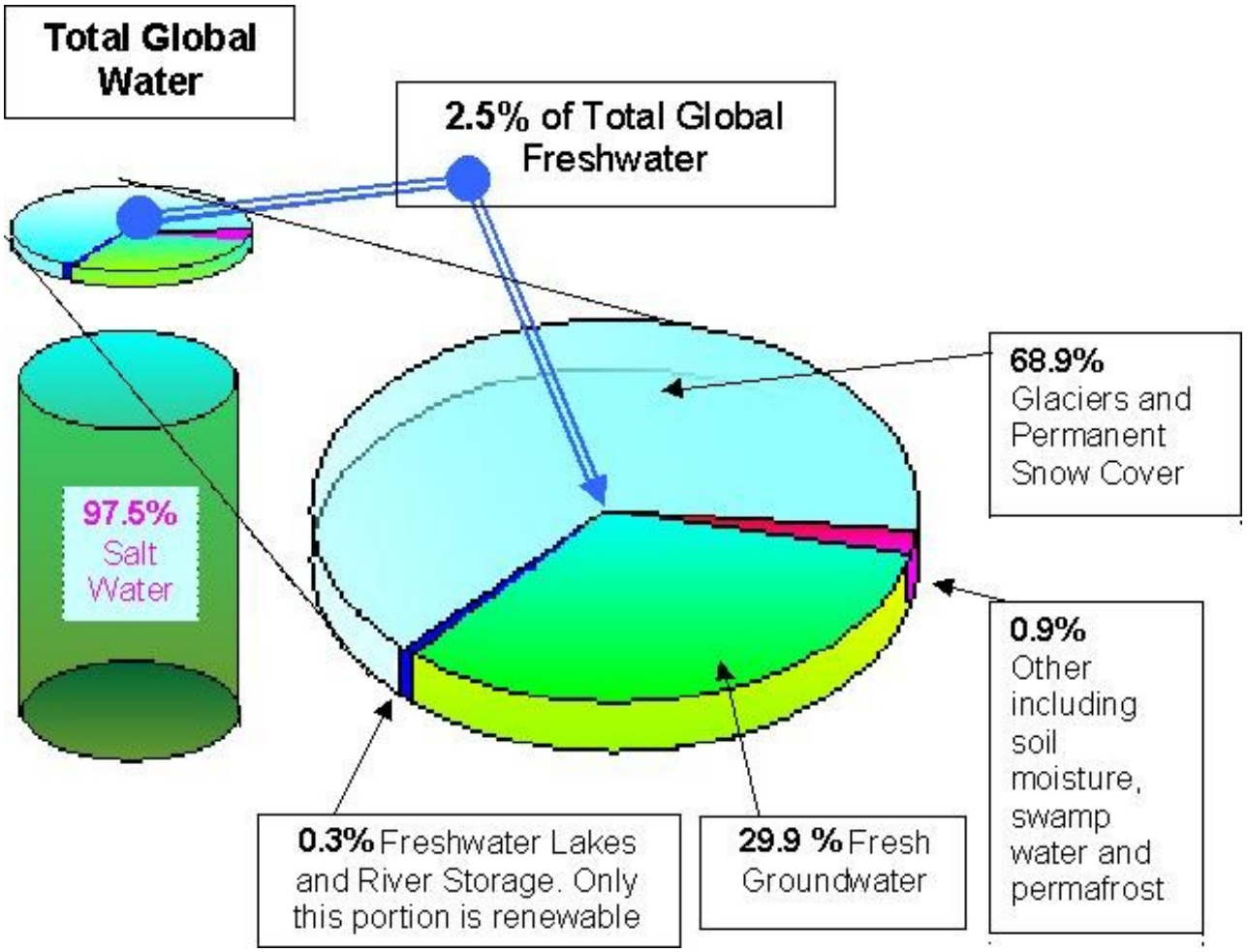
Super Fluxo

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

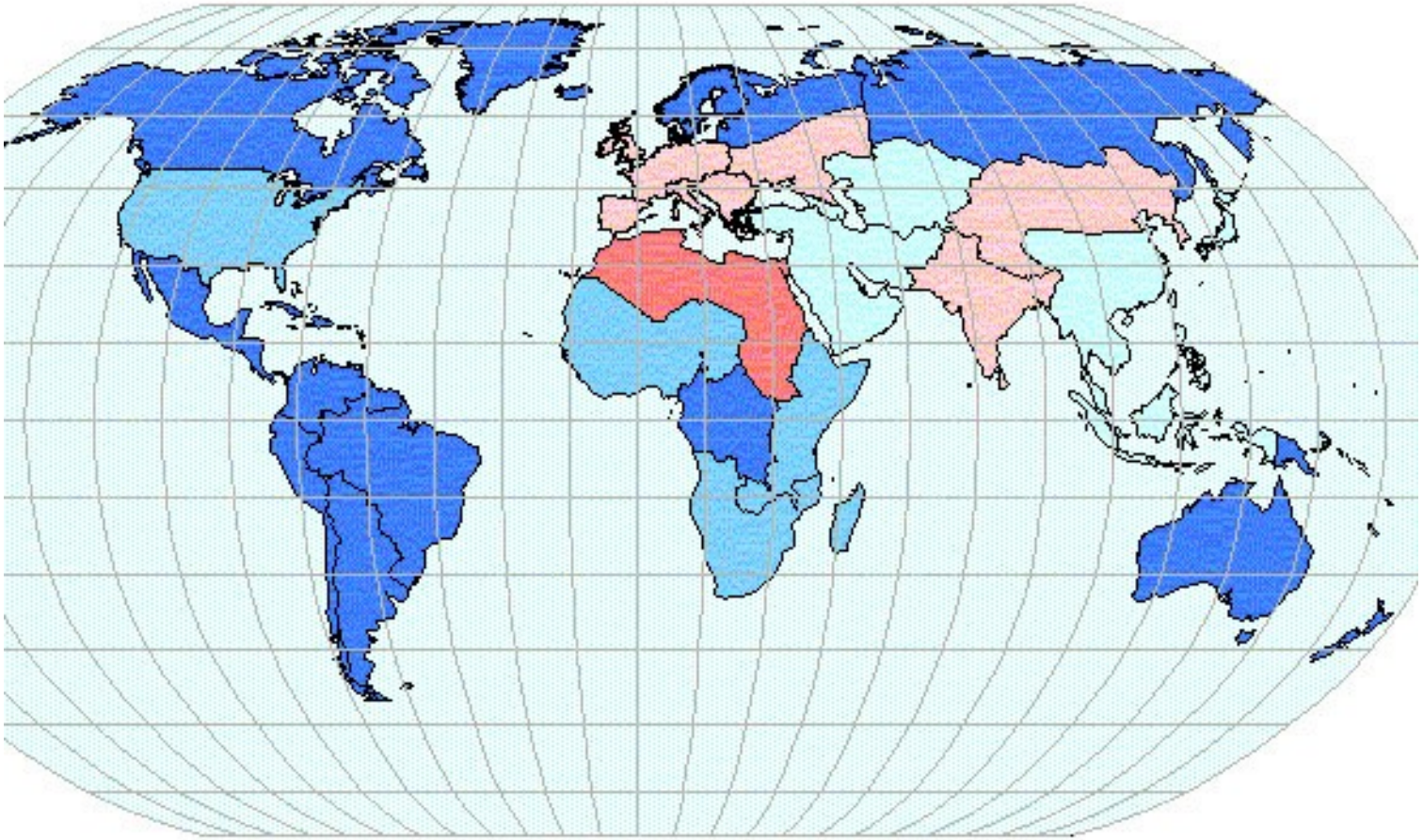


Por que se importar?

Água

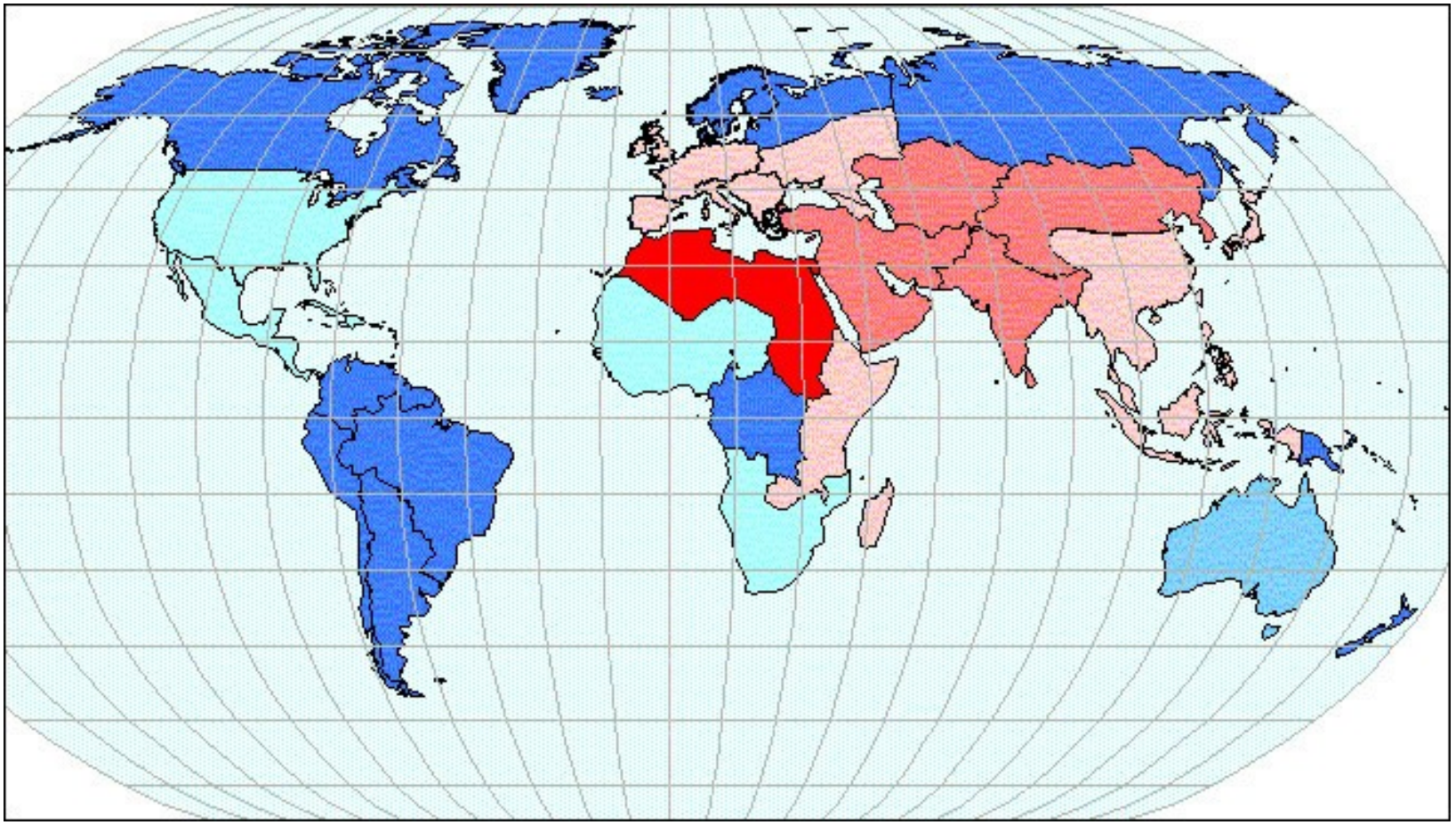

Total Global Water
2.5% of Total Global Freshwater
97.5% Salt Water
68.9% Glaciers and Permanent Snow Cover
0.9% Other including soil moisture, swamp water and permafrost
0.3% Freshwater Lakes and River Storage. Only this portion is renewable
29.9 % Fresh Groundwater

Stress



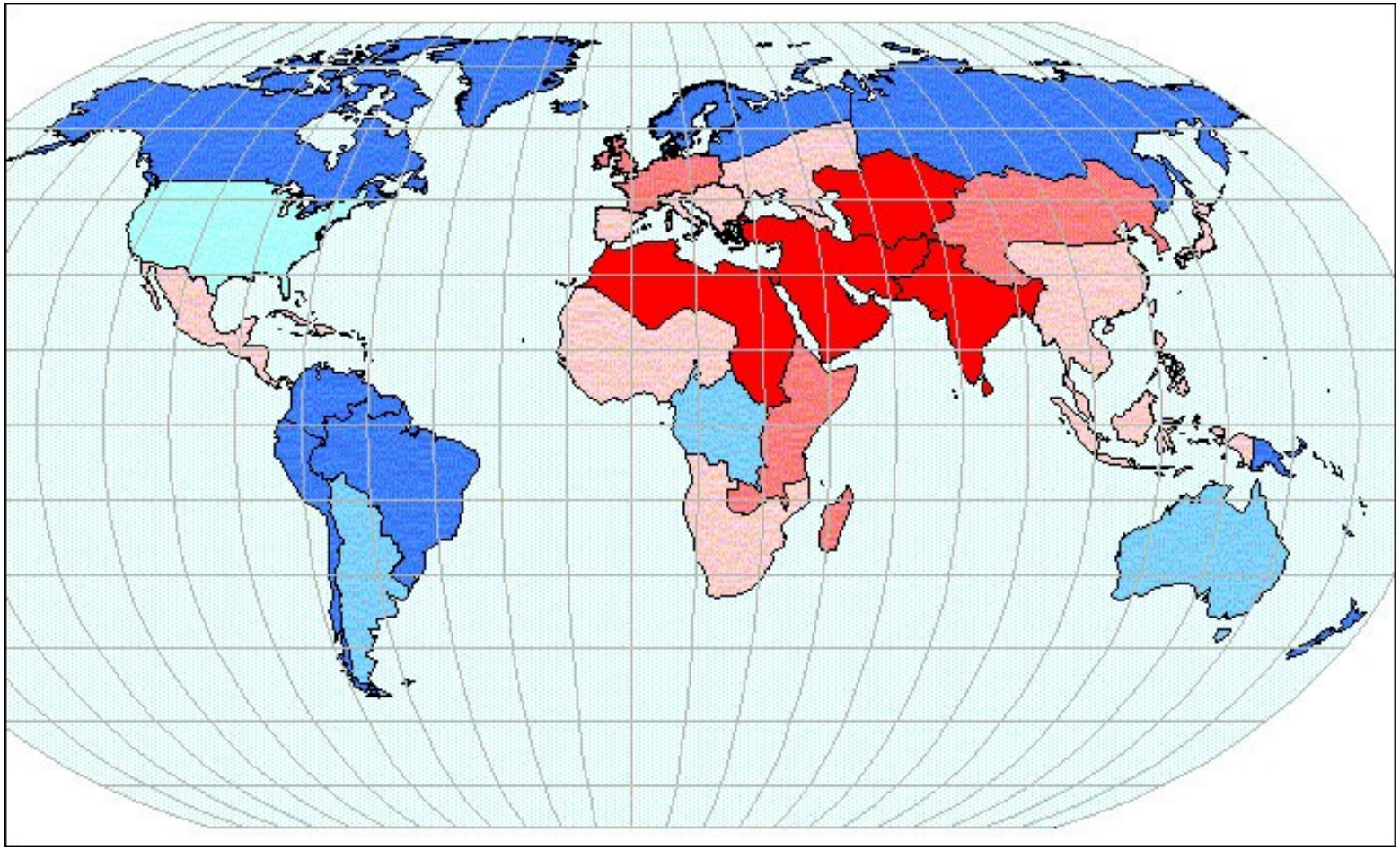
1950

Stress



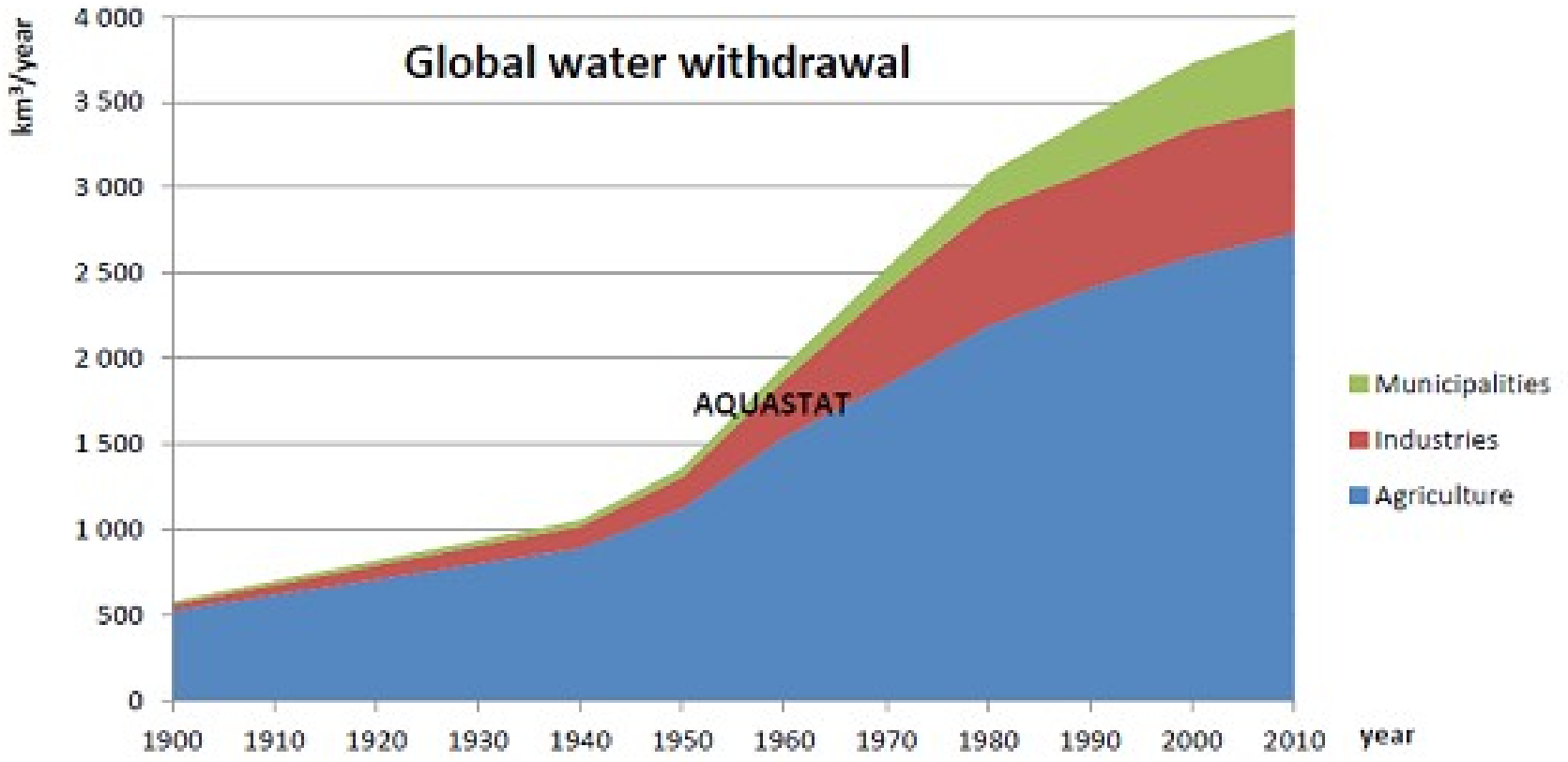
1995

Stress



2025

Água

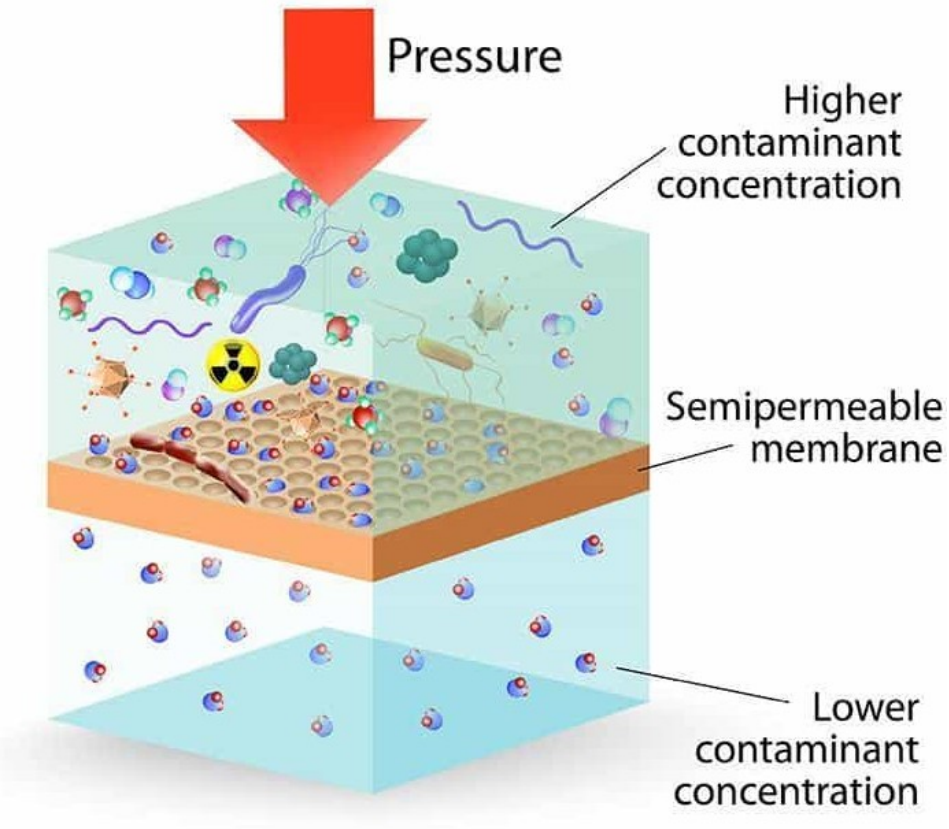

Global water withdrawal
km³/year
4 000
3 500
3 000
2 500
2 000
1 500
1 000
500
0
1900
1910
1920
1930
1940
1950
1960
1970
1980
1990
2000
2010
year
AQUASTAT
Municipalities
Industries
Agriculture

O QUE AS PESSOAS

TEM

FEITO?

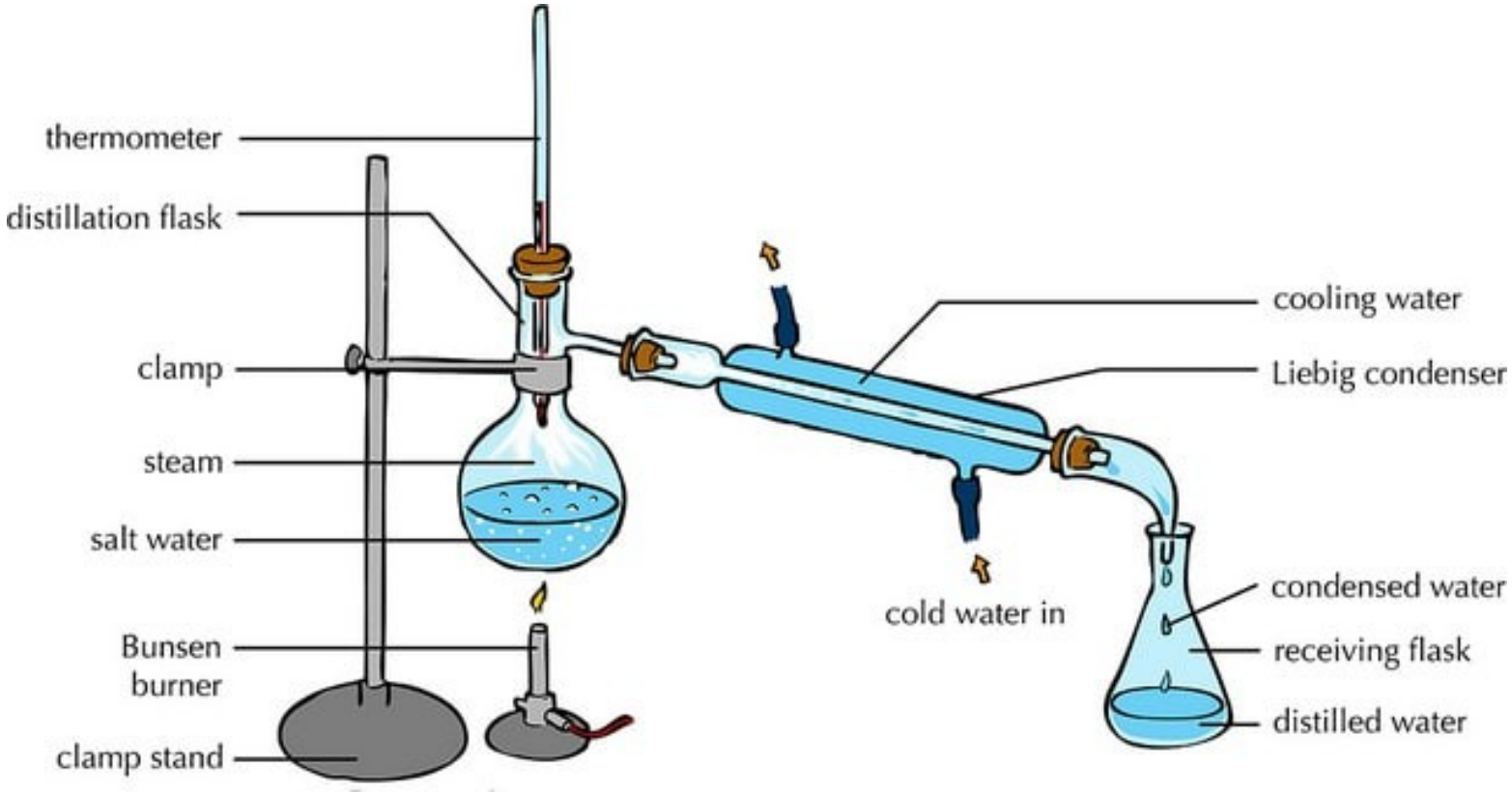
Osmose Reversa



Problema da Osmose Reversa: Tamanho e Energia



Distilação


thermometer
distillation flask
clamp
steam
salt water
Bunsen burner
clamp stand
cooling water
Liebig condenser
cold water in
condensed water
receiving flask
distilled water

Problema da Distilação: Tamanho e Energia



QUAL A NOSSA IDEIA?

Água tem mais de 70 anomalias

Elas são úteis para a vida

Por que não usar depois de compreender esta anomalia para ter água potável?

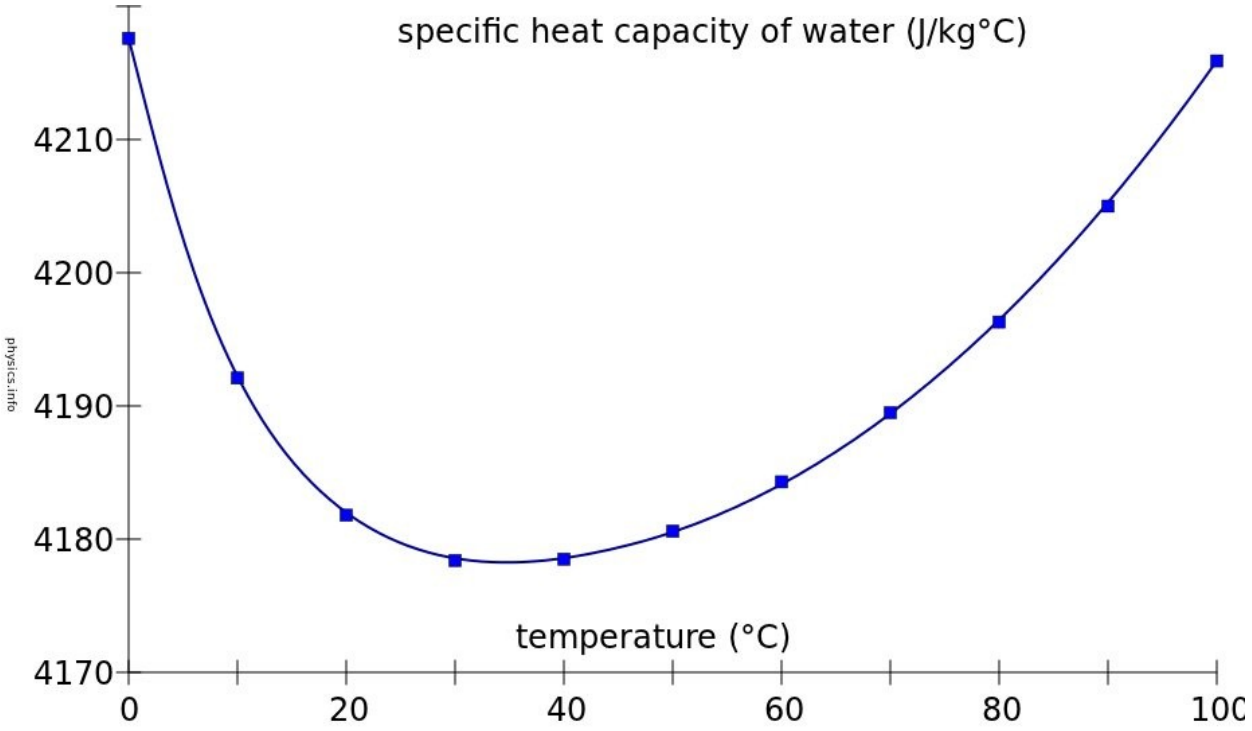
ANOMALIAS

DA

ÁGUA?

Calor Específico

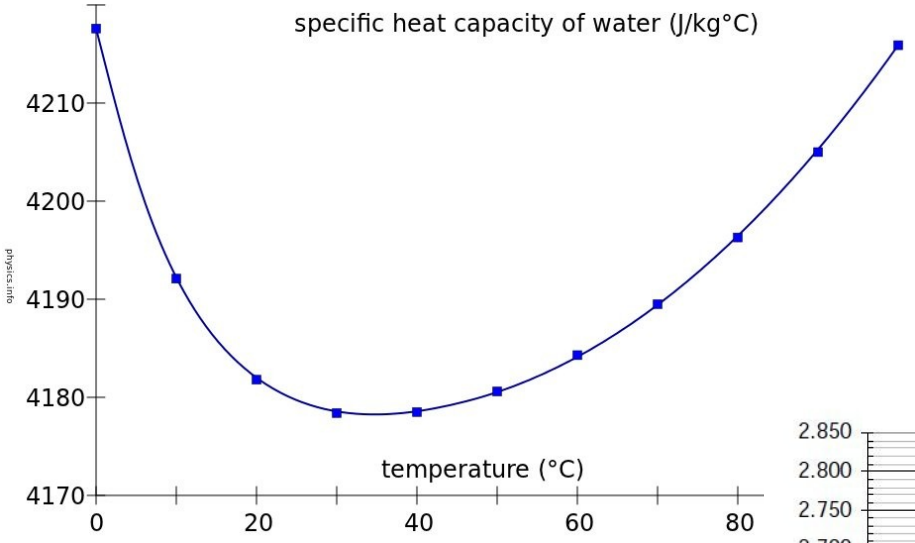
Methanol: Lombari, Ferrari, Salvetti, CPL 300 (99)
Water: G. S. Kell, J. Chem. Eng. Data 20, 97 (75)



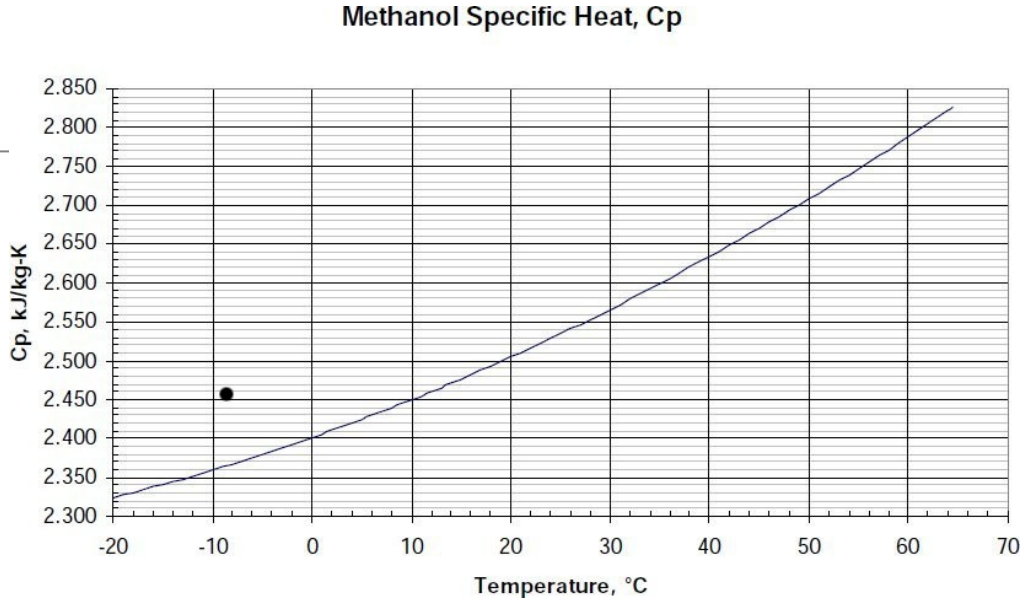
$$C_p = dQ_P/dT$$

Calor Específico

Methanol: Lombari, Ferrari, Salvetti, CPL 300 (99)
Water: G. S. Kell, J. Chem. Eng. Data 20, 97 (75)



$$C_p = dQ_P/dT$$



Qual é a importância?

Calor Específico



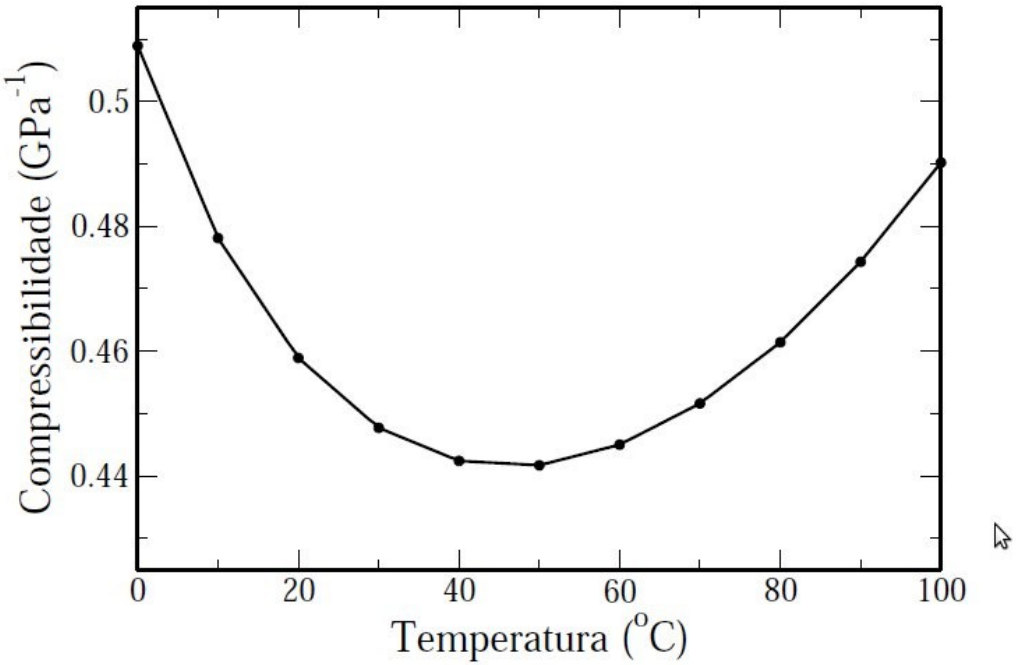
Água → 4,18 kJ/kg°C

Sílica → 0,68 kJ/kg°C

Compressibilidade

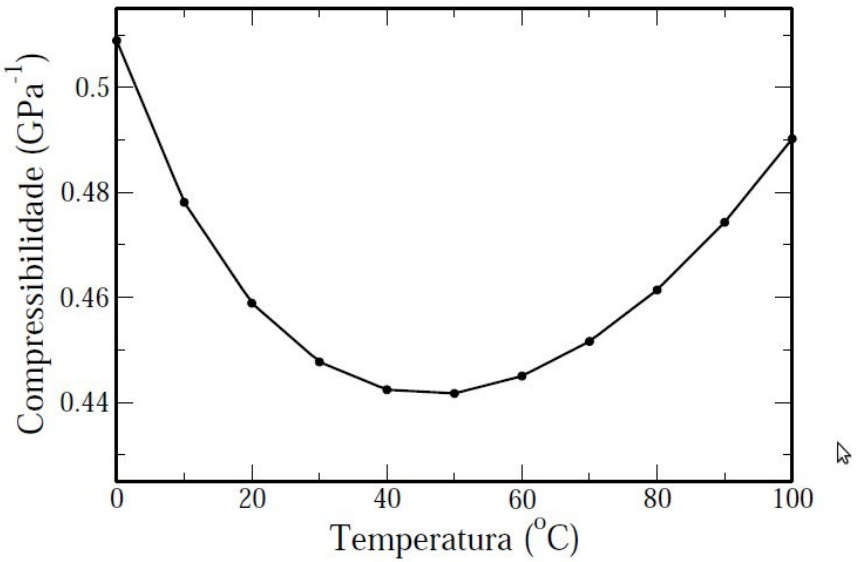
water: Speedy, Angell, JCP 65, 351 (76)
toluene: Minassian, Bouzar, Alba, JPC 92, 487 (88)

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

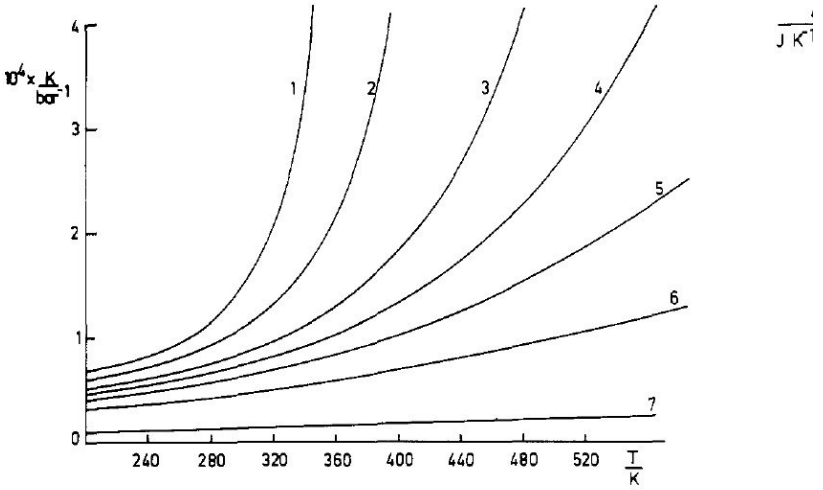


Compressibilidade

water: Speedy, Angell, JCP 65, 351 (76)
toluene: Minassian, Bouzar, Alba, JPC 92, 487 (88)



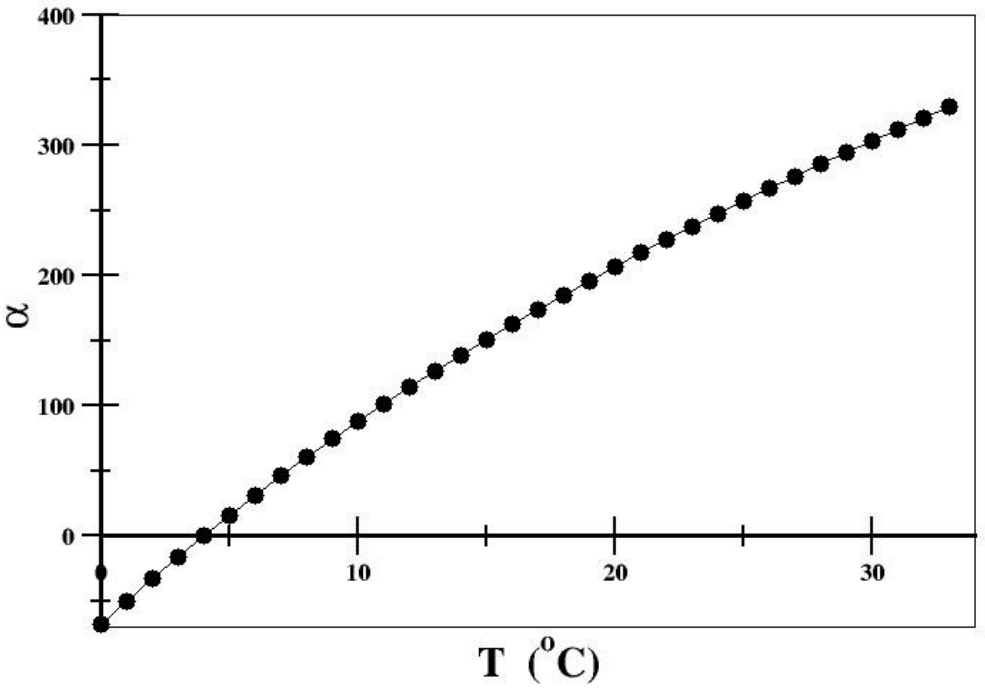
$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T ,$$



Coeficiente Expansão Térmica

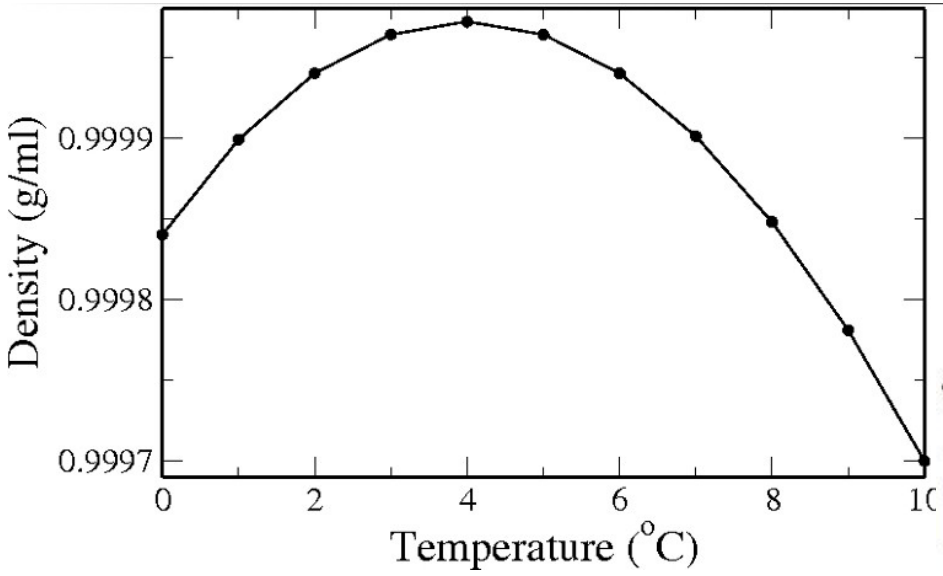
water: Kell, J. Chem. Eng. Data 20, 97 (75)

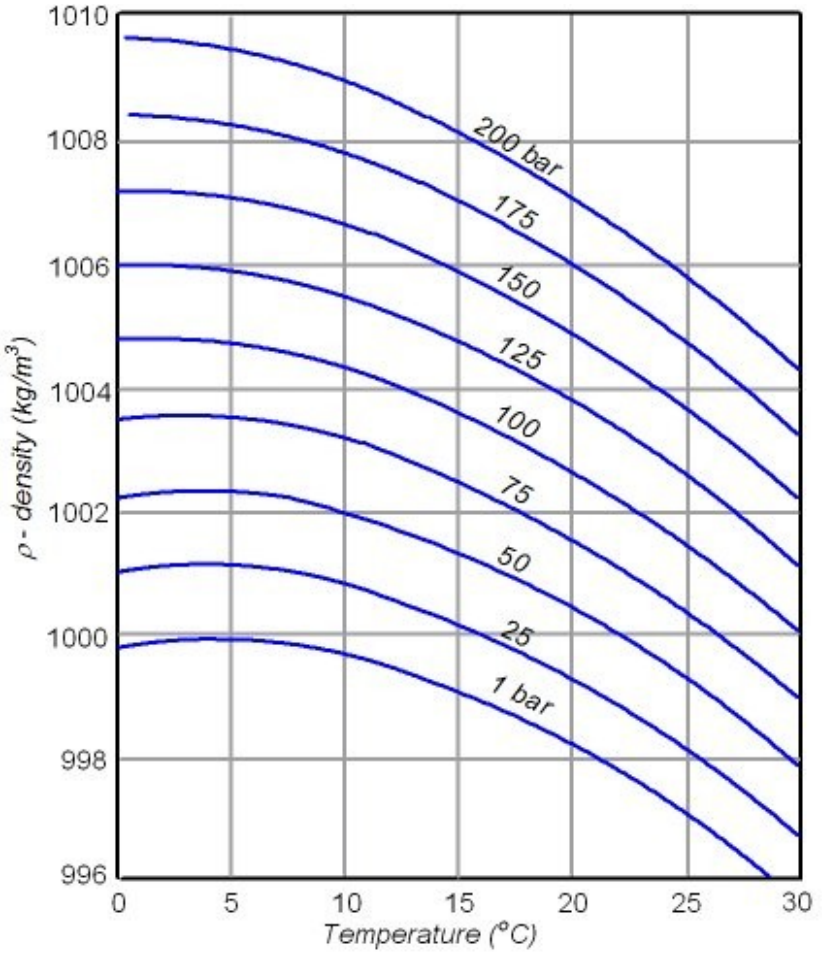
$$\alpha = \alpha_V = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p$$



Densidade várias Pressões

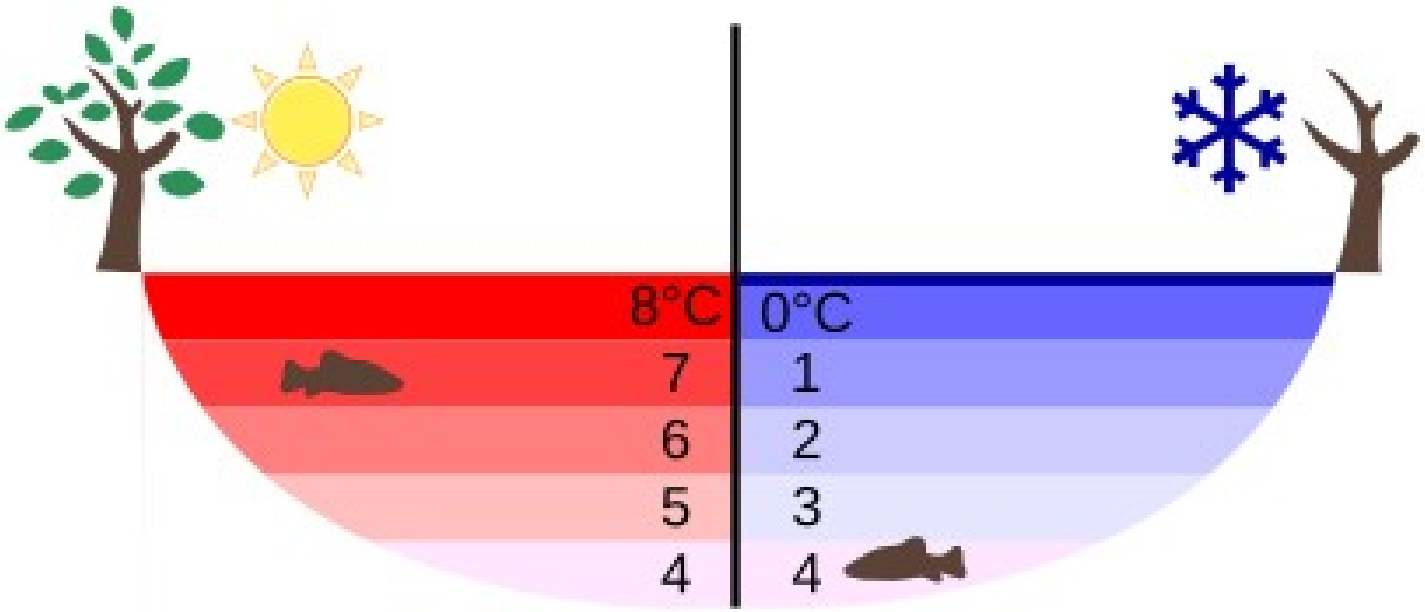
water: Kell, J. Chem. Eng. Data 20, 97 (75)





Densidade e a Vida

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



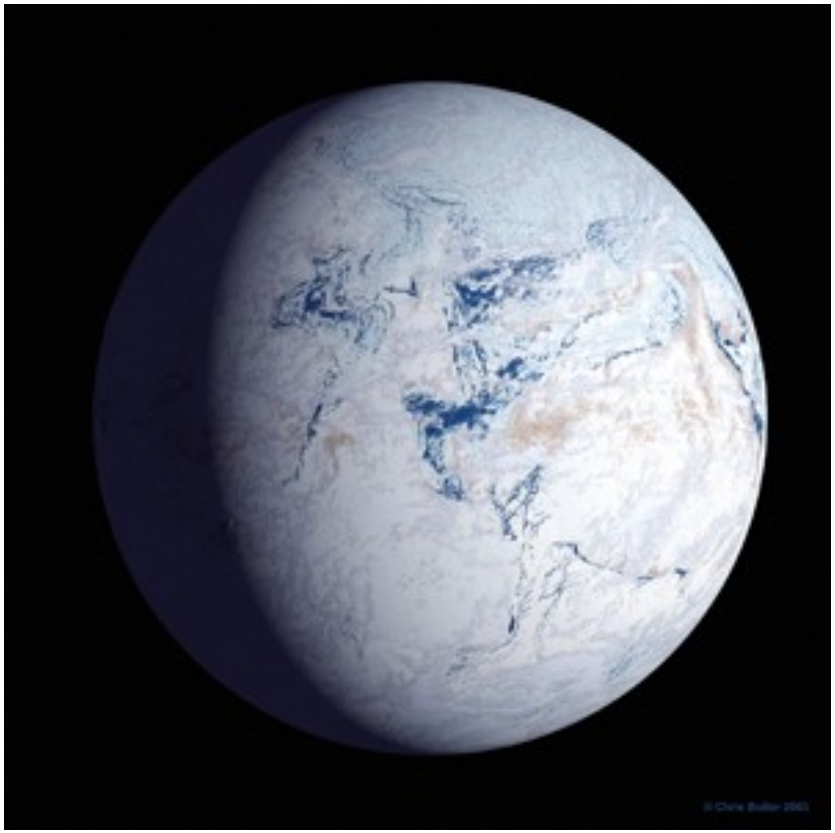
Densidade e Outros Materiais

Gelo vs. Parafina



Água – Vida - Gelo

Ice Age



An artist's impression of 'Snowball Earth.' (Image: NASA)

Jupiter's moon Europa
NASA's Galileo
Credit:
NASA/JPL-Caltech/SETI

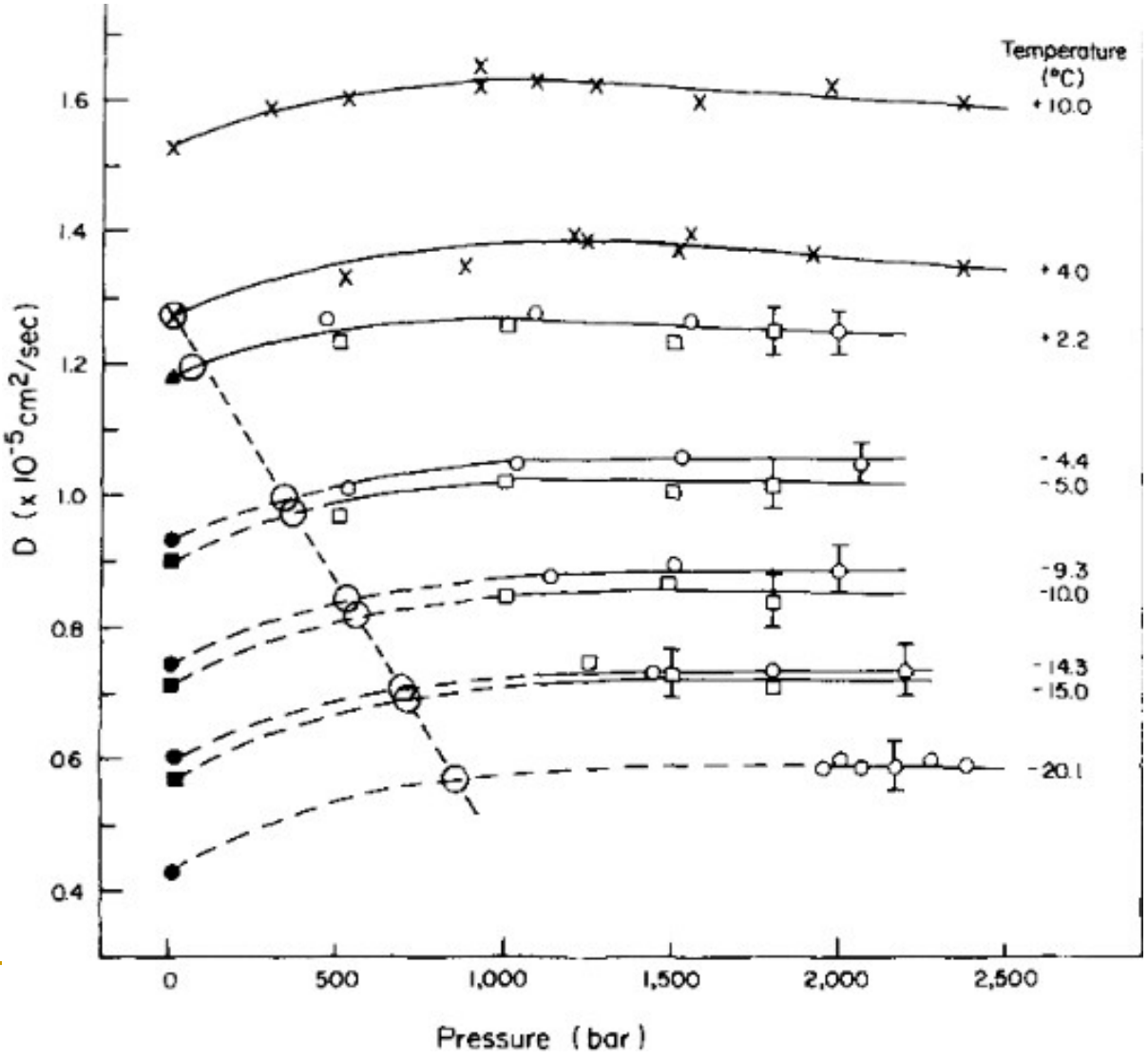


Difusão

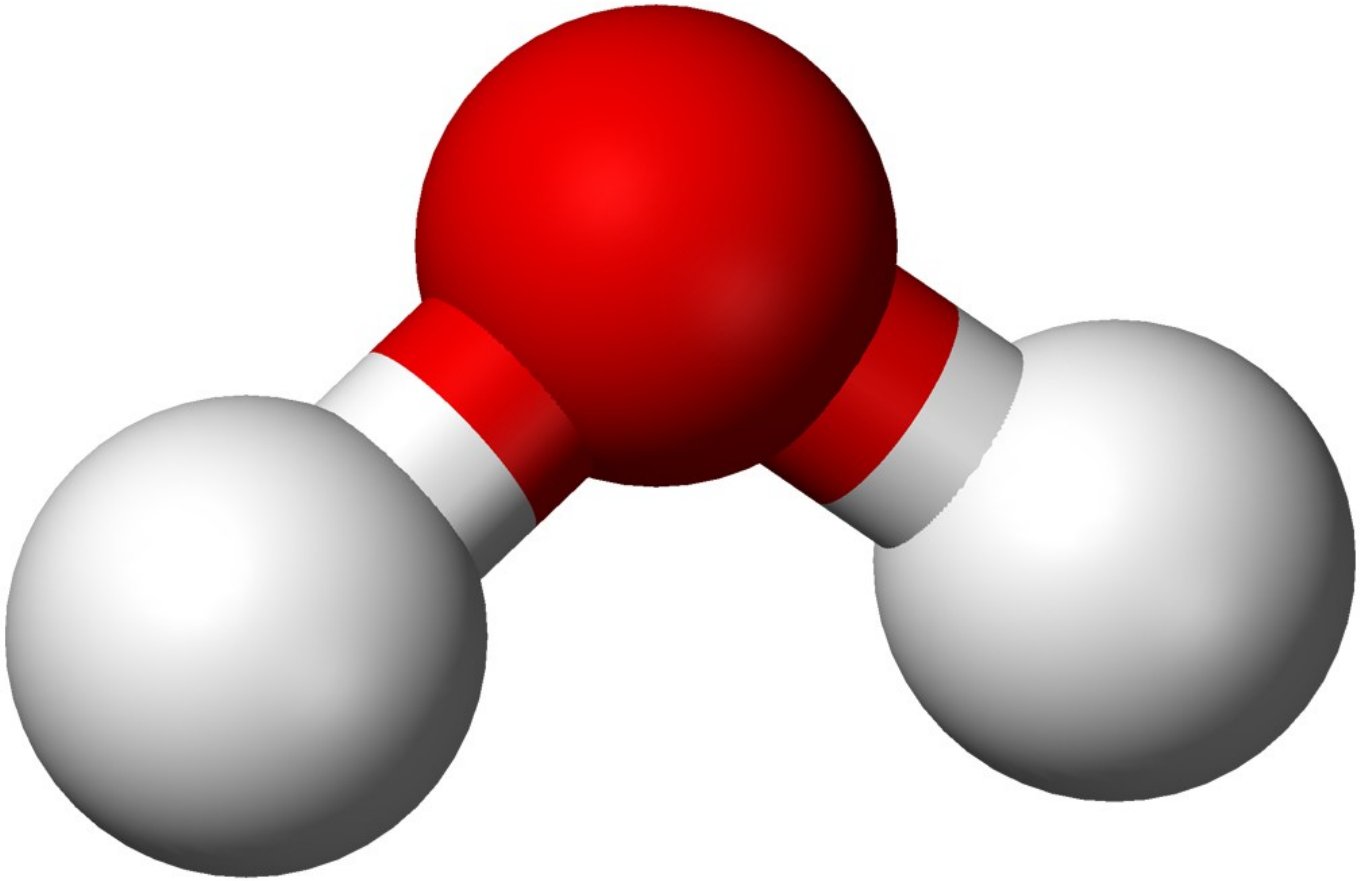
Angell, Finch, Bach JCP 65, 3063 (76)

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

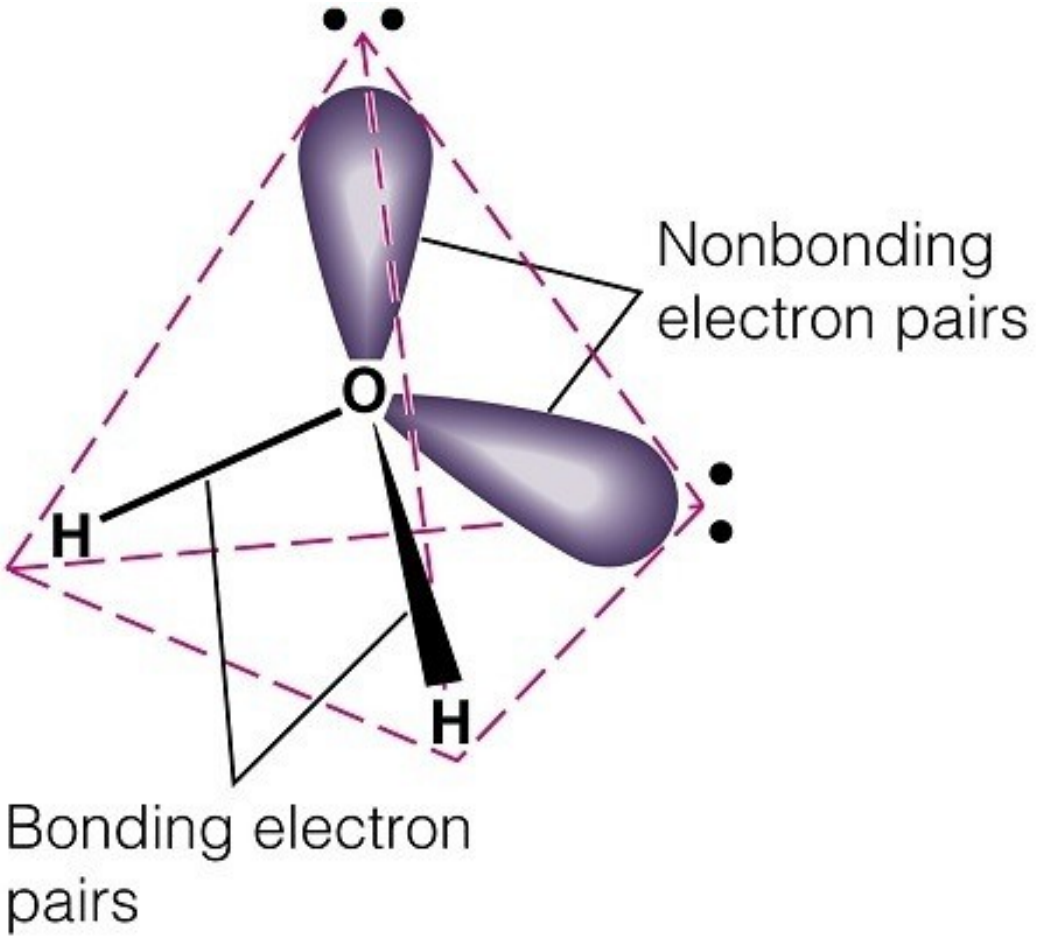
$$<\Delta^2 r(t)> \sim 6Dt$$



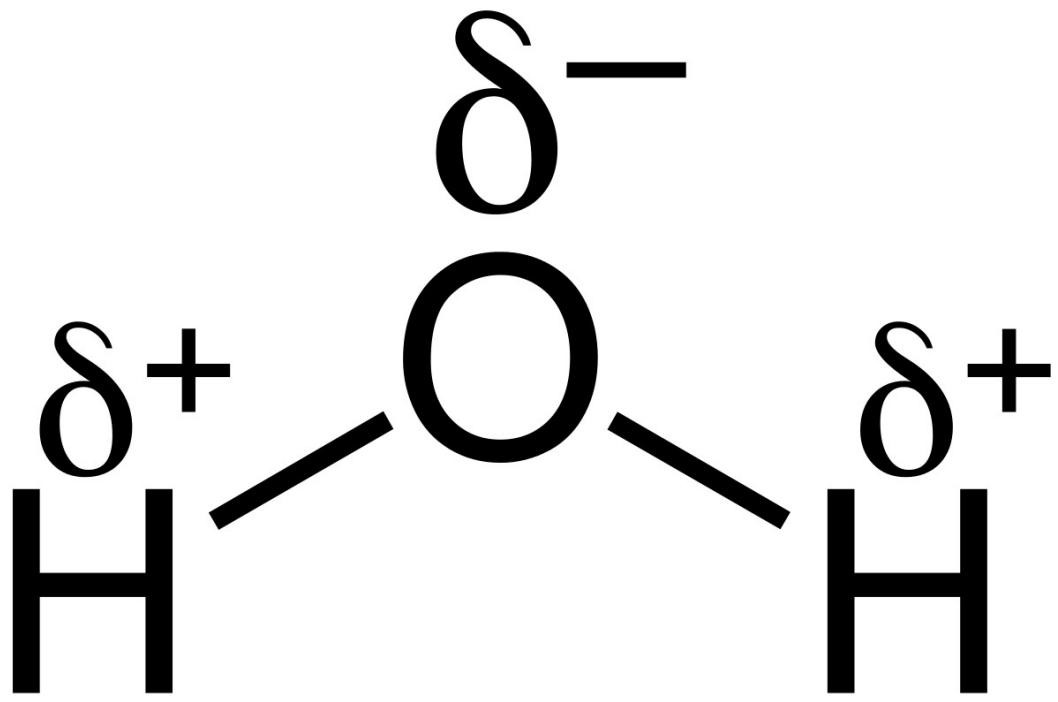
Água



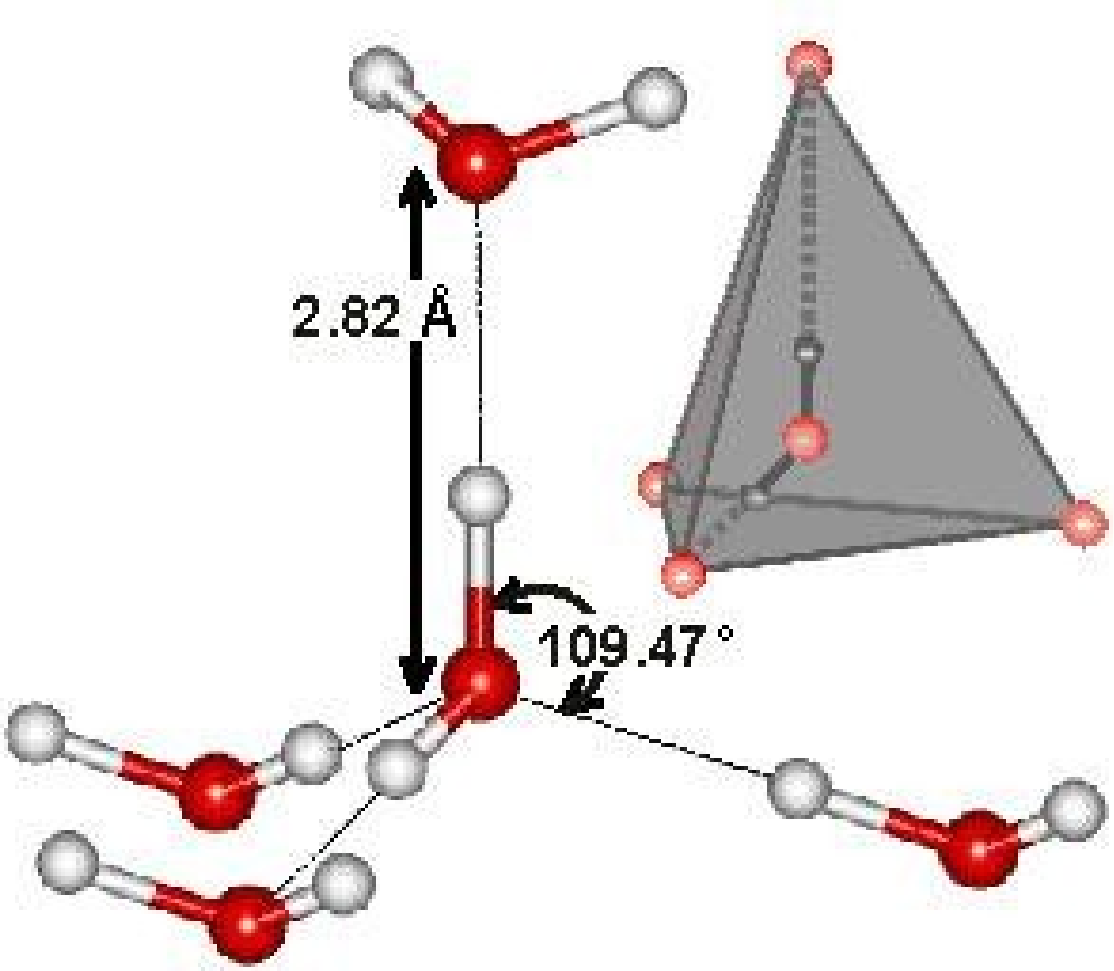
Água



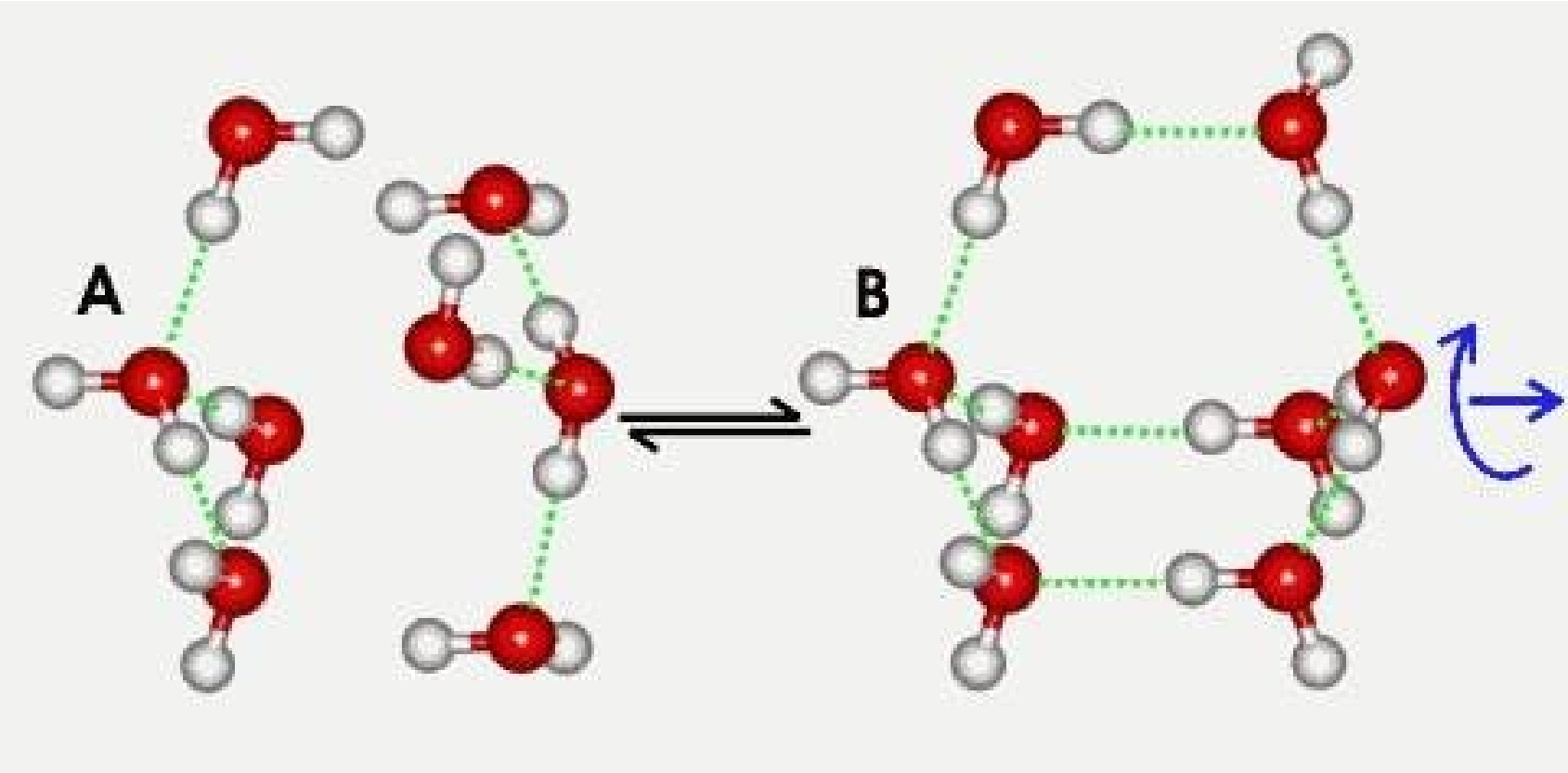
Água



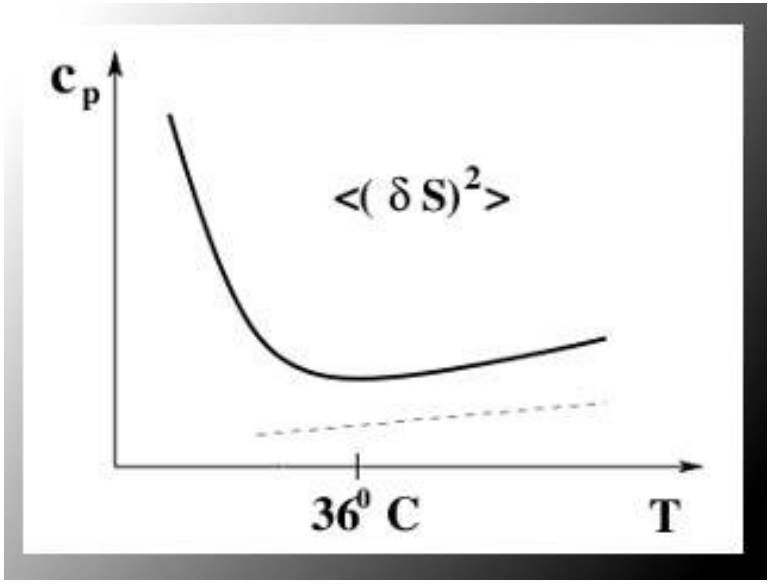
Ligações de Hidrogêni

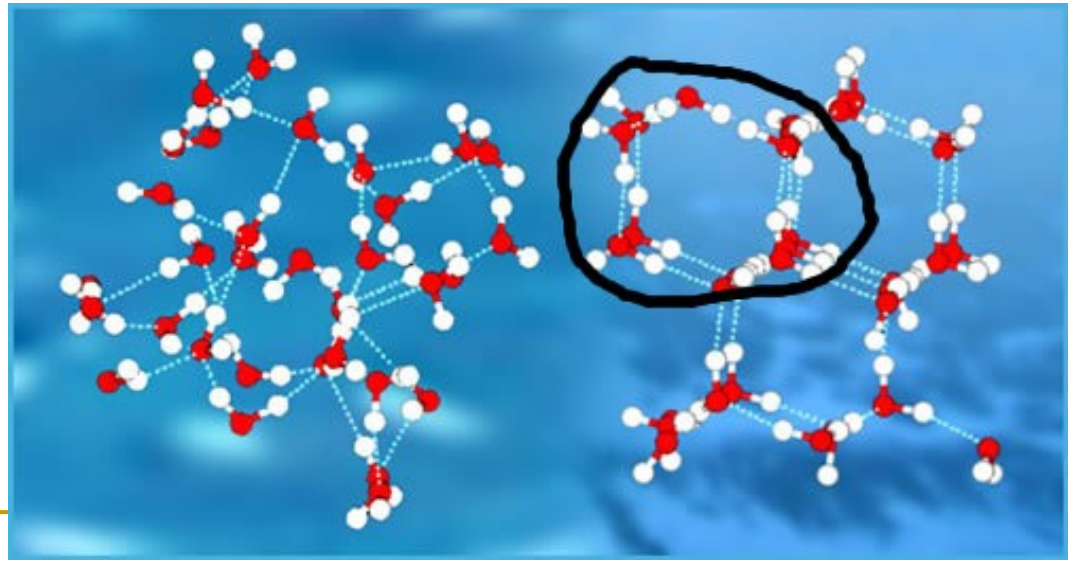


Tetrâmeros Abertos e Fechados

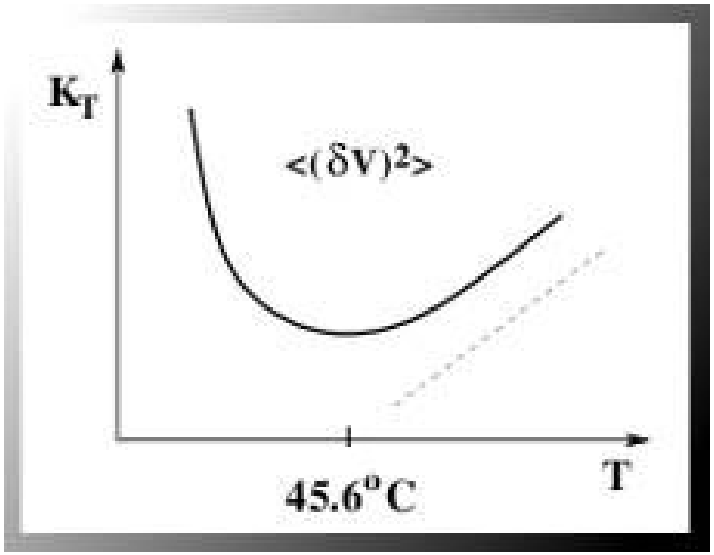


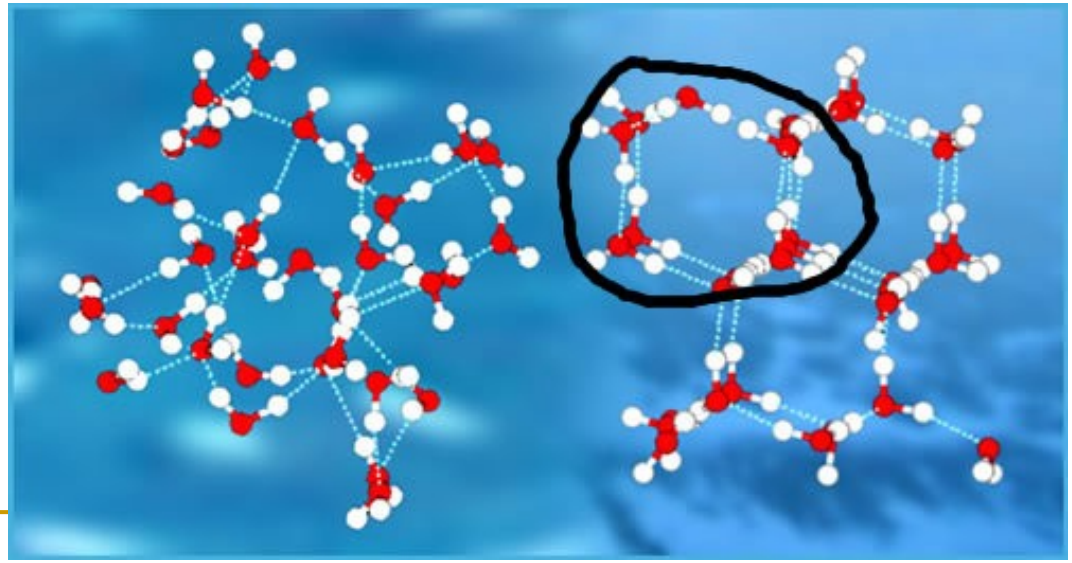
Calor Específico



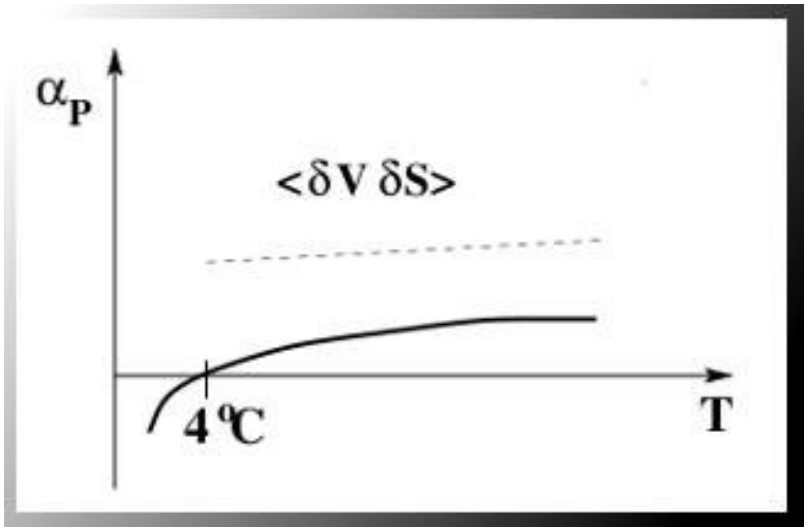


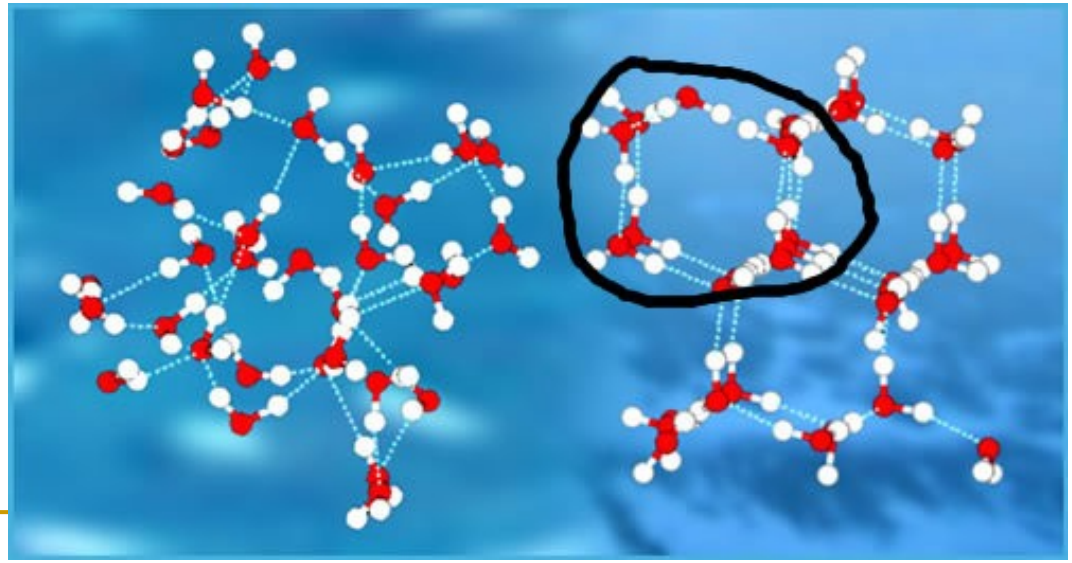
Compressibilidade





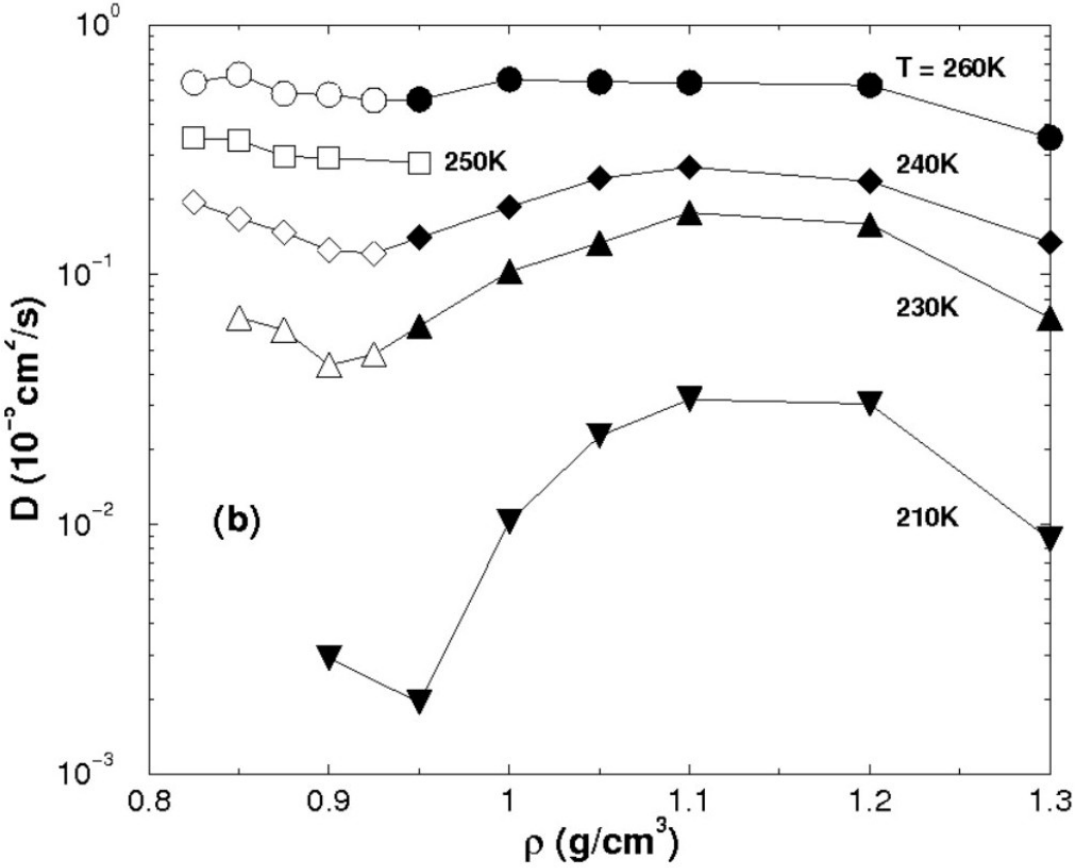
Expansão Térmica





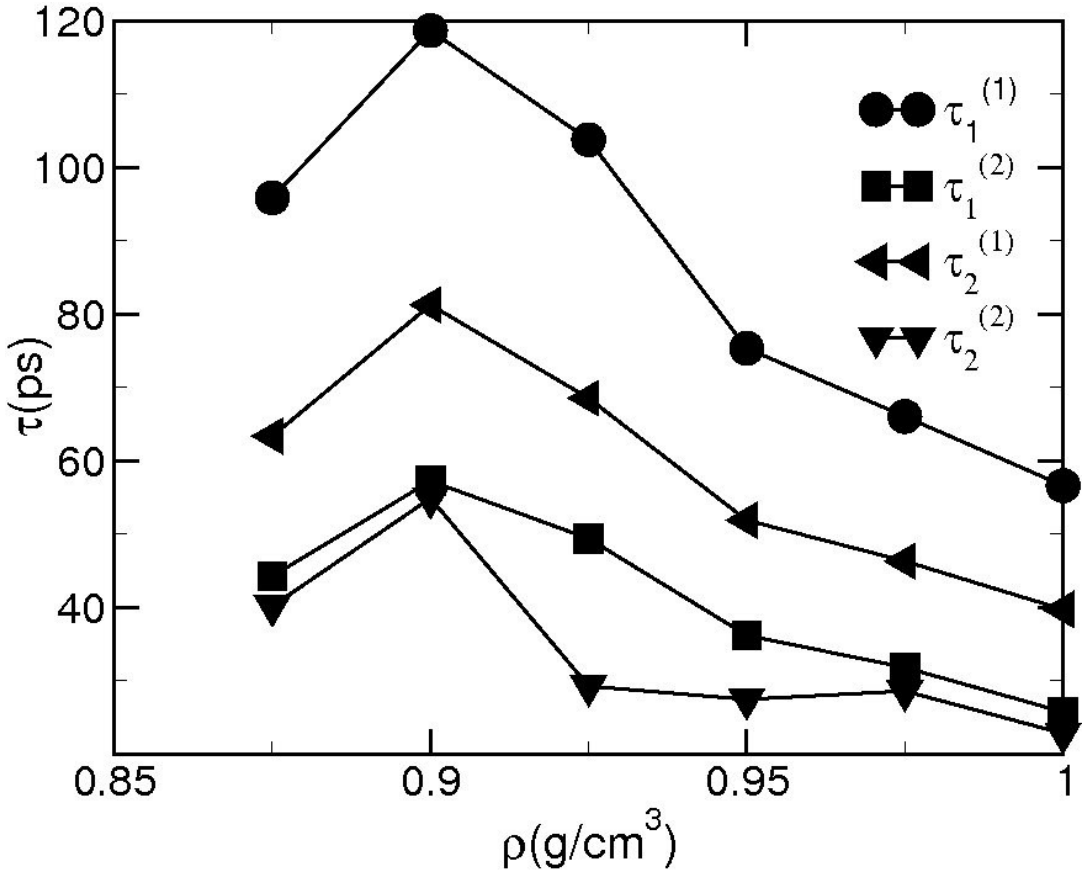
Simulações de Difusão

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



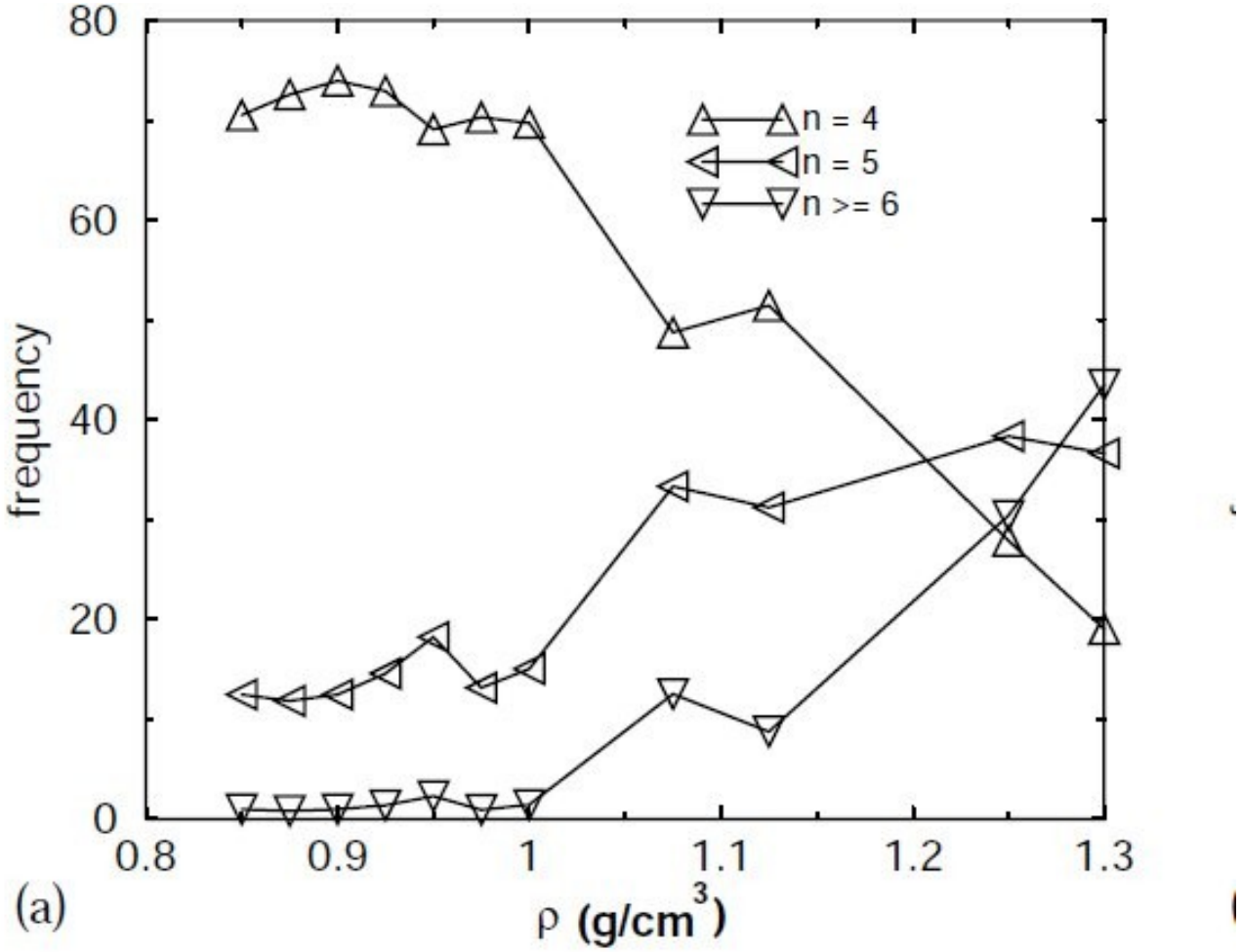
Simulação de Rotação

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

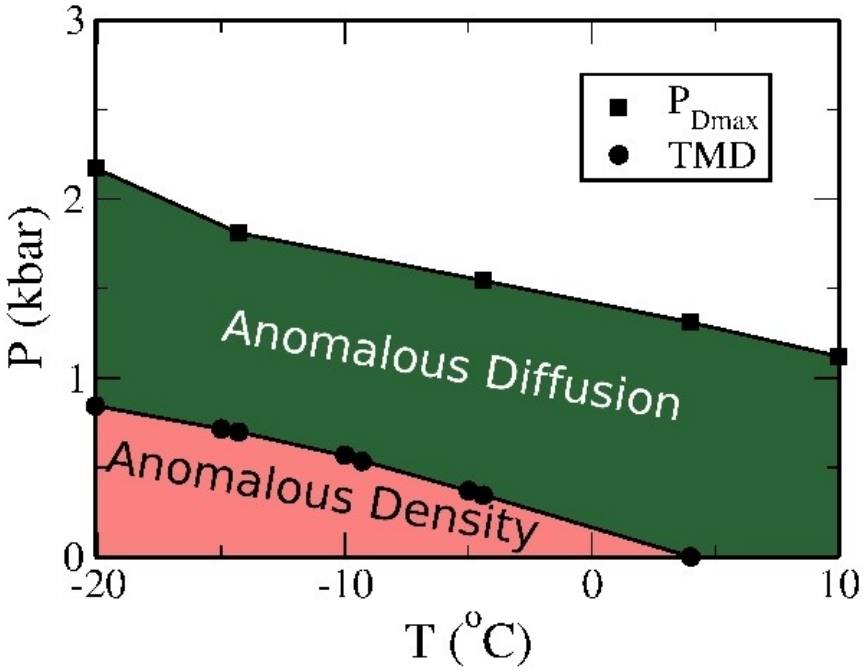


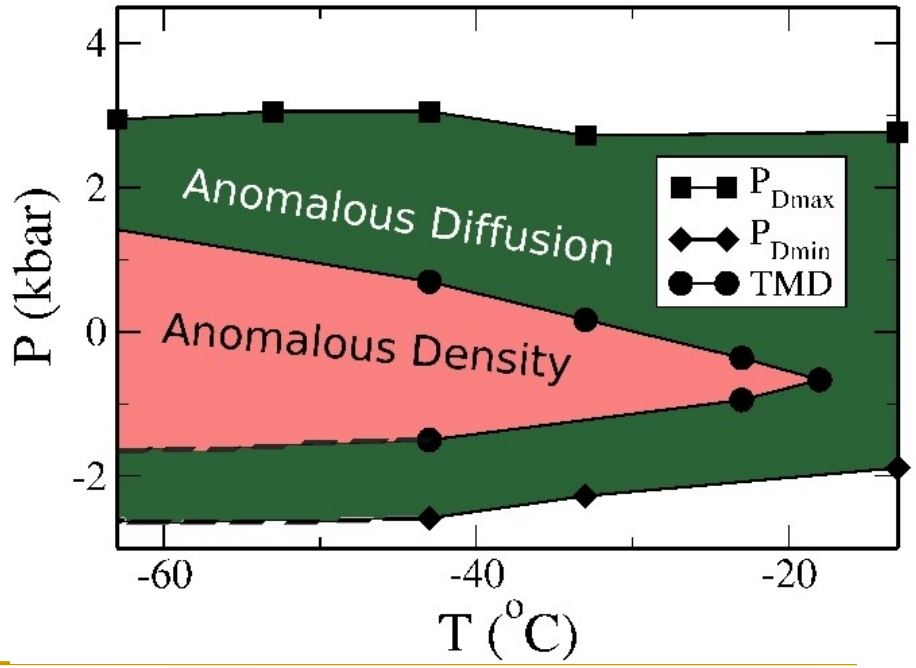
Número de Vizinhos

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

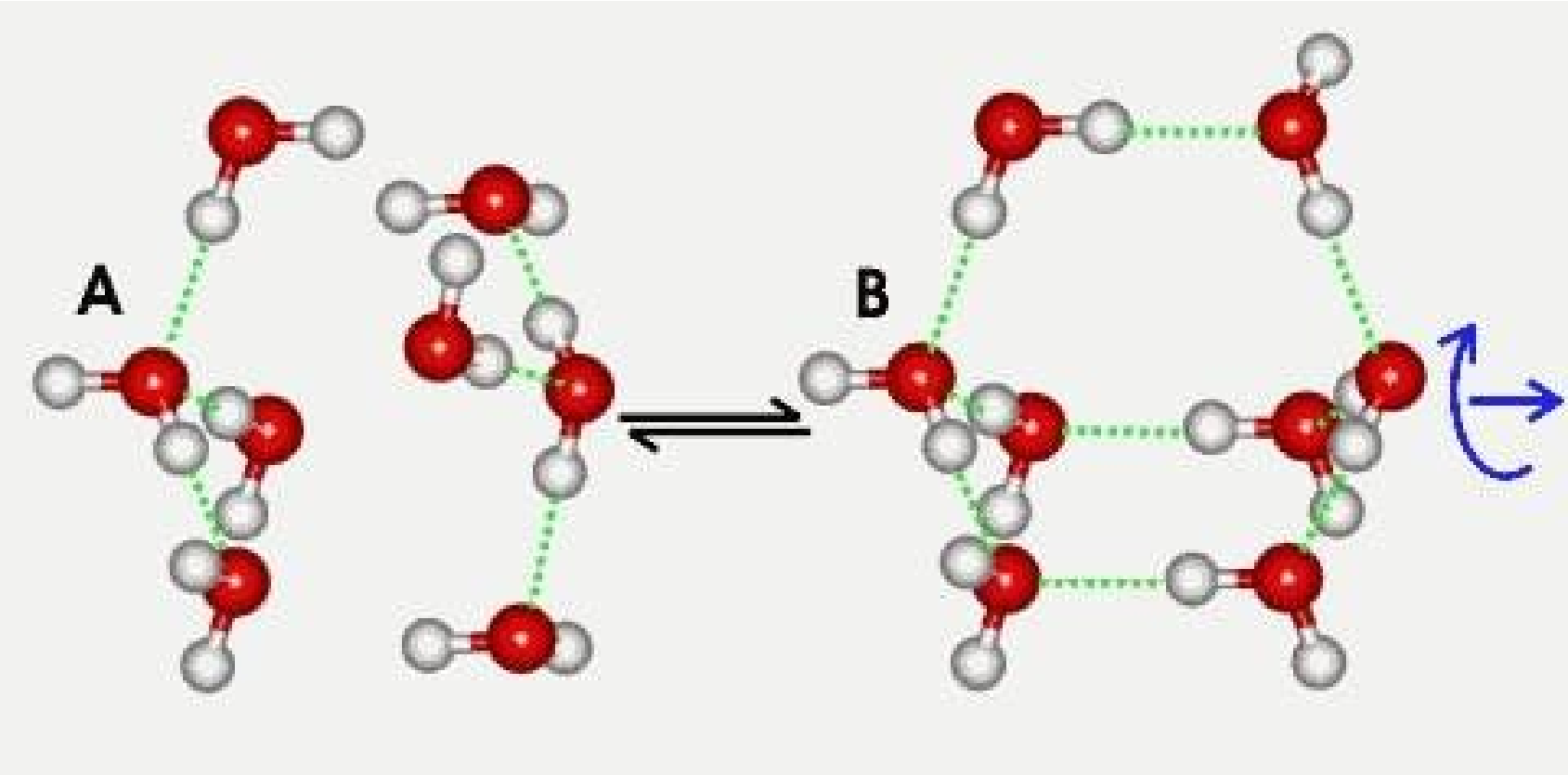


Simulação vs. Experimentos

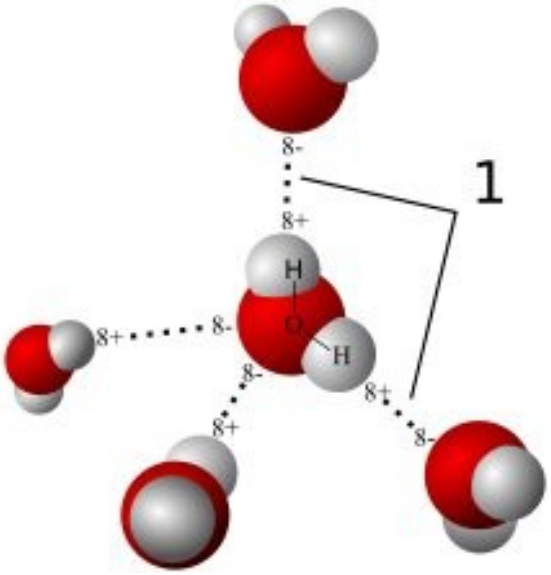


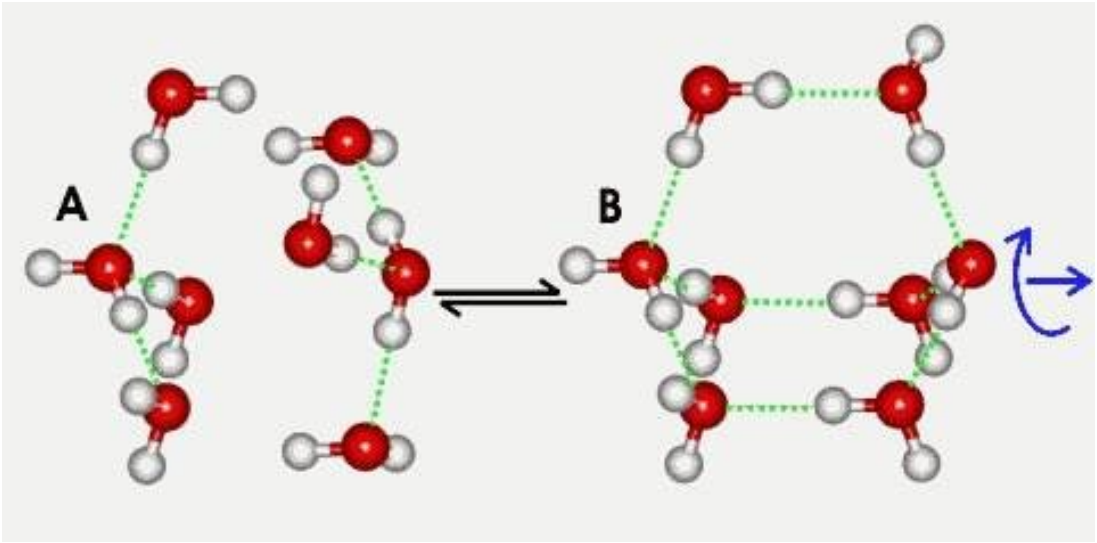


Unidade Básica
O Tetrâmero

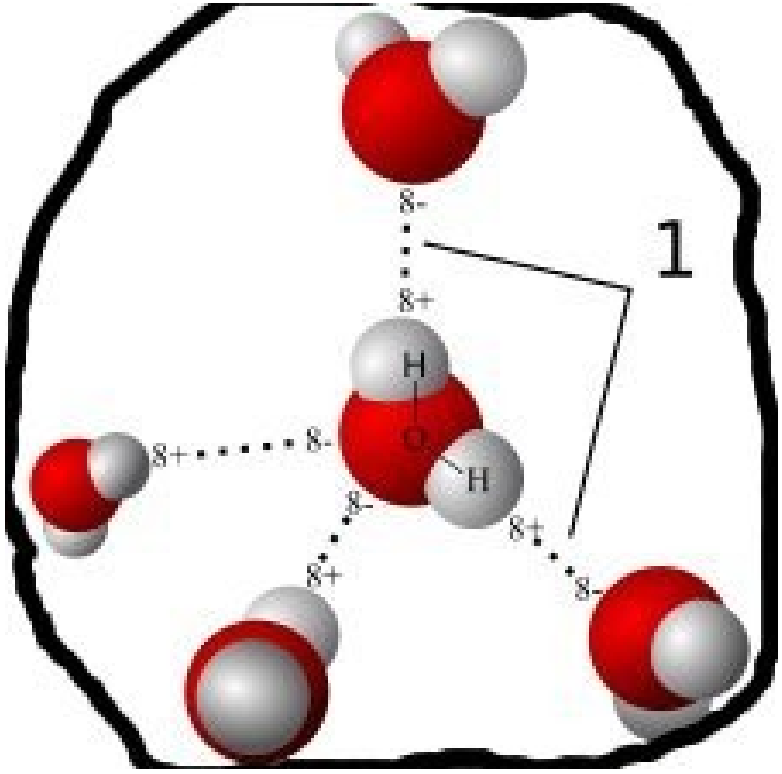


Potencial Efetivo

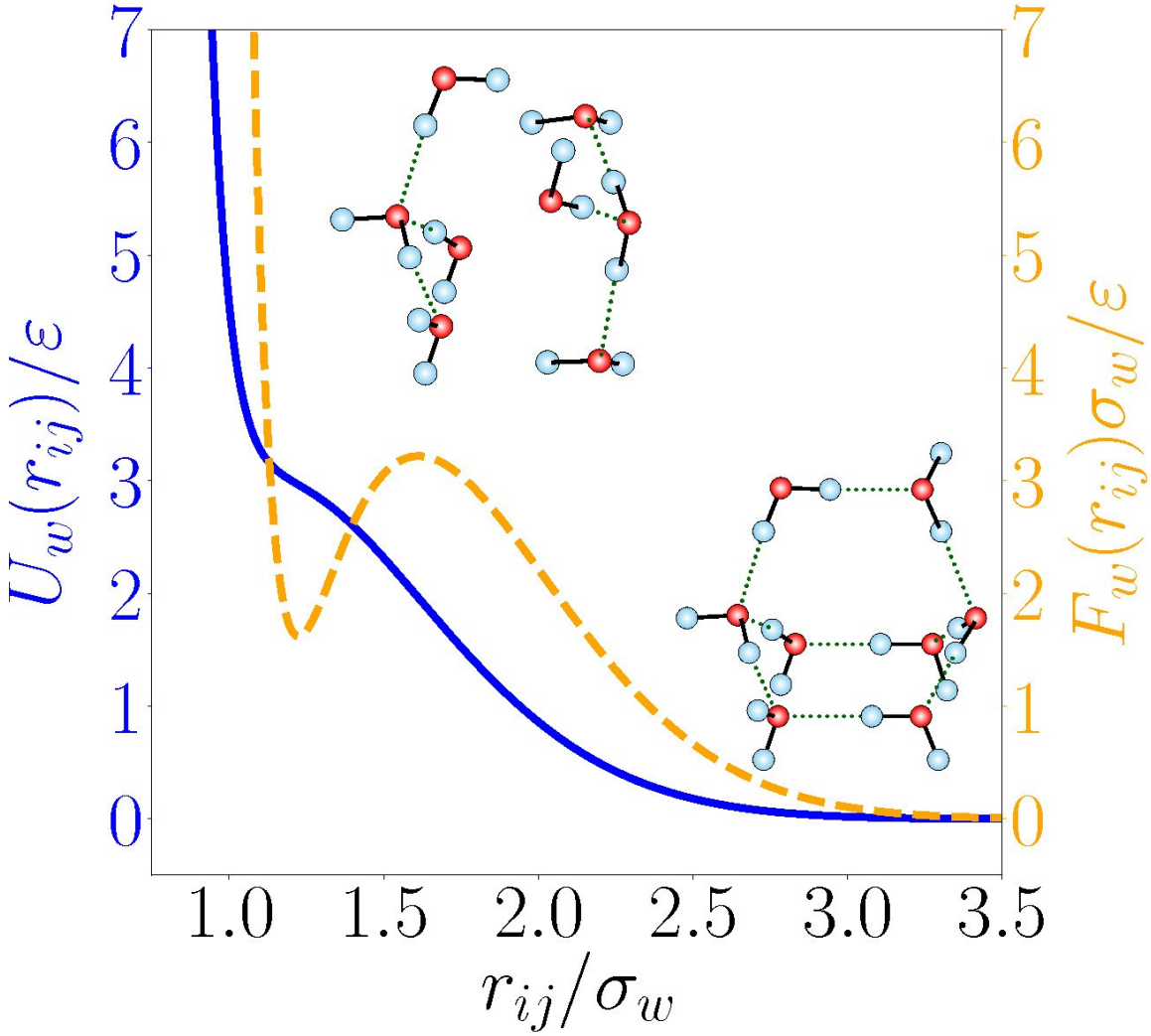




Potencial Efetivo

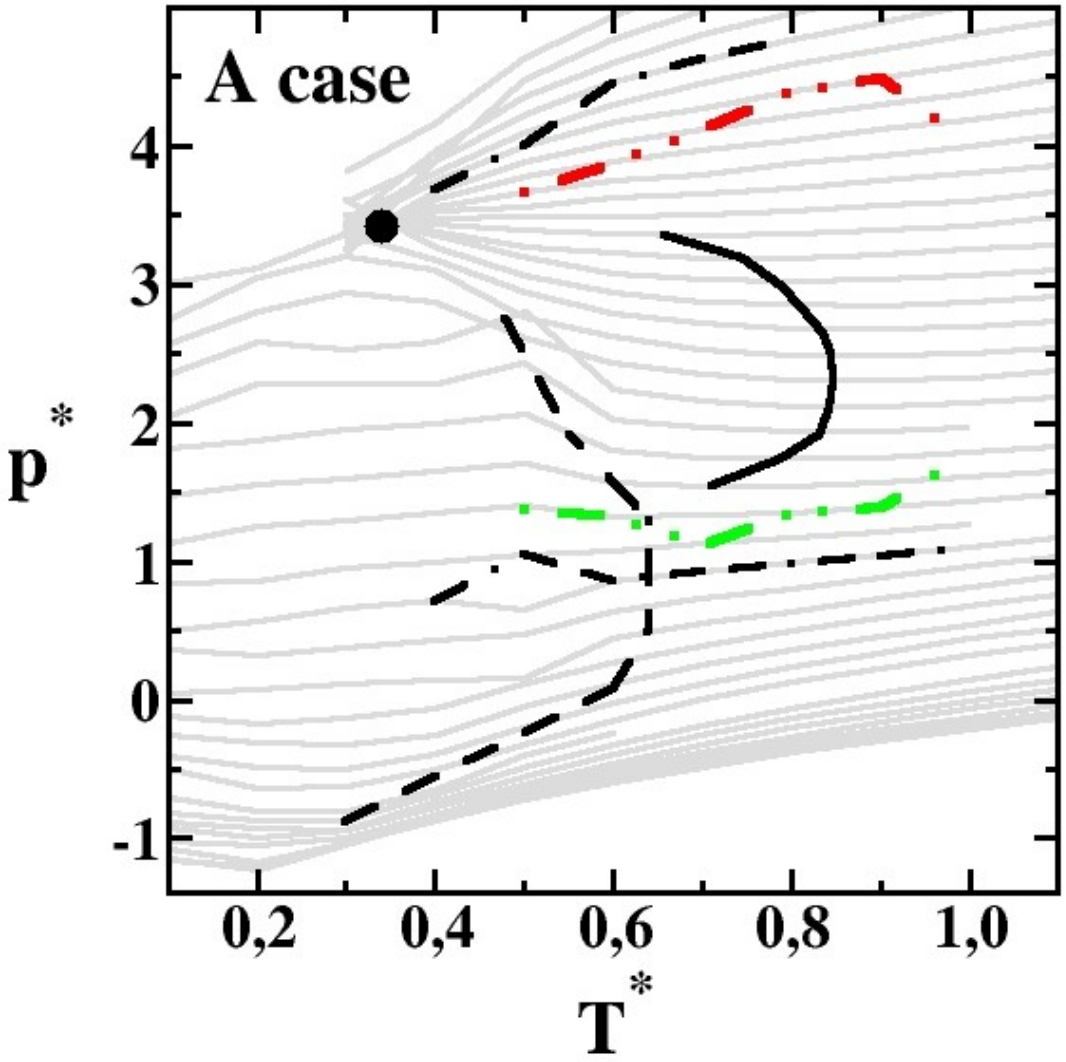


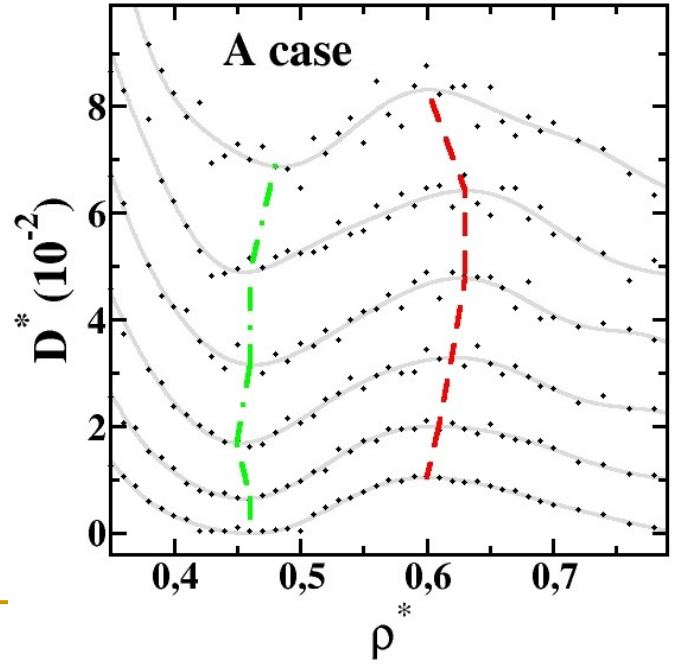
Potencial Efetivo



Potencial Efetivo

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





ANOMALIAS

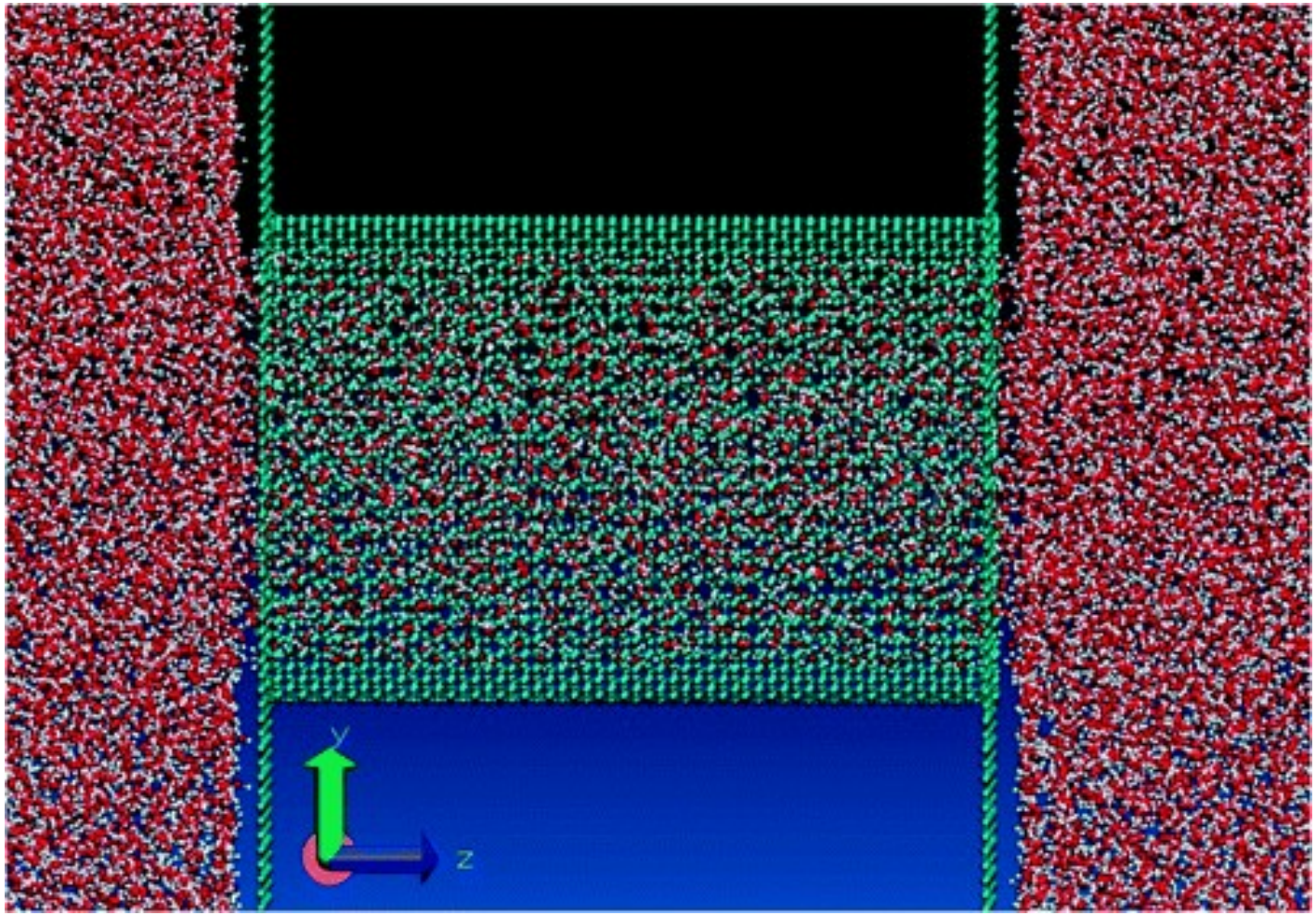
EM

SISTEMA NANO?

DIFUSÃO

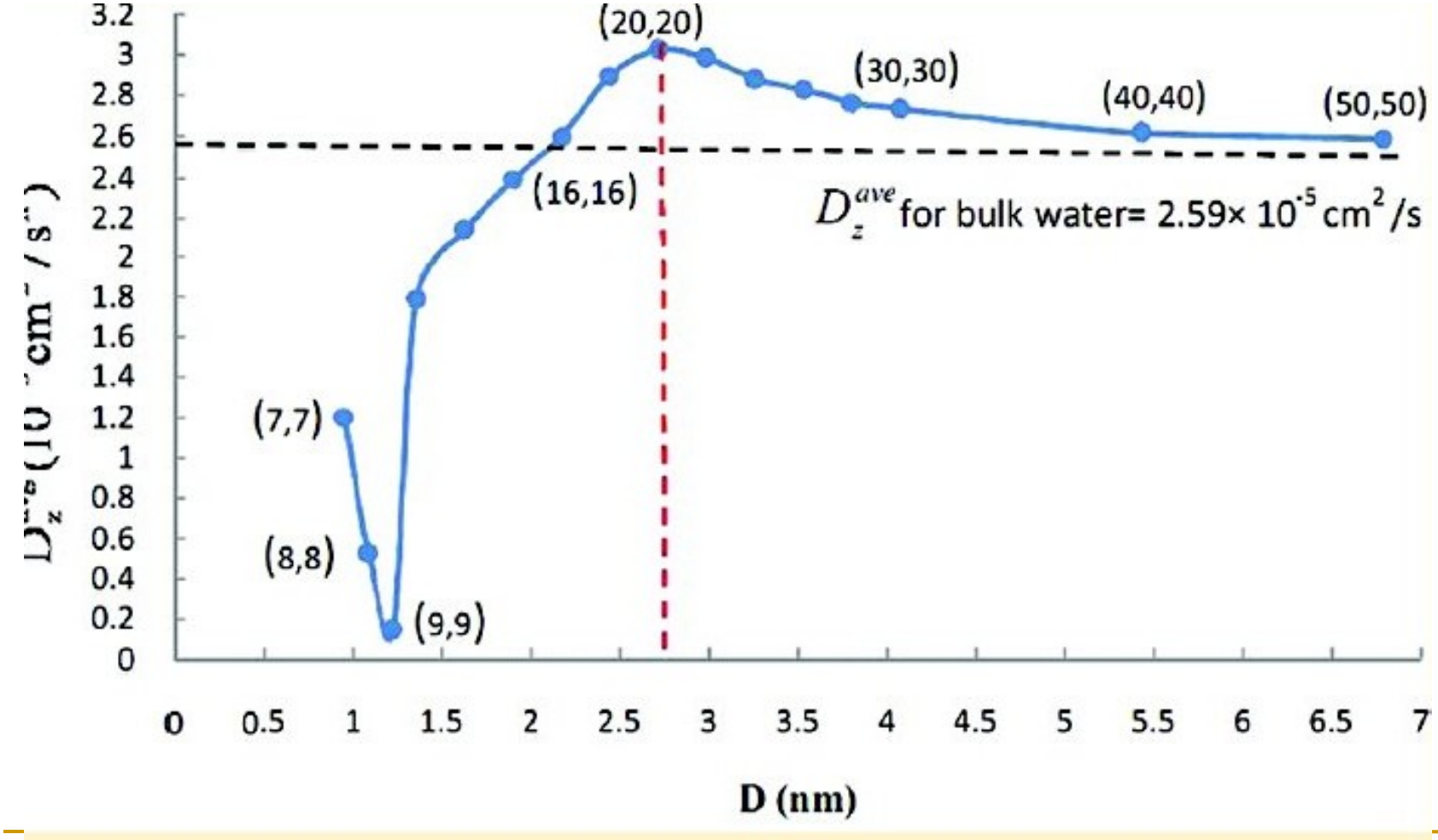
Água Confinada

A.B. Farinami, JPCB 115, 12145 (2012)



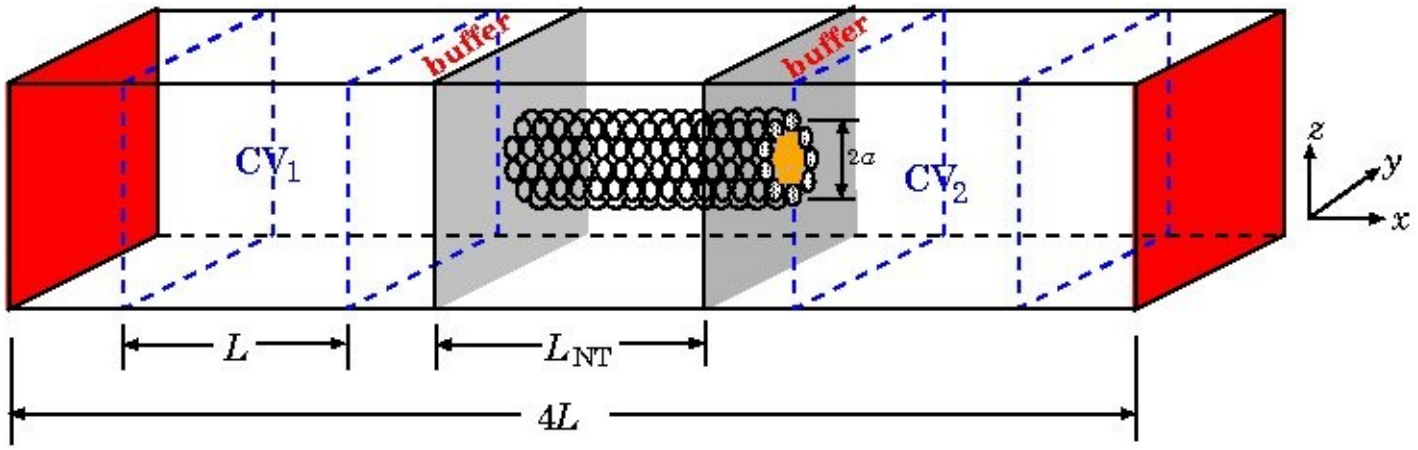
Difusão

A.B. Farinami, JPCB 115, 12145 (2011)



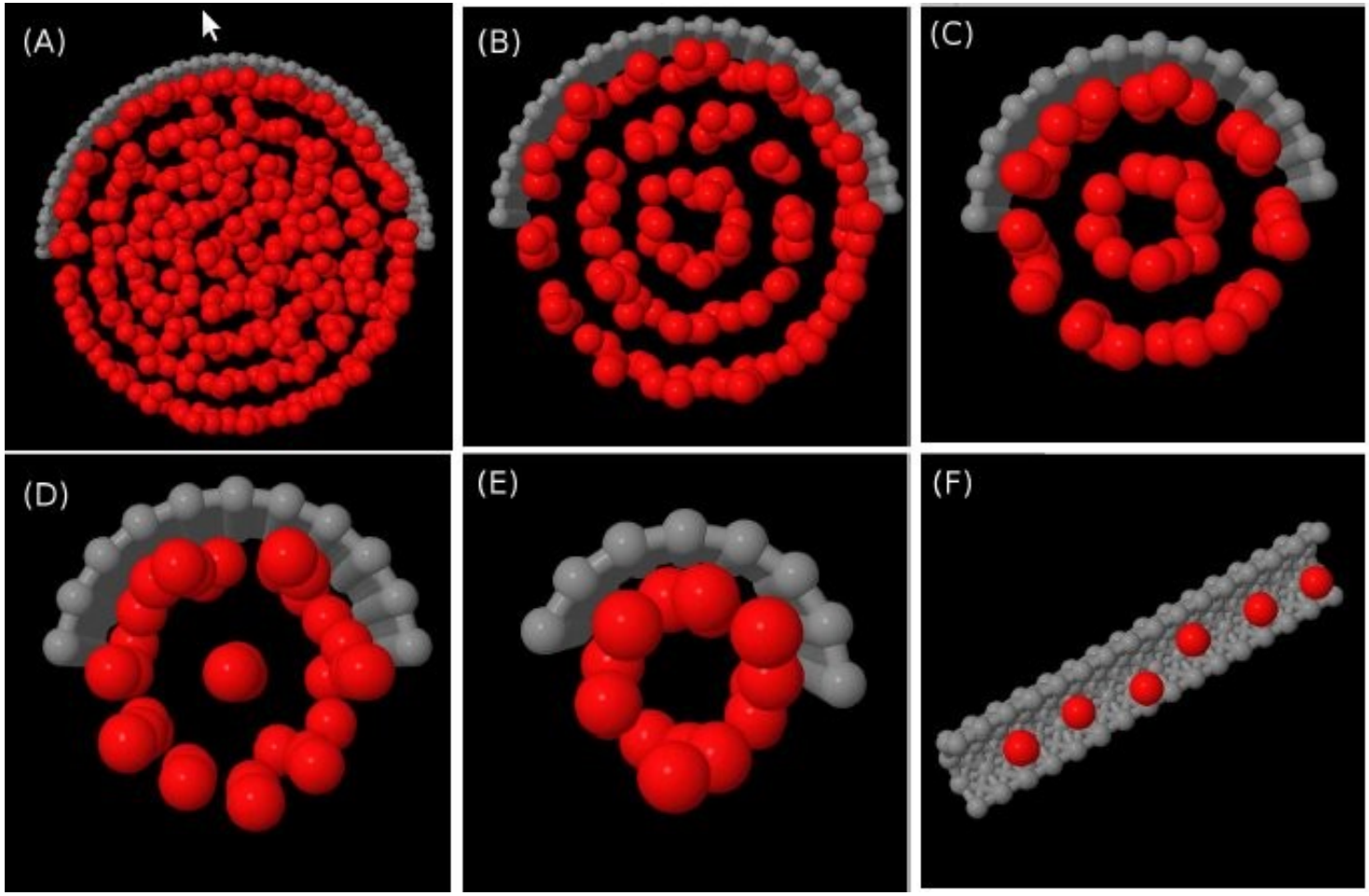
Sistema Efetivo Confinado

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



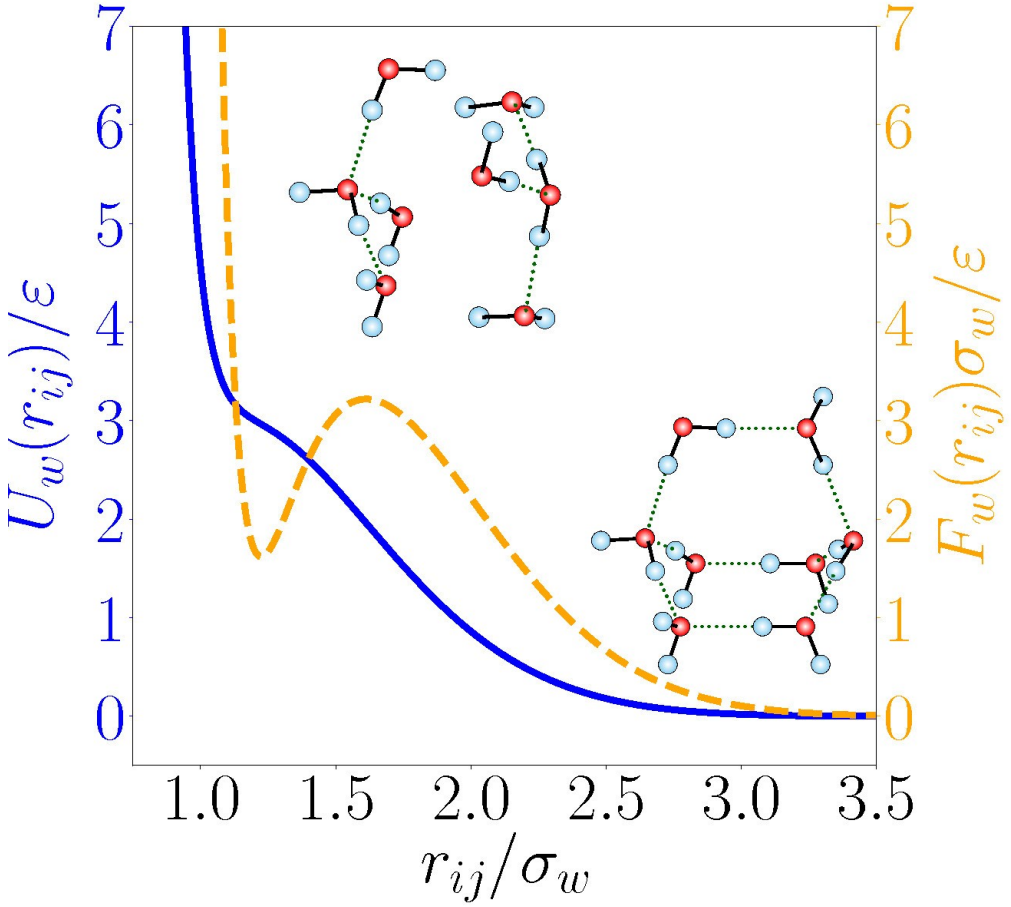
Sistema Efetivo Confinado

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



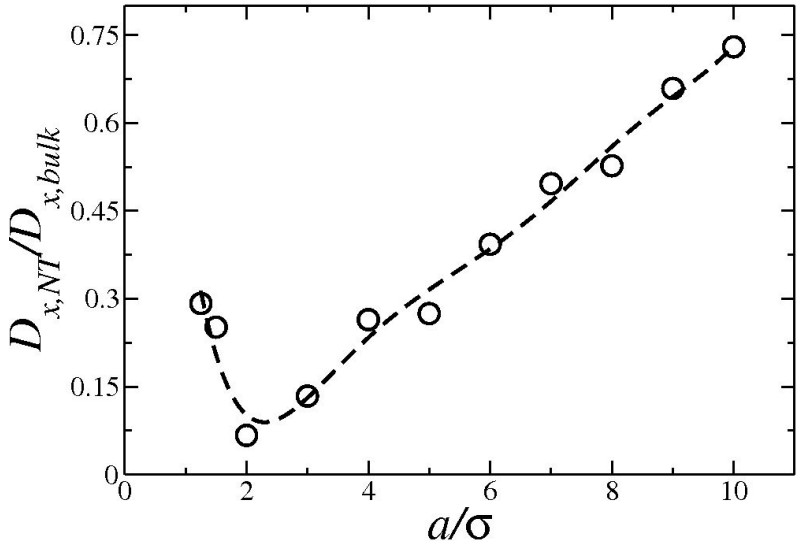
Potencial Efetivo

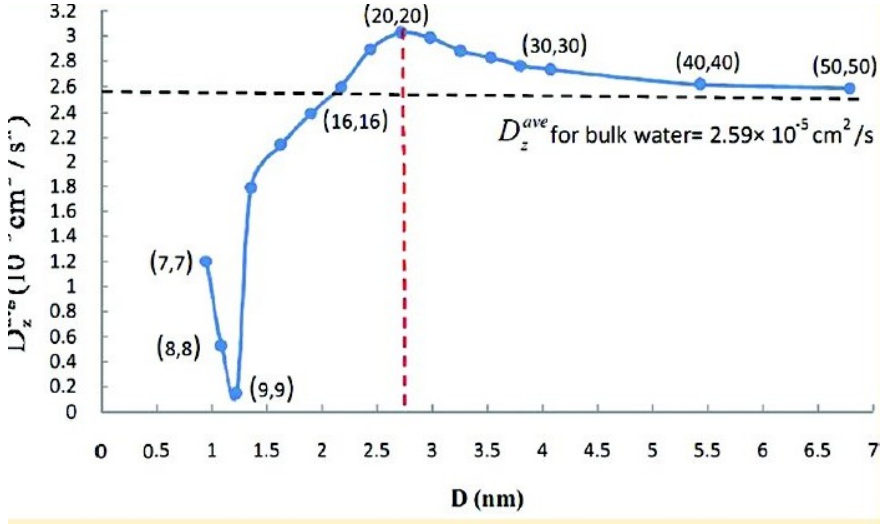
J. R. Bordin, A. Diehl and MCB, JCP 137, 084504 (2012)



Difusão

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

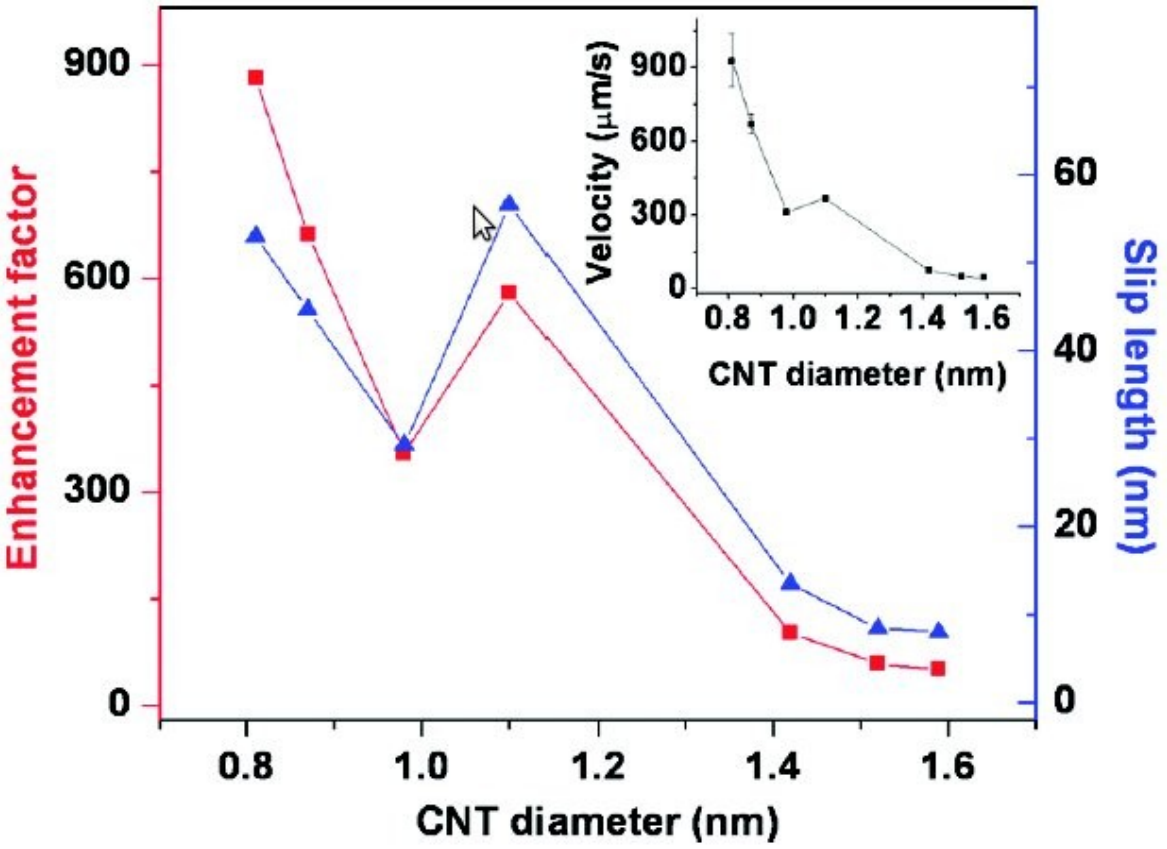




FLUXO

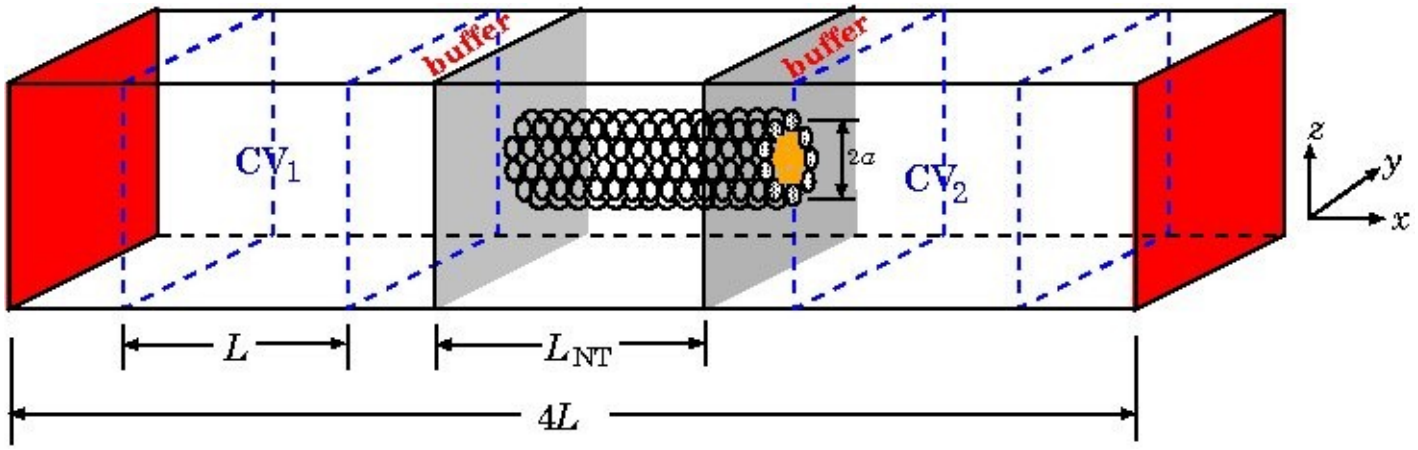
Super Fluxo

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

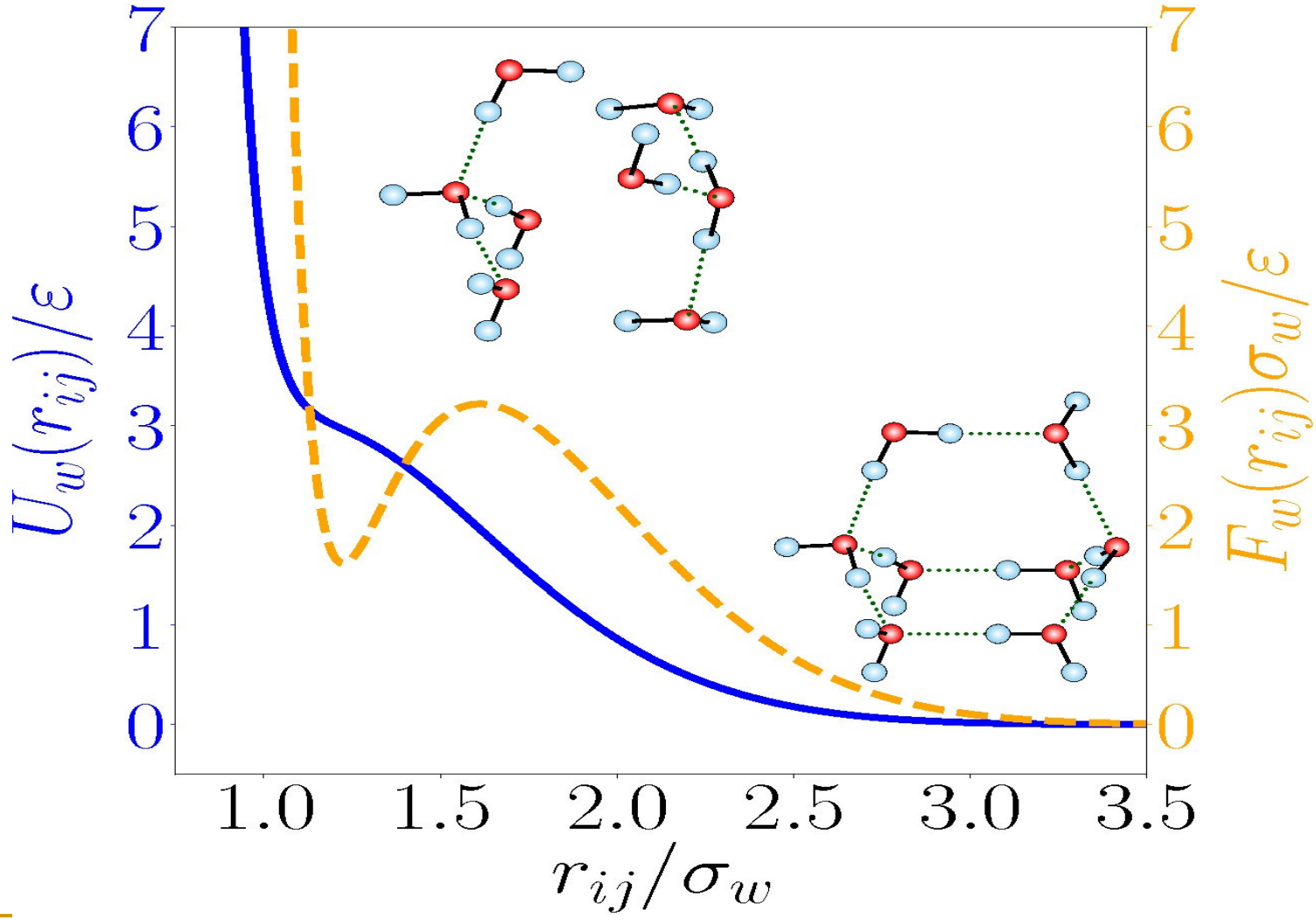


Sistema Efetivo

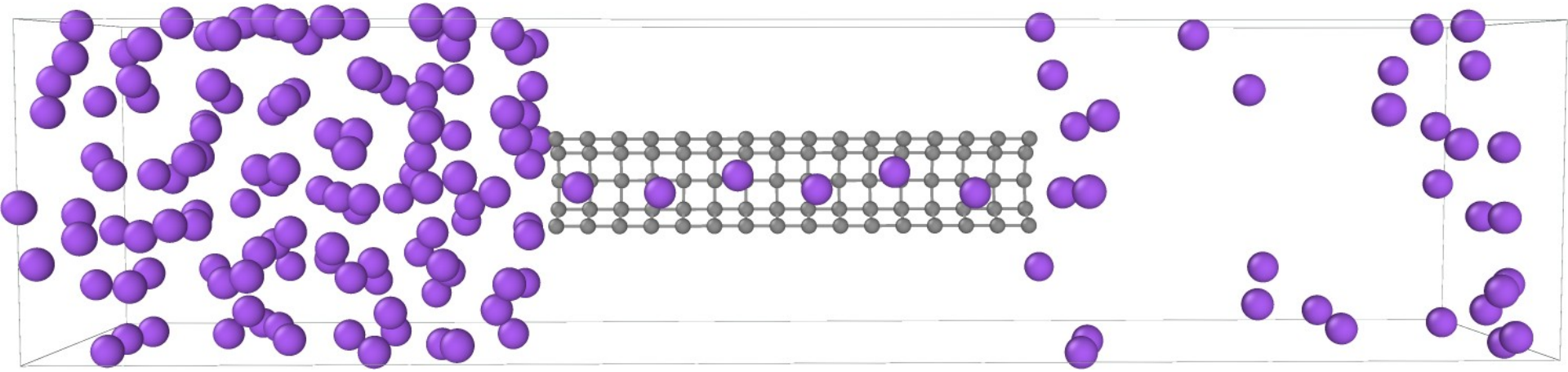
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)



Potencial Efetivo

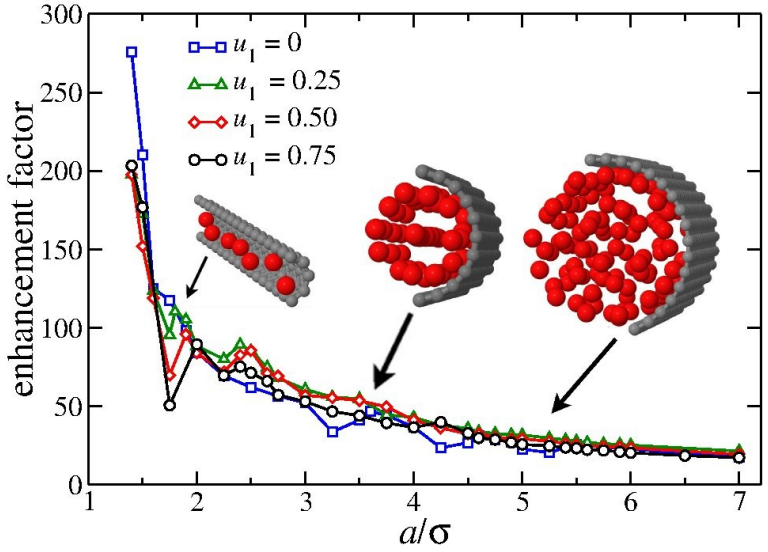


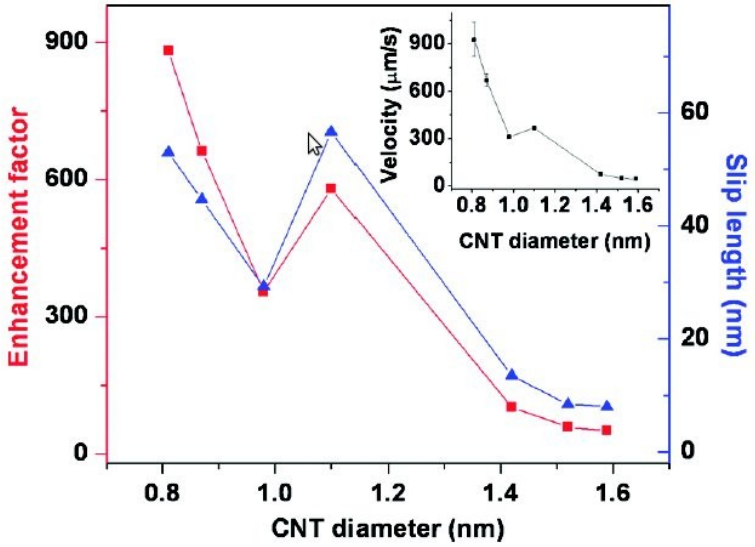
Potencial Efetivo



Super Fluxo

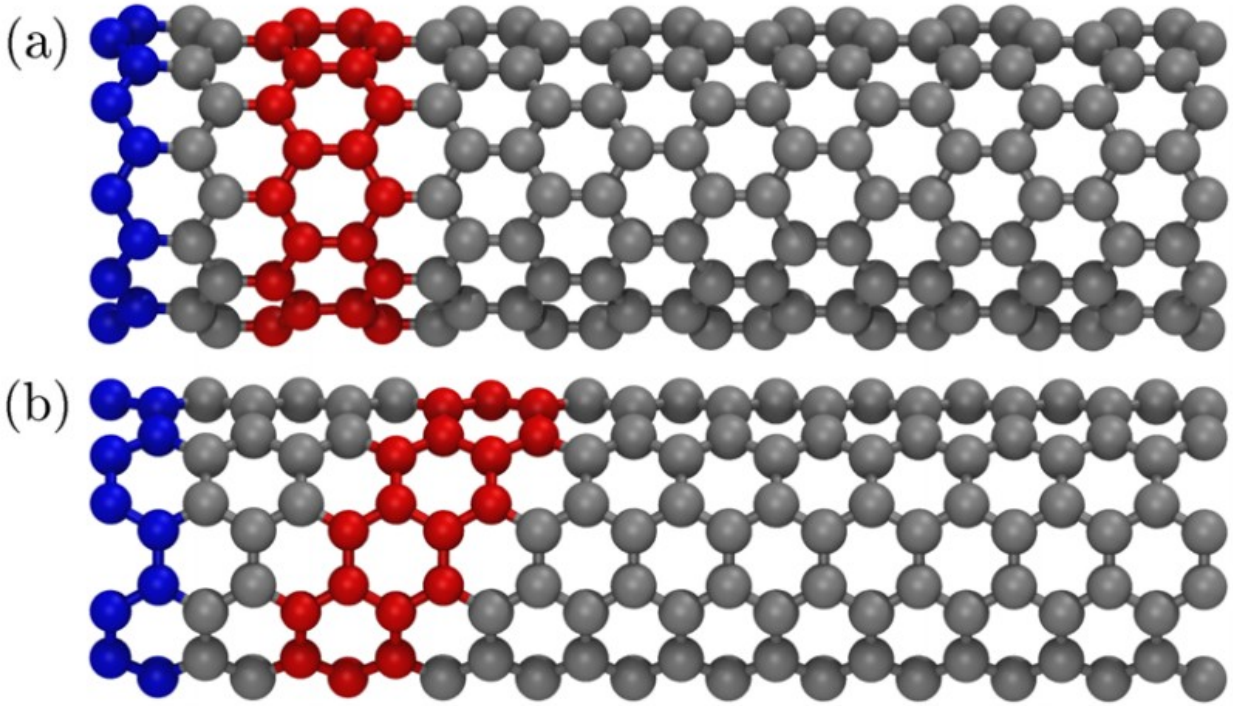
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)
X. Qin et al, Nanoletters 11, 2173 (2011) - experimental





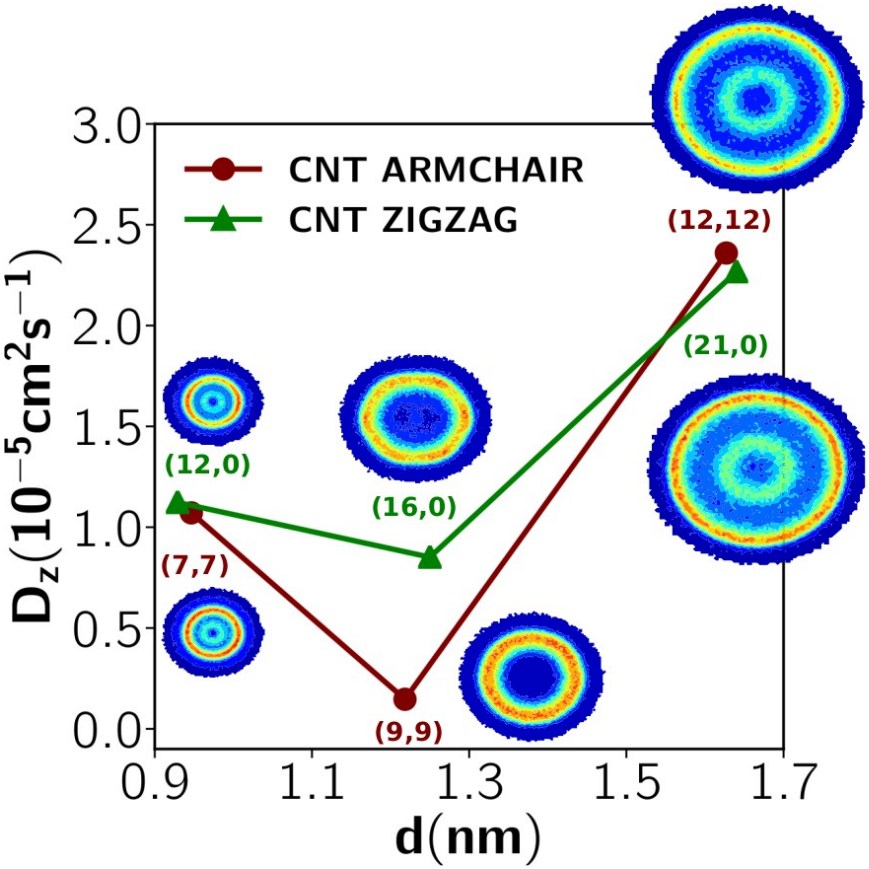
Chiralidade

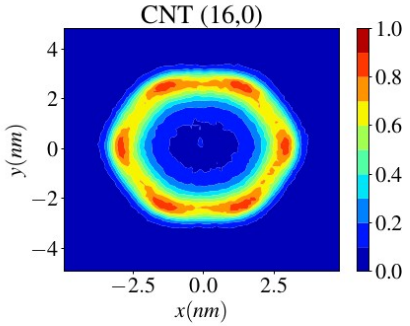
Mendonça, Ternes, Salcedo, Oliveira and MCB
JCP 152 024708 (2020)

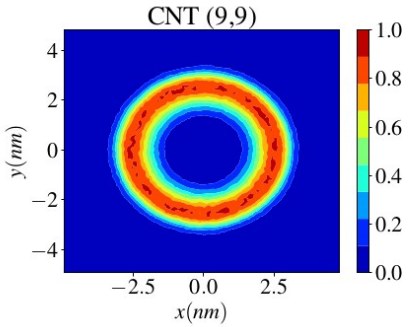


Chiralidade

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





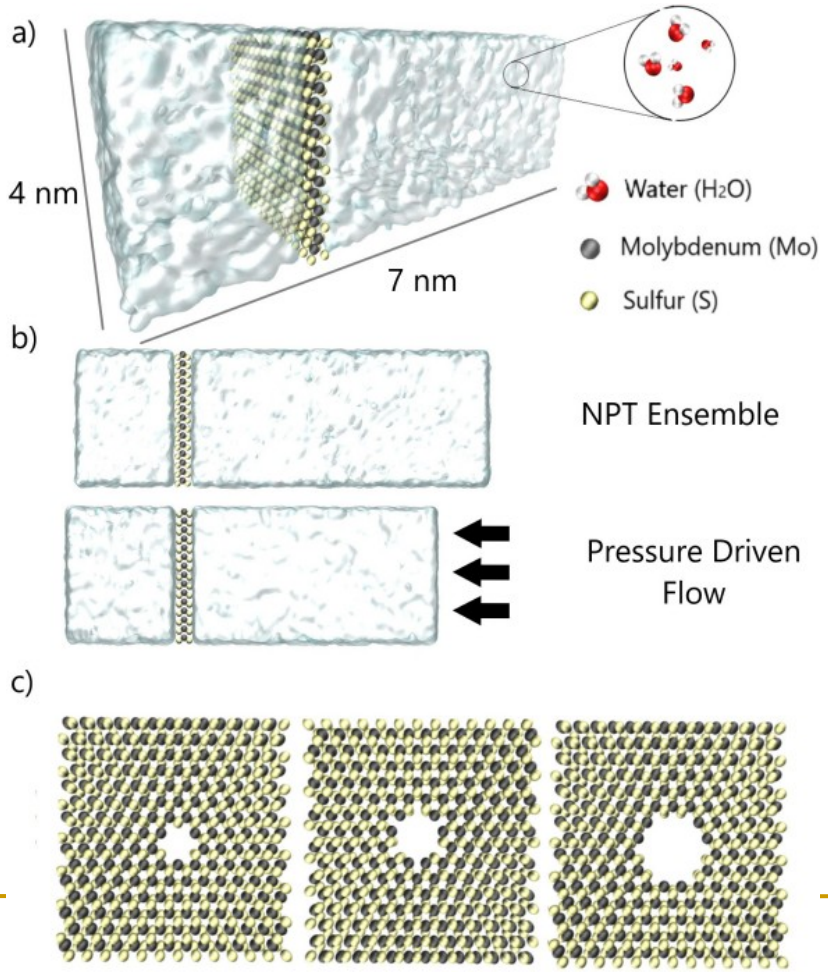


COMO OBTER ÁGUA POTÁVEL USANDO NANOPOROS?

Poros com Distintas Cargas

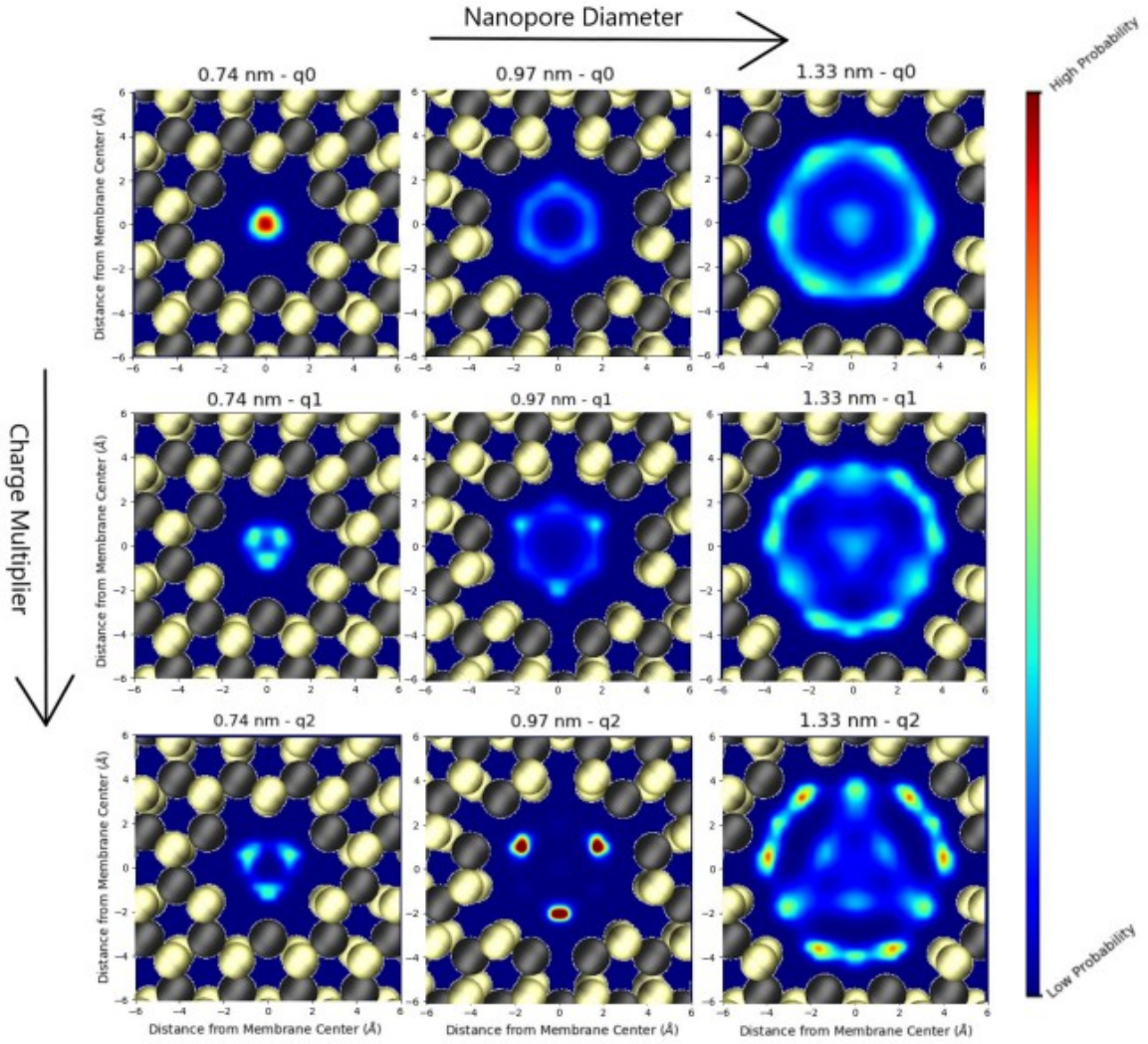
Abal, Barbosa

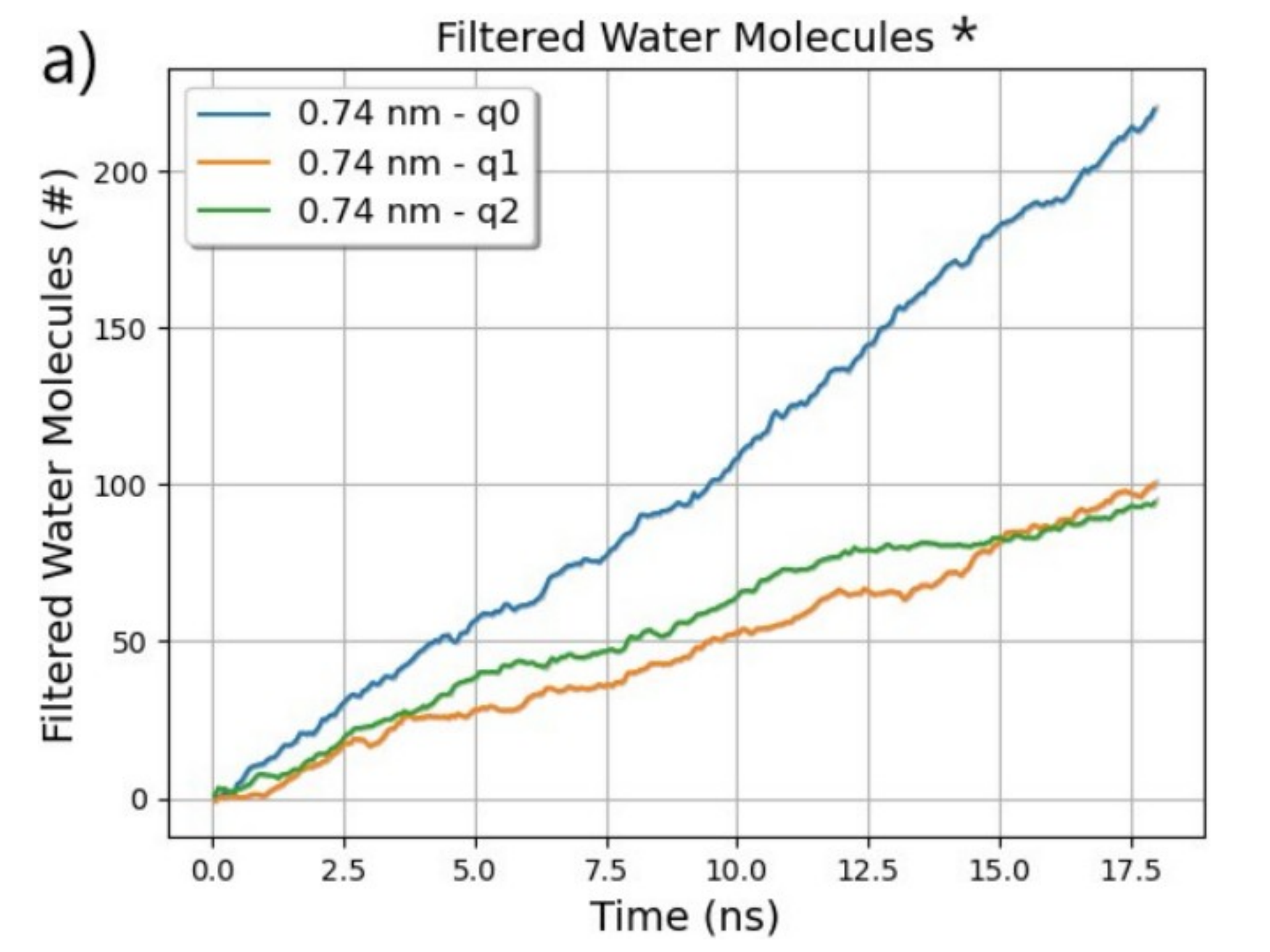
Phys. Chem. Chem. Phys. 23, 12075 (2021)

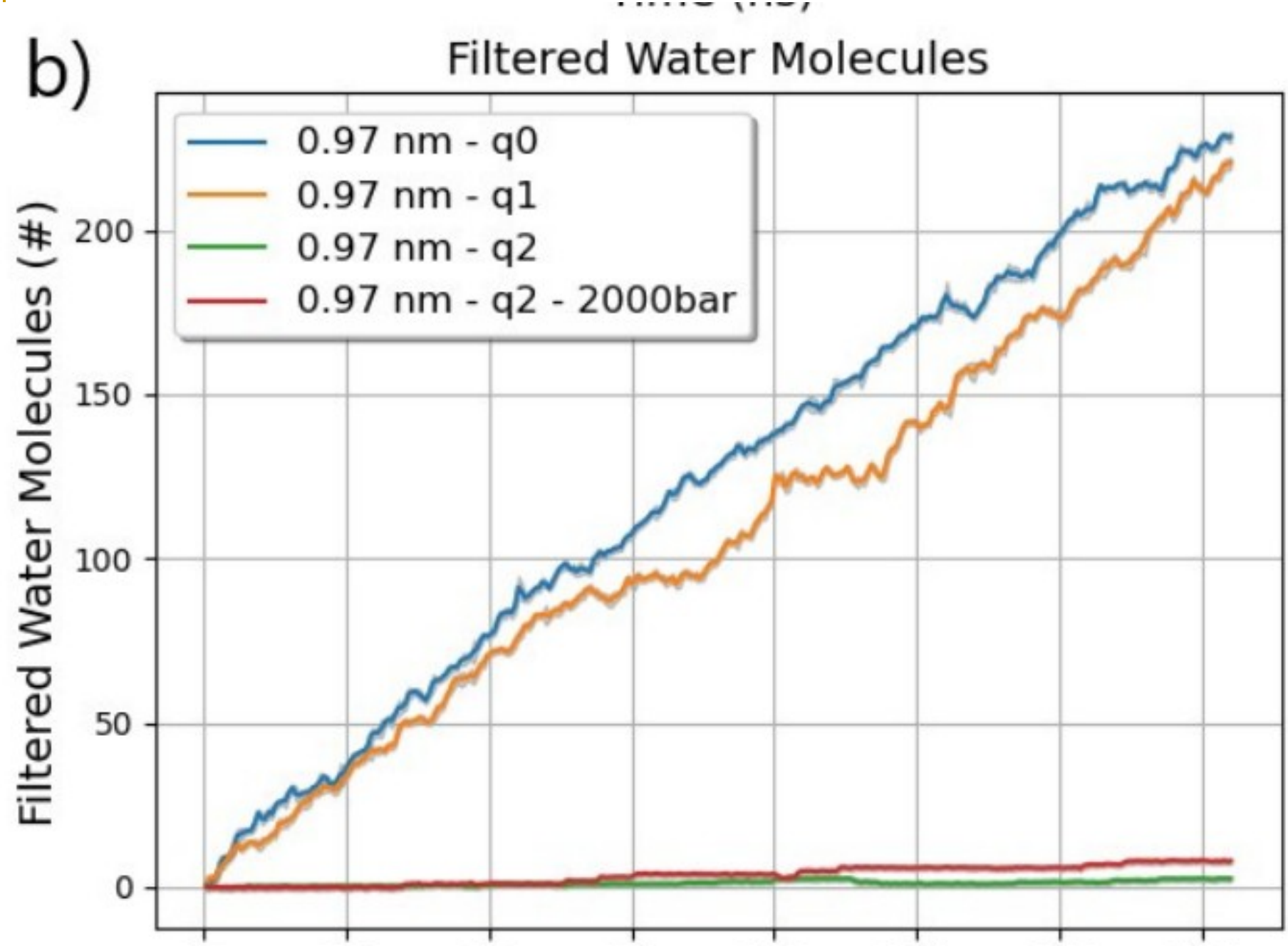


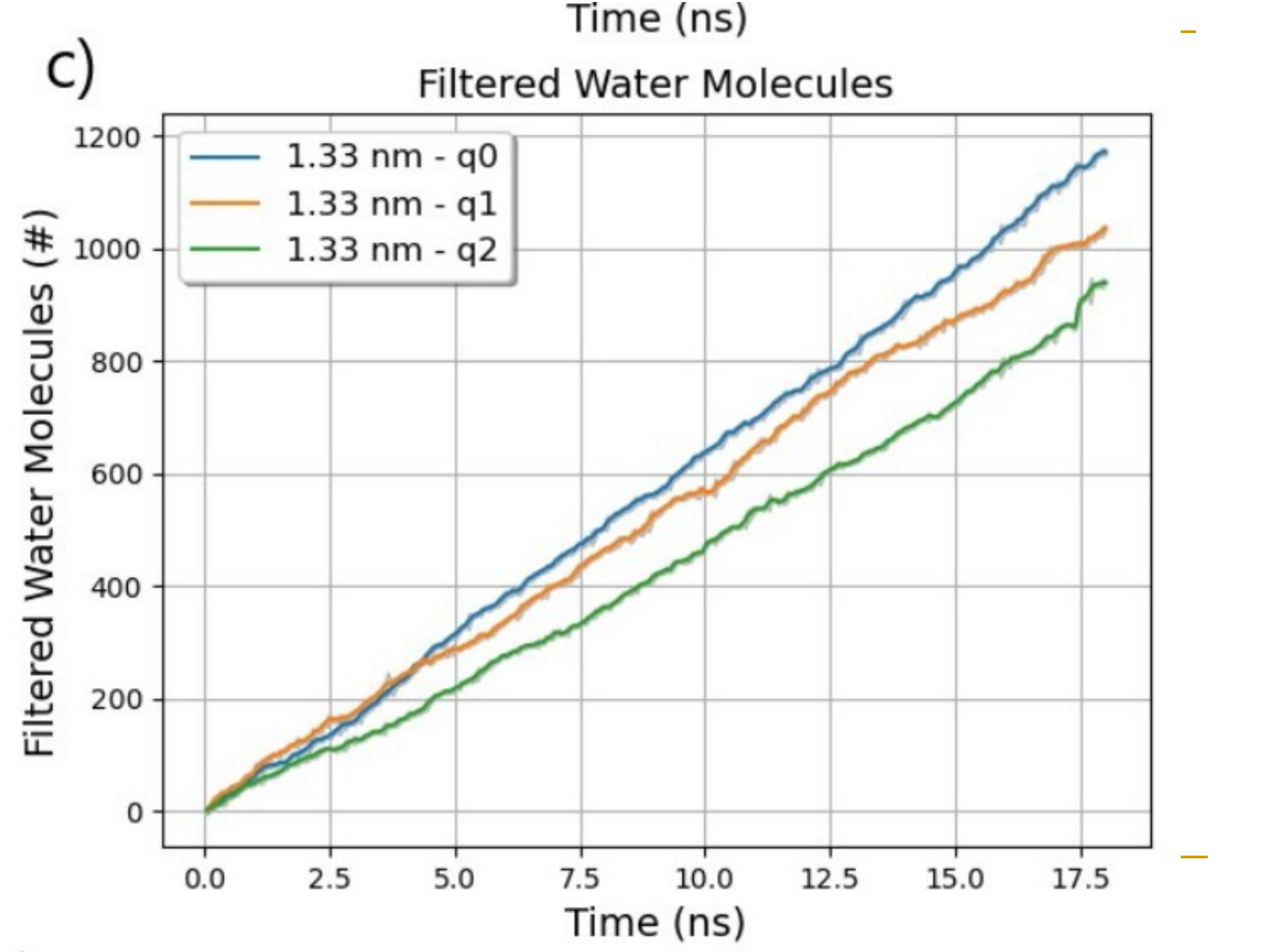
Poros com Distintas Cargas

DOI: 10.1039/D1CP00613D




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


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

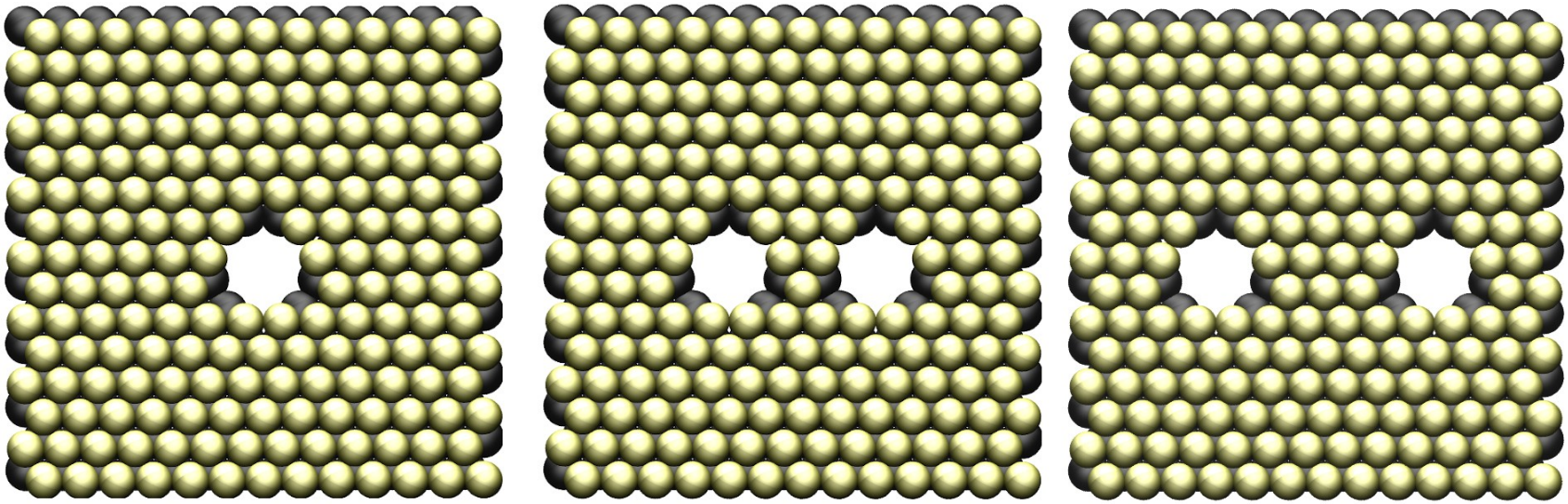

Time (ns)
c)
Filtered Water Molecules
1.33 nm - q0
1.33 nm - q1
1.33 nm - q2
Filtered Water Molecules (#)
1200
1000
800
600
400
200
0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Time (ns)

Poros Competem?

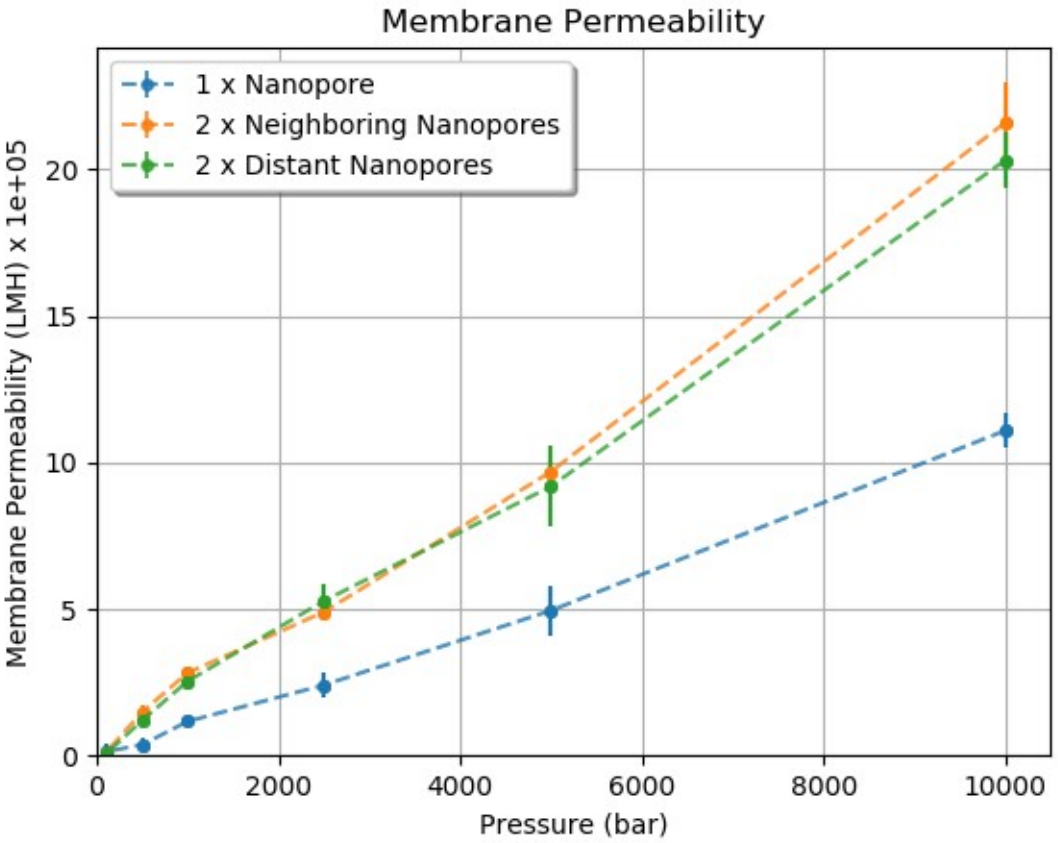
Abal, Barbosa

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

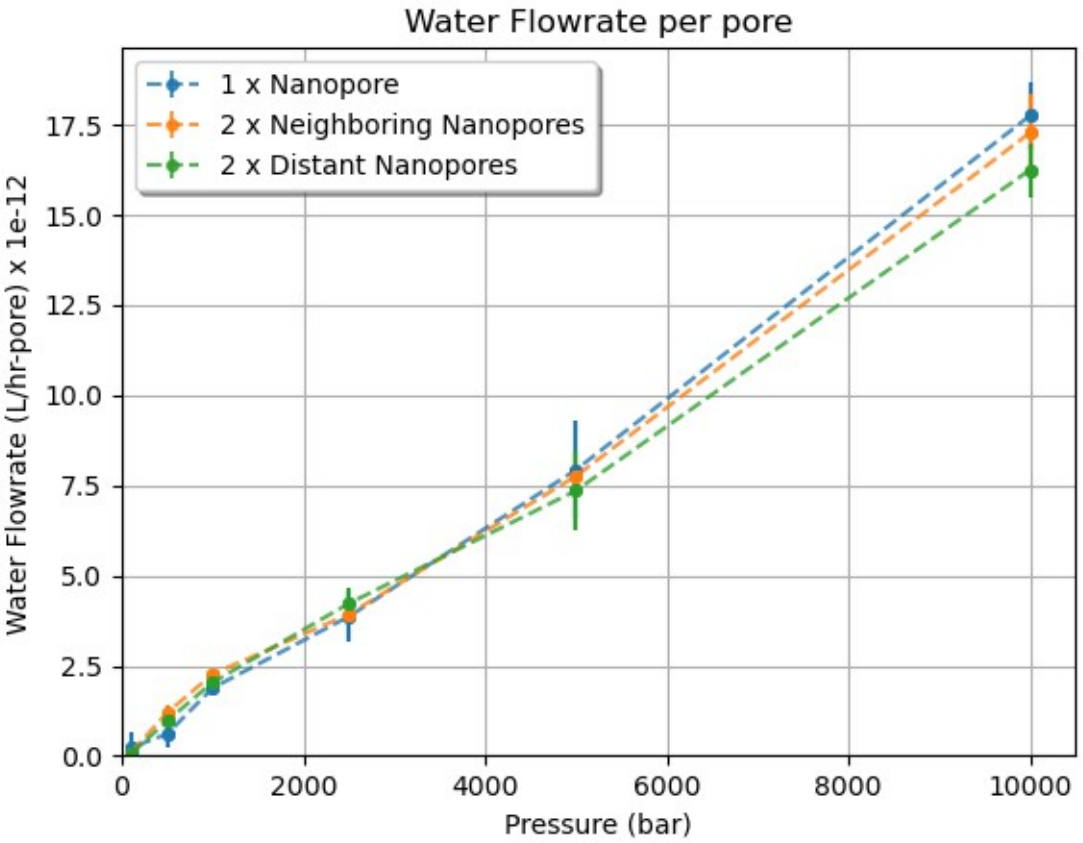
J. Chem. Phys. 154, 134506 (2021)



Permeabilidade



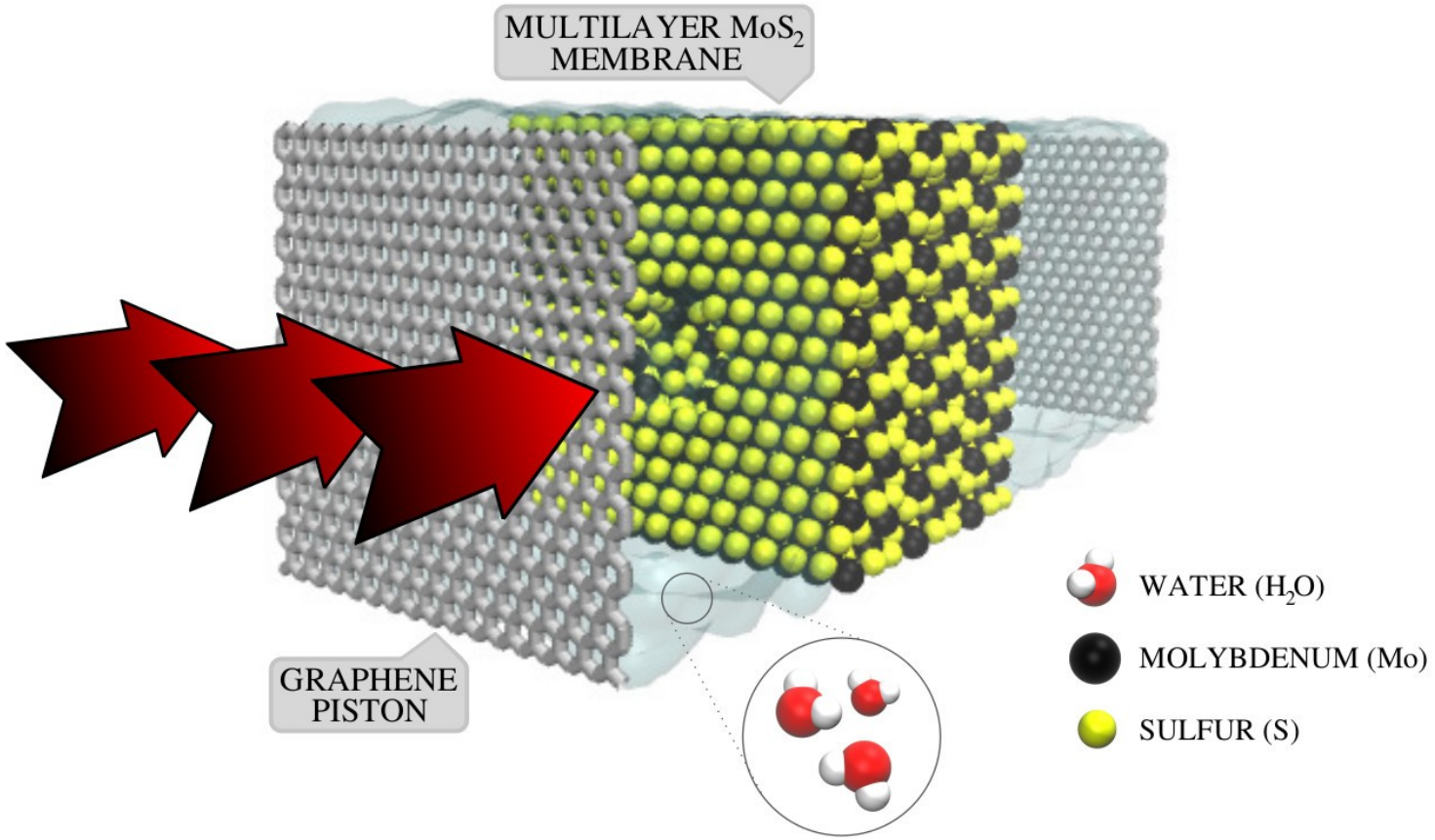
Rejeição de Sal



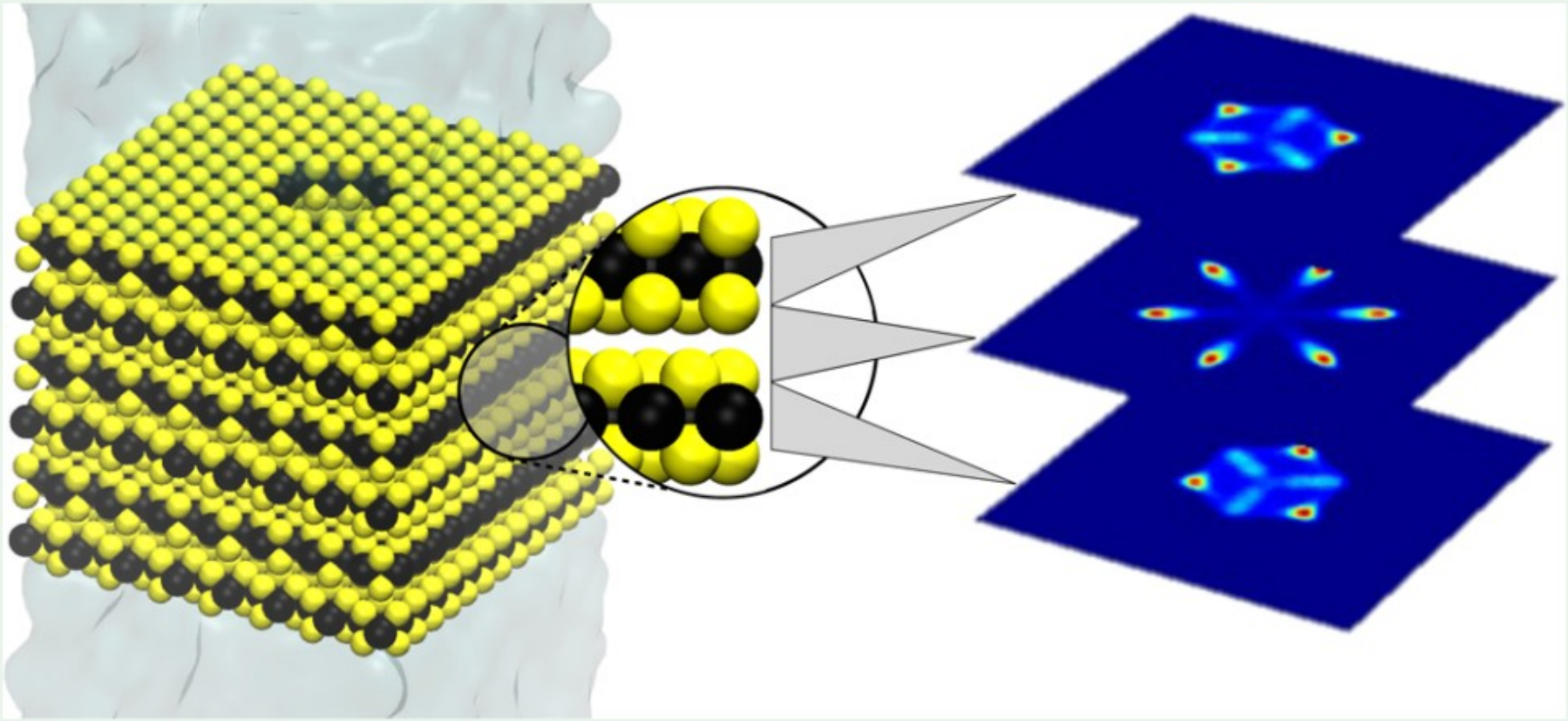
O que acontece se tentar fazer um nanotubo com várias folhas?

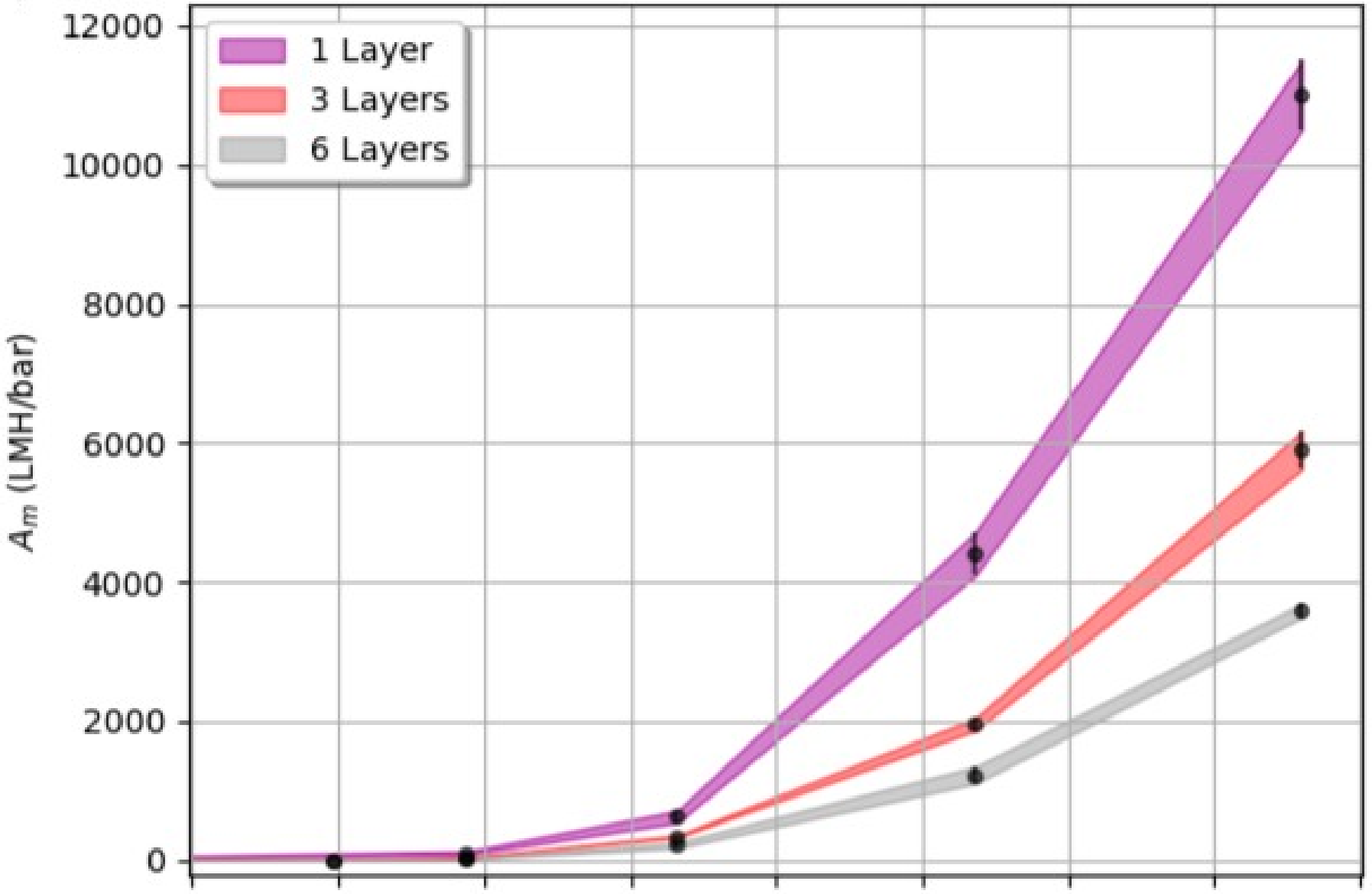
Multicamada

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



Multicamada



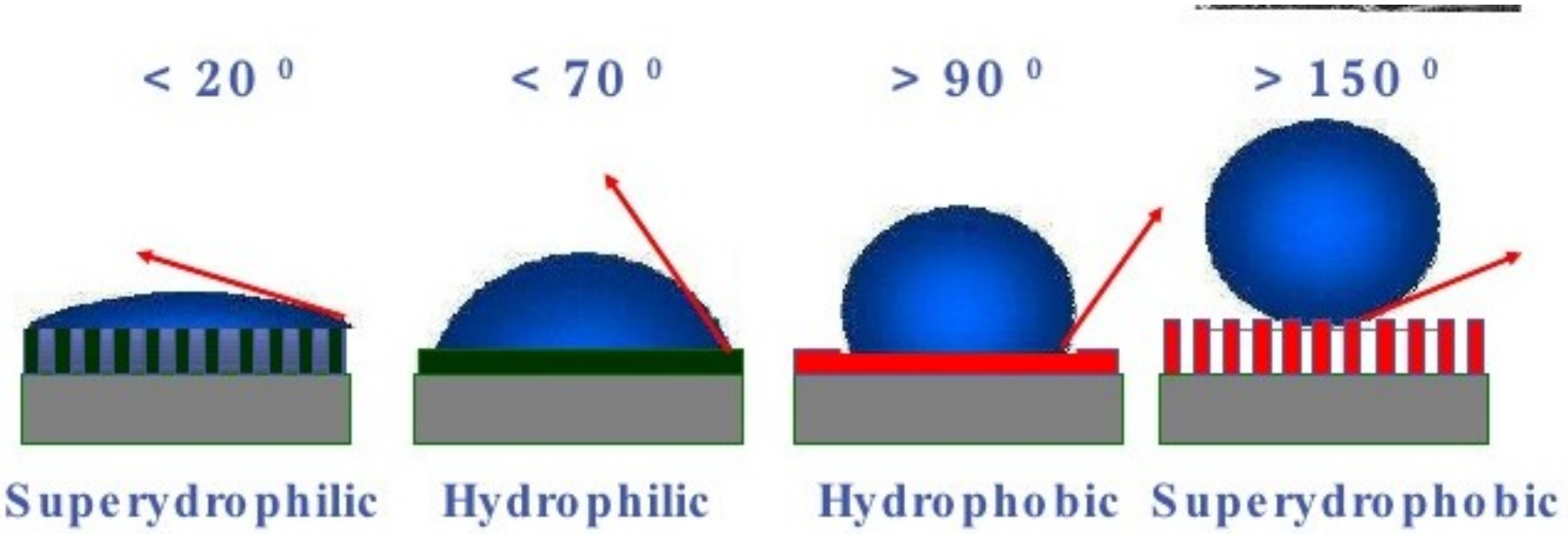

12000
10000
8000
6000
4000
2000
0
A_m (LMH/bar)
1 Layer
3 Layers
6 Layers

AMOR E ÓDIO

DA

ÁGUA

Hidrofóbico e Hidrofílico



Hidrofóbico

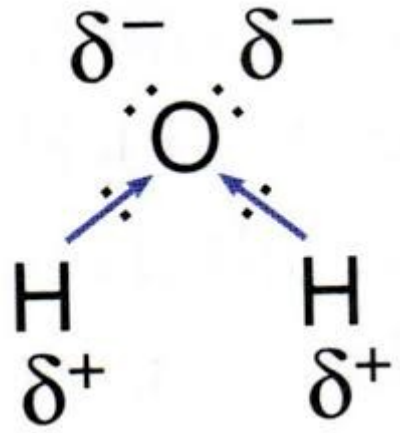


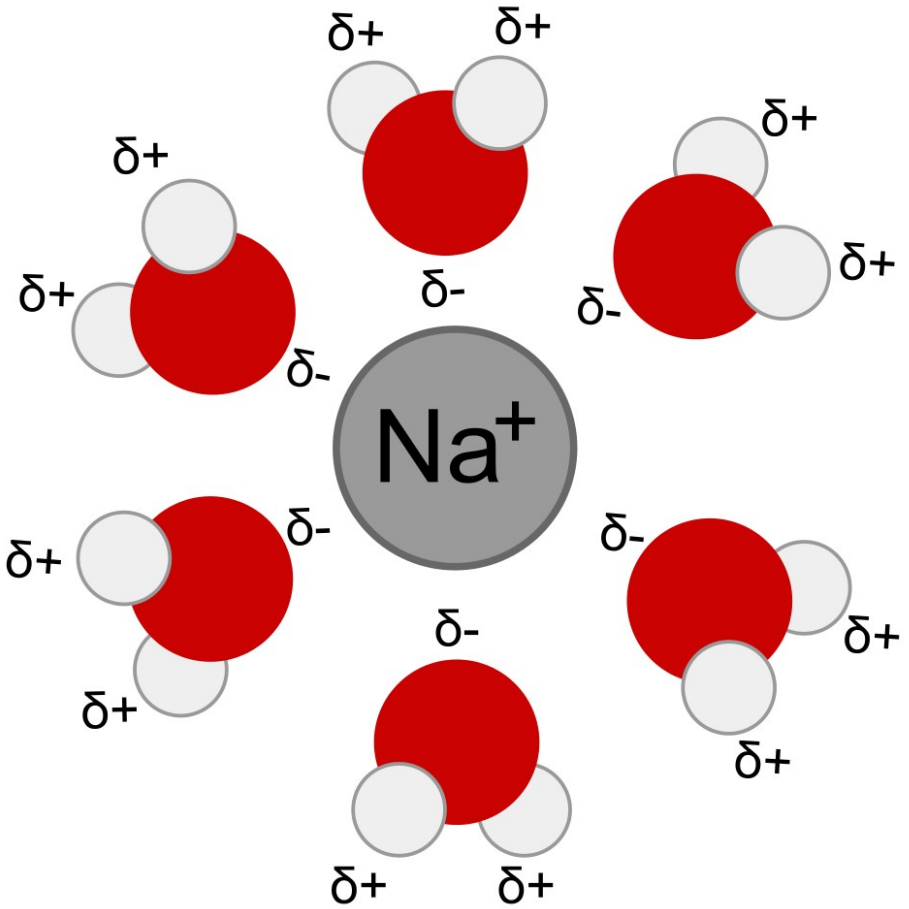
MATERIAIS

QUE A ÁGUA

AMA

Água e Íons

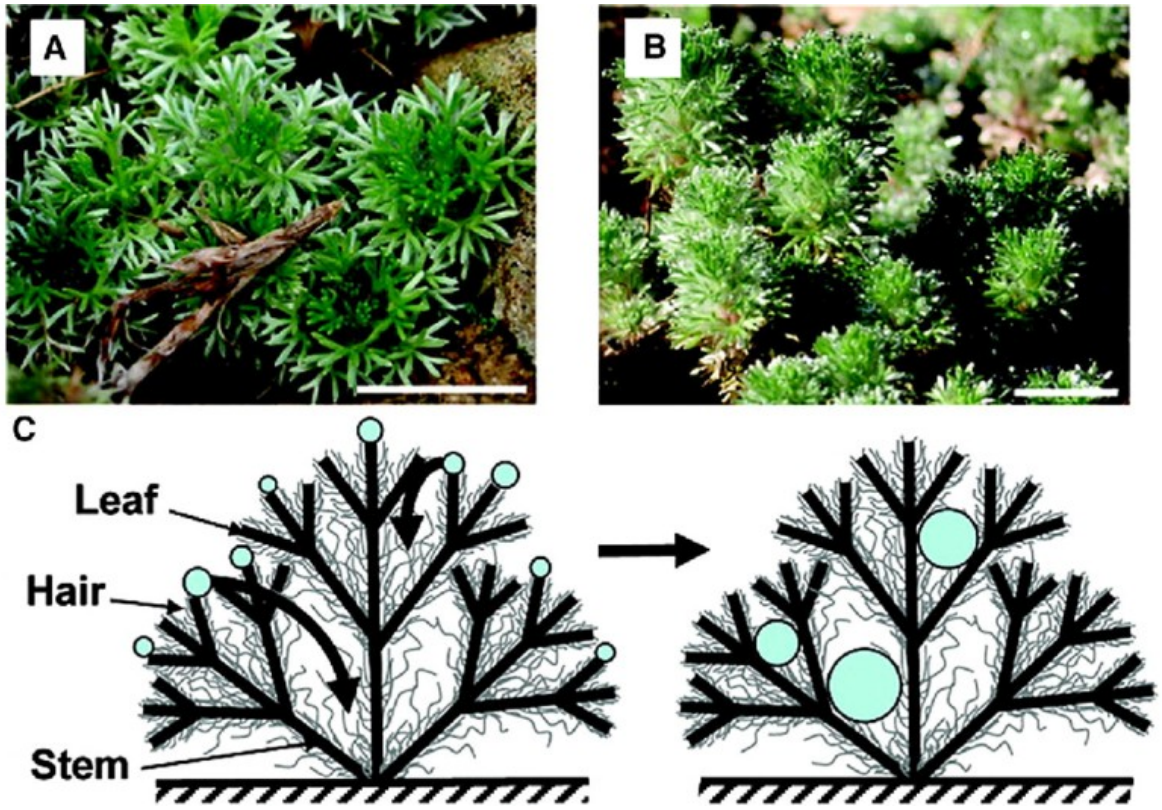




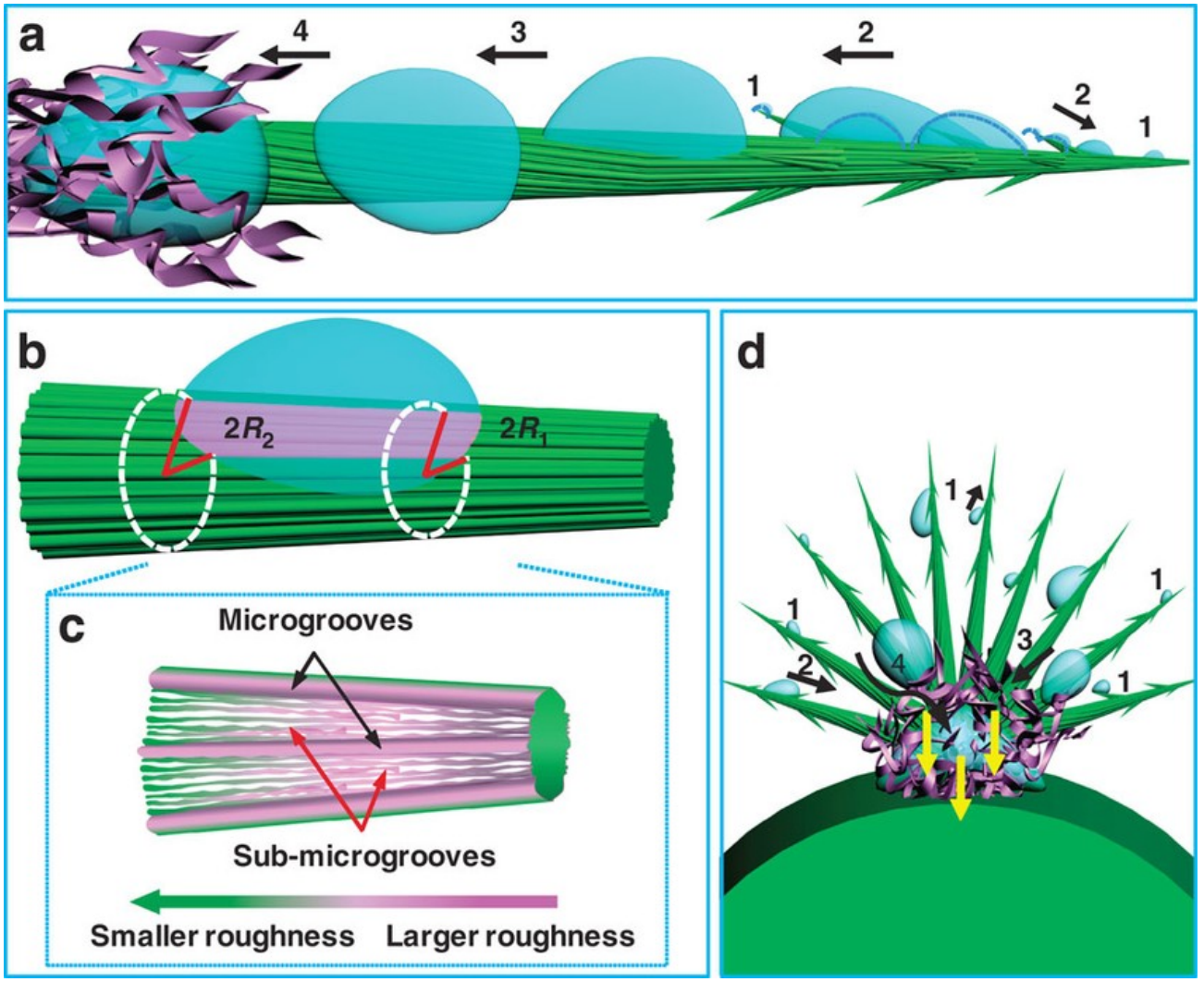
Besouro é Nano



Cotula Fallax



Cactus



Ju, Bai, Zheng, Zhao, Fang, Ziang, NATURE COMMUNICATIONS | 3:1247 (2012)

COMO CAPTAR

ÁGUA

USANDO

SEM ANOMALIA ?

Torre de Knapen



Hidrofílicos

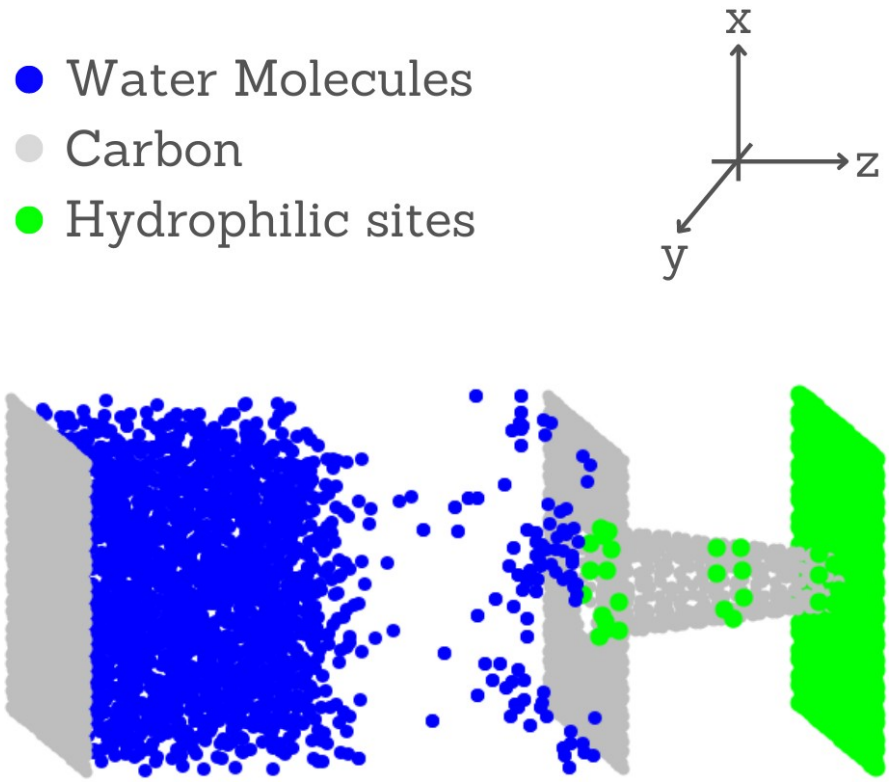


COMO CAPTAR

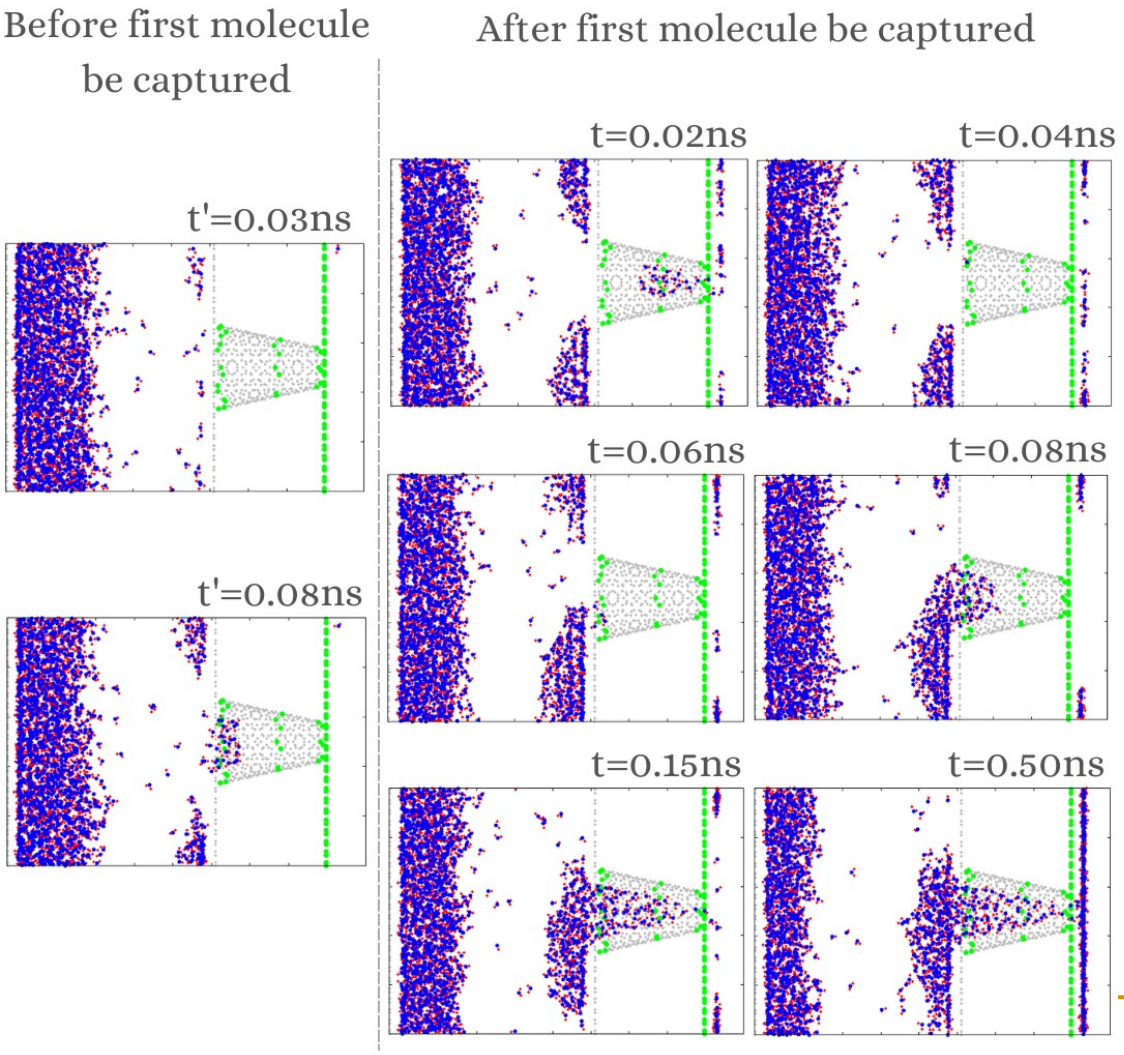
ÁGUA

COM ANOMALIA?

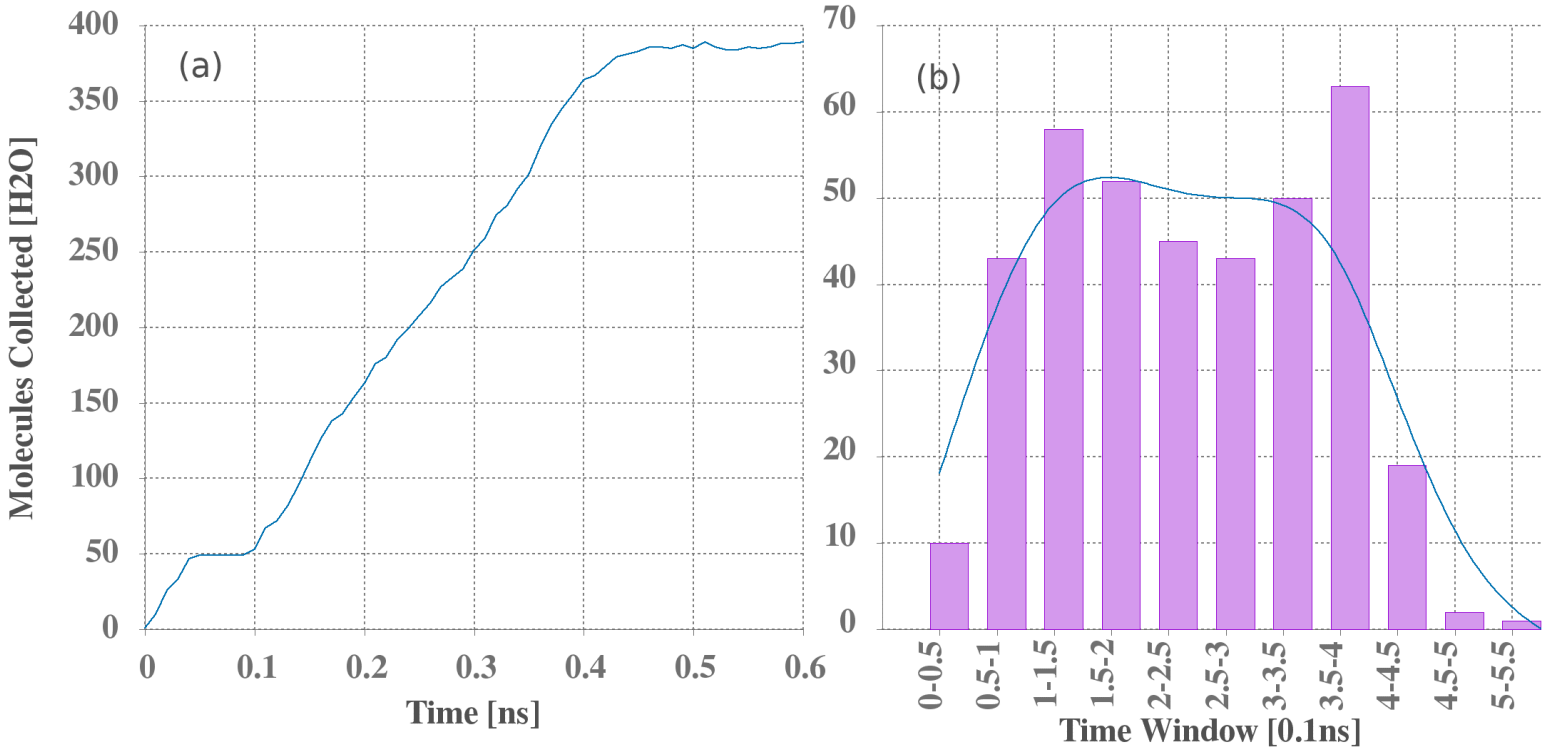
Nano Cone



Nano Cone


Before first molecule be captured
After first molecule be captured
t'=0.03ns
t'=0.08ns
t=0.02ns
t=0.04ns
t=0.06ns
t=0.08ns
t=0.15ns
t=0.50ns

Nano Cone

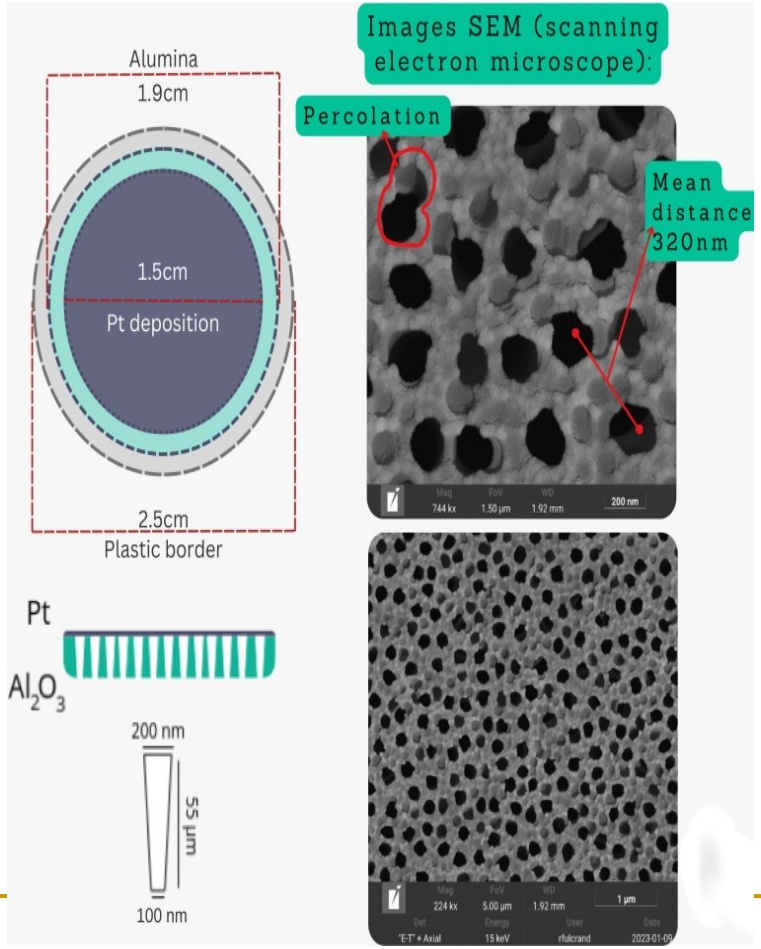

(a)
Molecules Collected [H2O]
400
350
300
250
200
150
100
50
0
0
0.1
0.2
0.3
0.4
0.5
0.6
Time [ns]
(b)
70
60
50
40
30
20
10
0
0-0.5
0.5-1
1-1.5
1.5-2
2-2.5
2.5-3
3-3.5
3.5-4
4-4.5
4.5-5
5-5.5
Time Window [0.1ns]

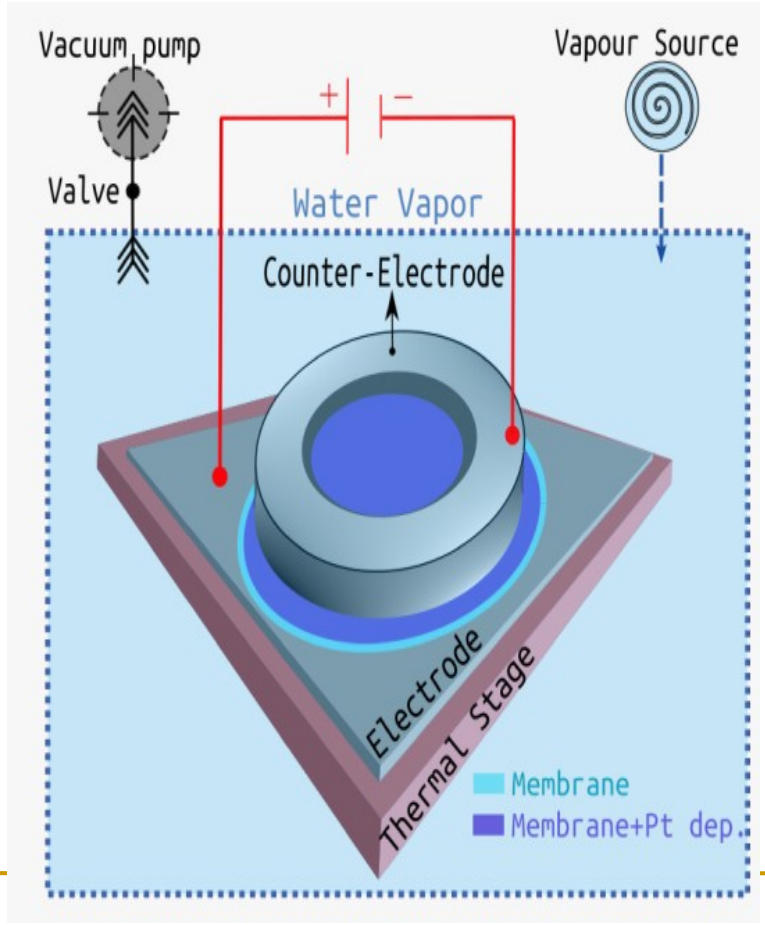
COMO CAPTAR

ÁGUA

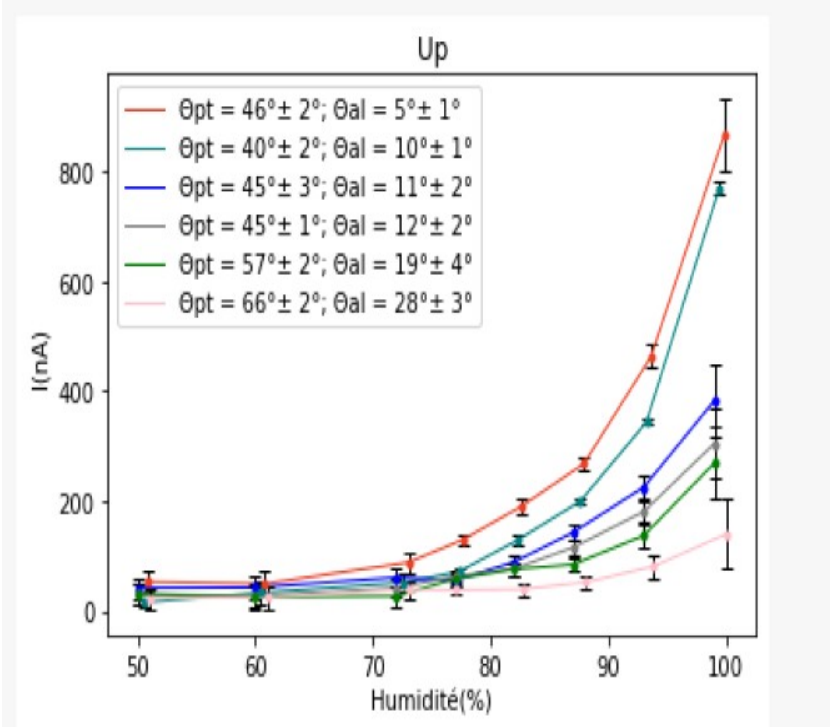
EXPERIMENTALMENTE?

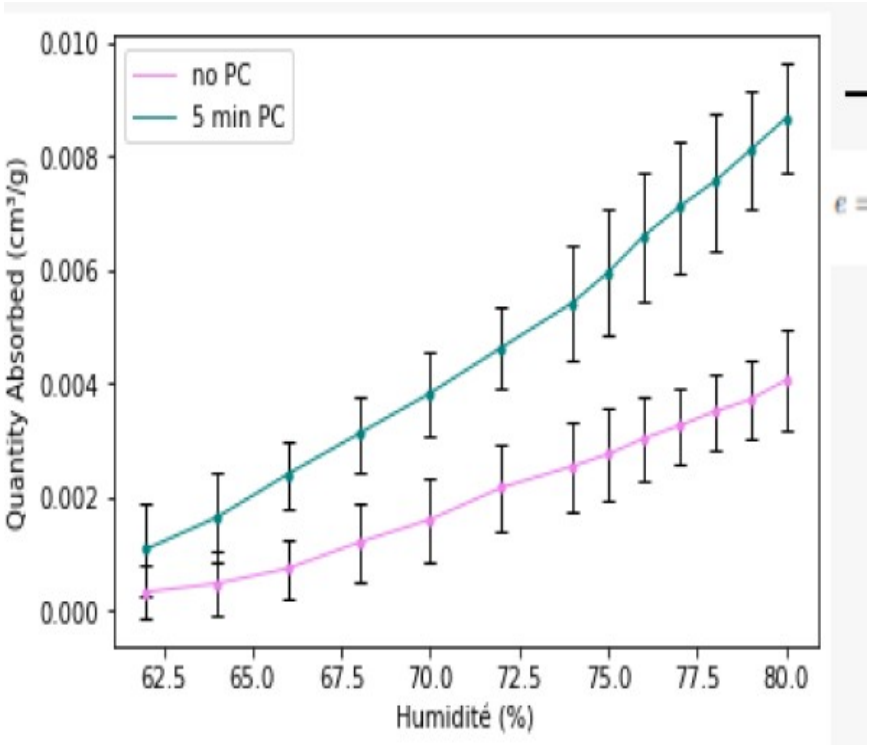
Nano Cone


Alumina
1.9cm
1.5cm
Pt deposition
2.5cm
Plastic border
Pt
Al_2O_3
200 nm
55 µm
100 nm
Images SEM (scanning electron microscope):
Percolation
Mean distance 320nm

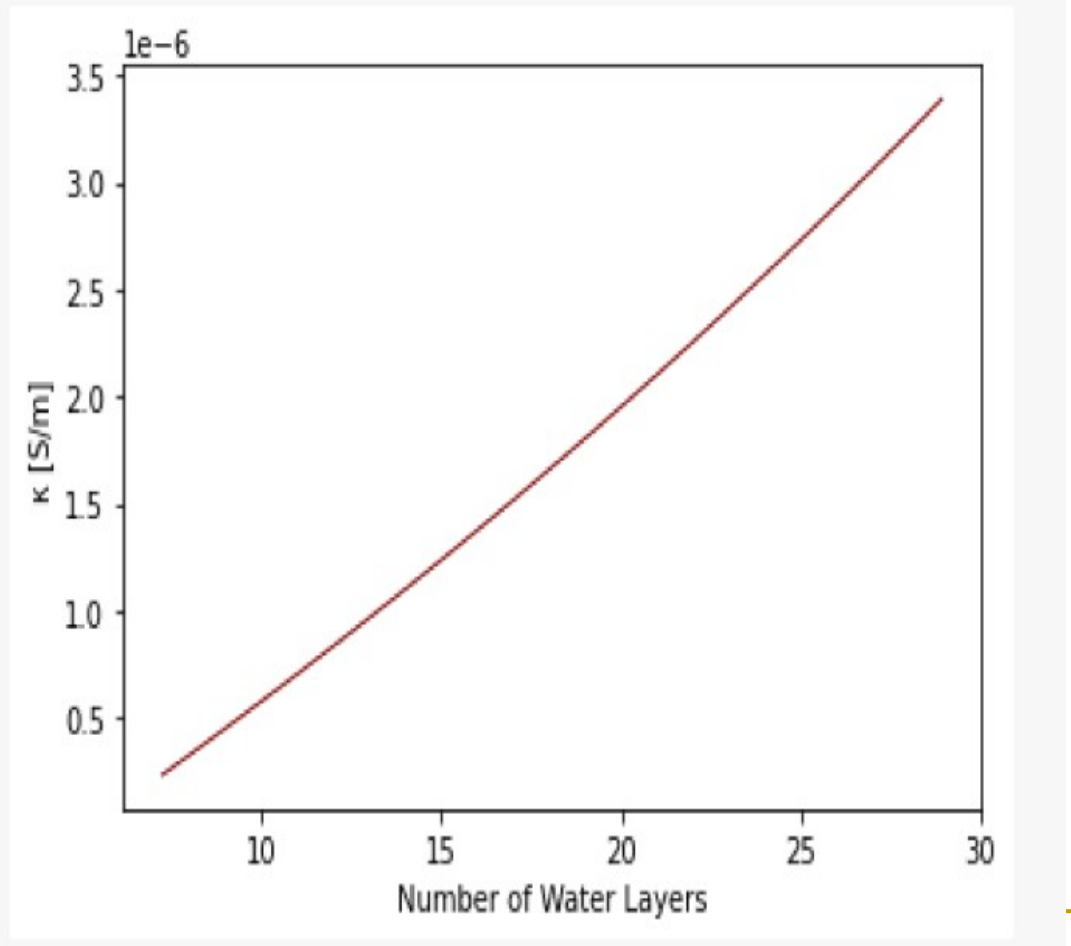

Vacuum pump
Vapour Source
Valve
Water Vapor
Counter-Electrode
Electrode
Thermal Stage
Membrane
Membrane+Pt dep.

Humidade


Up
Θpt = 46°± 2°; Θal = 5°± 1°
Θpt = 40°± 2°; Θal = 10°± 1°
Θpt = 45°± 3°; Θal = 11°± 2°
Θpt = 45°± 1°; Θal = 12°± 2°
Θpt = 57°± 2°; Θal = 19°± 4°
Θpt = 66°± 2°; Θal = 28°± 3°
I(nA)
0
200
400
600
800
50
60
70
80
90
100
Humidité(%)


no PC
5 min PC
Quantity Absorbed (cm³/g)
0.000
0.002
0.004
0.006
0.008
0.010
62.5
65.0
67.5
70.0
72.5
75.0
77.5
80.0
Humidité (%)

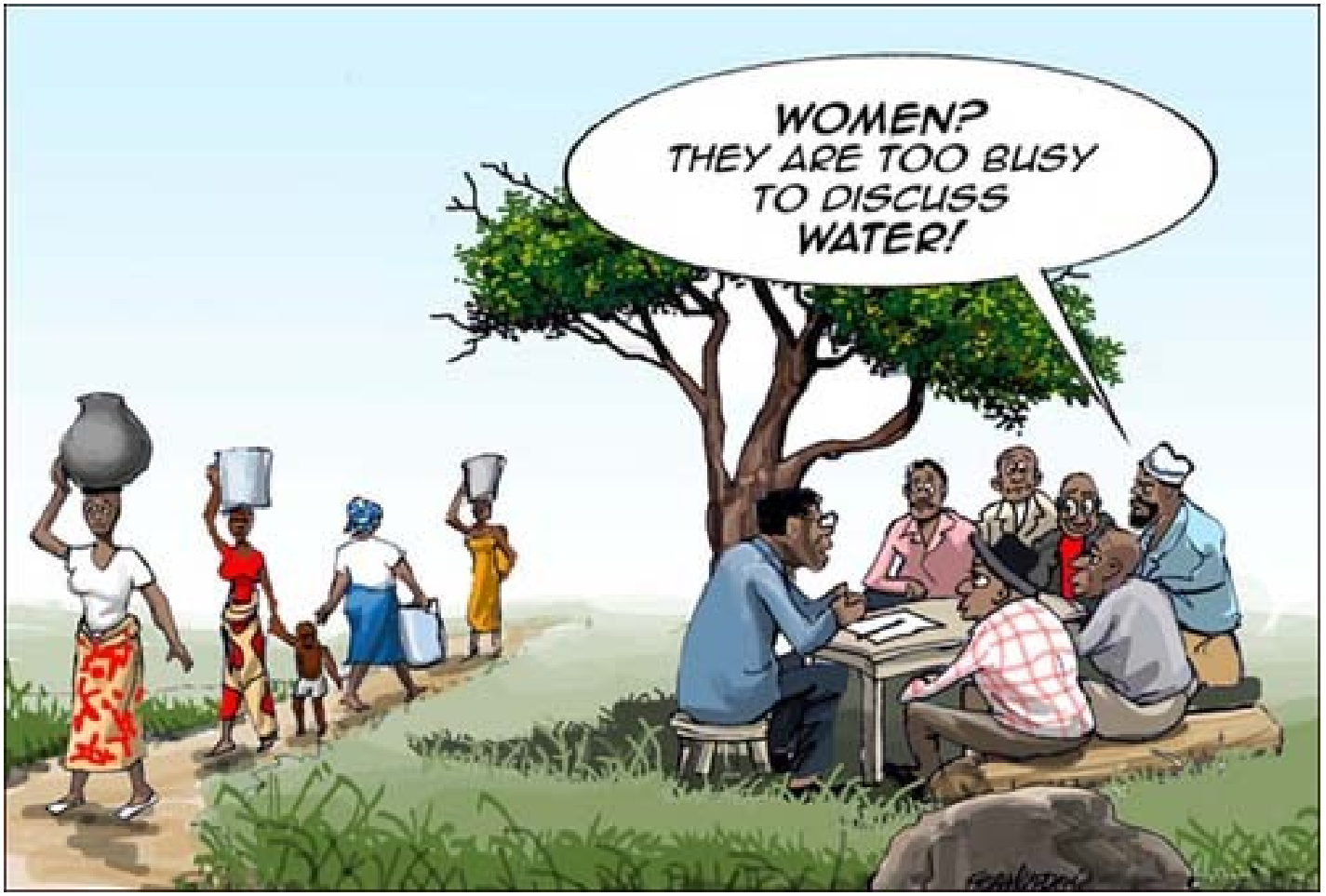
Condutividade



Conclusões

- **Anomalias são importantes para a vida**
- **Podemos usar as anomalias para criar mais água potável**

Diversidade




GRUPO DE
COMPLEXOS

Futuro?

