Enhanced flow of core-softened fluids through nanotubes

What is the mistery?

Why should we care?

What is our assumption?

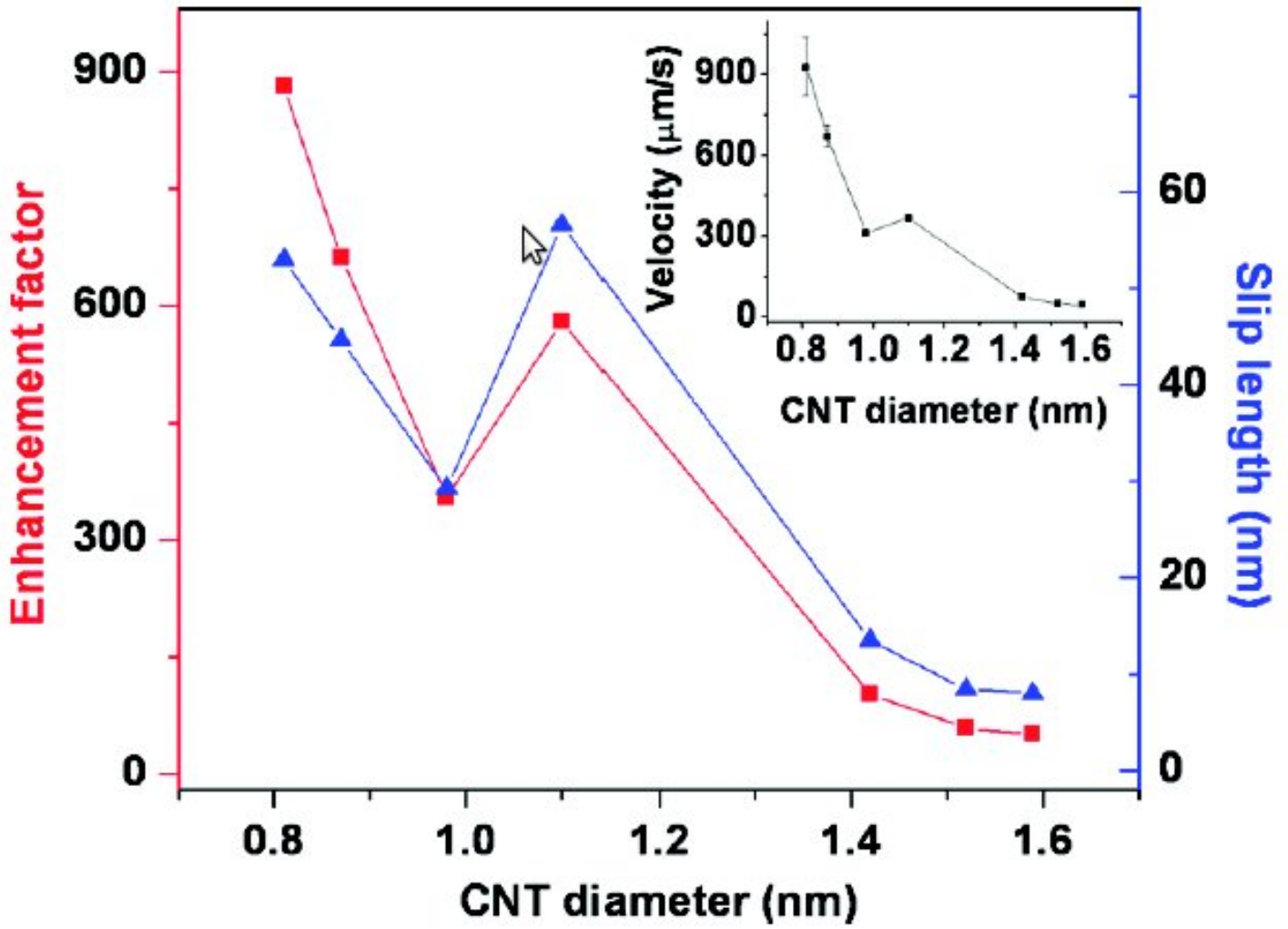
What are our results?

Conclusions

Our Group

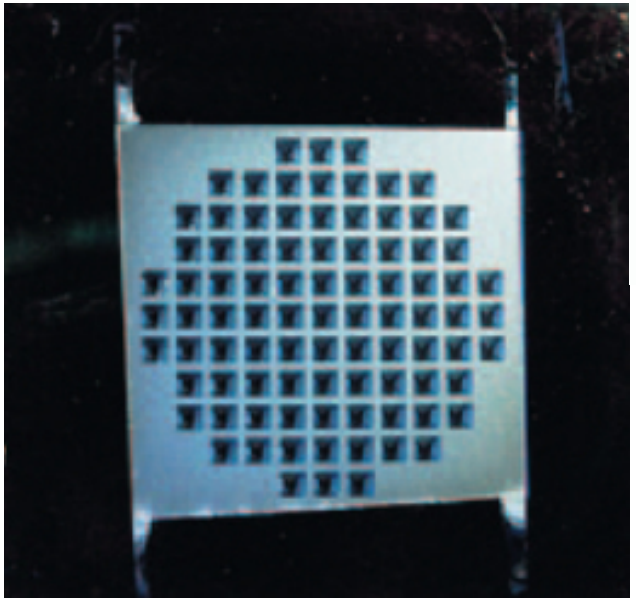
What is the mistery?

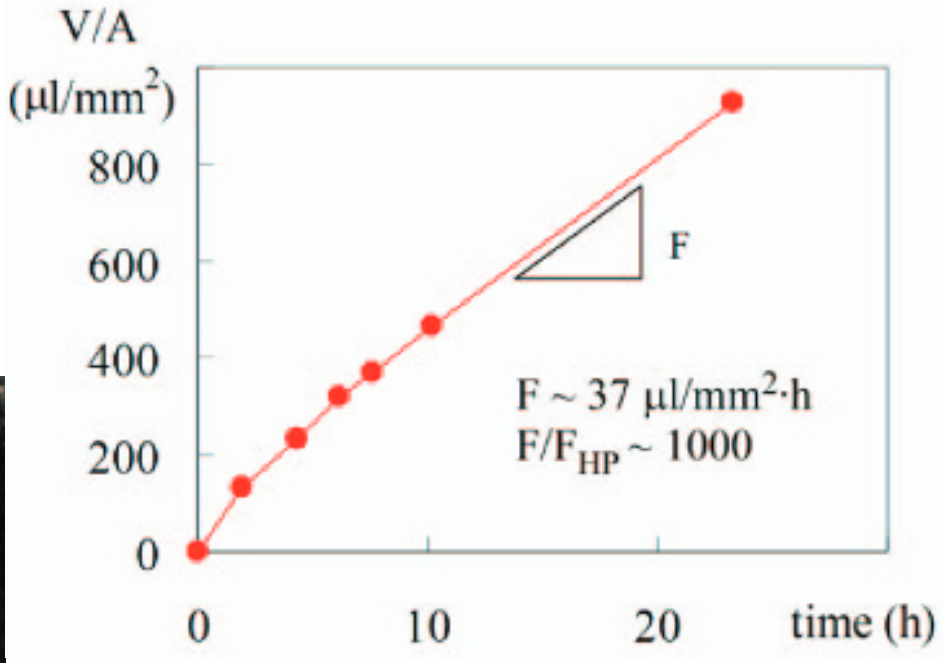
X. Qin et al, Nanoletters 11, 2173 (2011) - experimental - SPC/E



Nanotube Filter

Fornasiero, Park, Holt, Stadermann, Costas,GGrigoropoulos, Noy, Bakajin, PNAS 2008

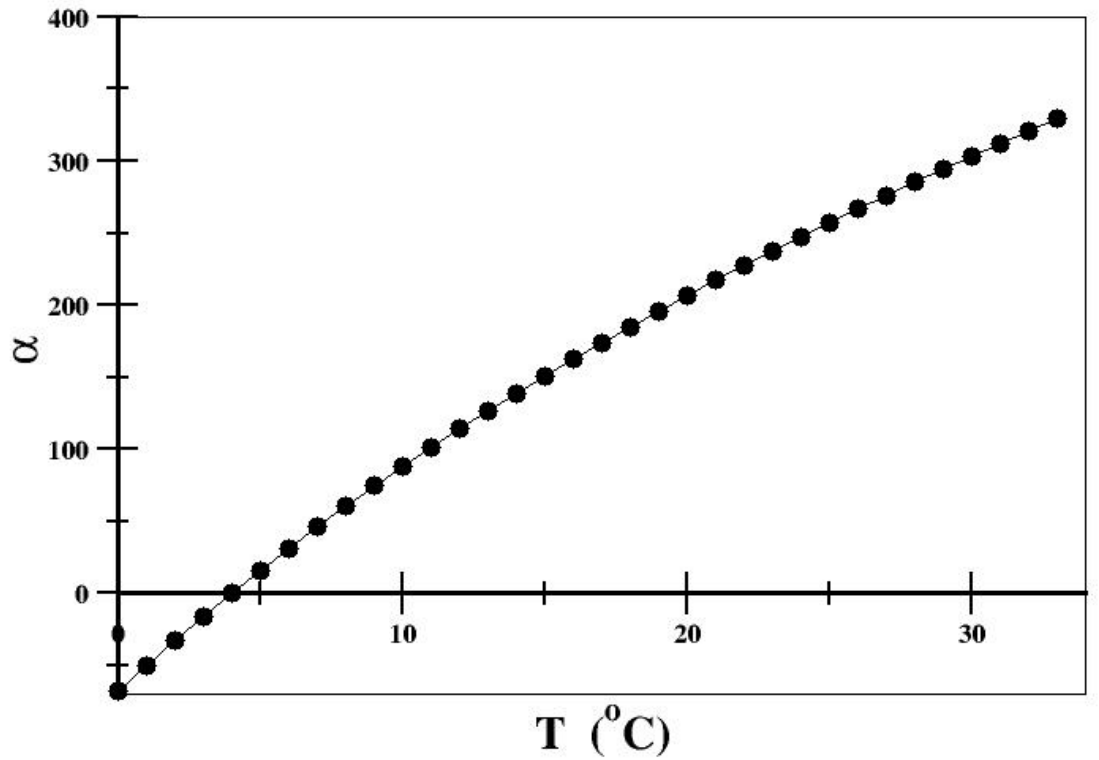




Thermal Expansion

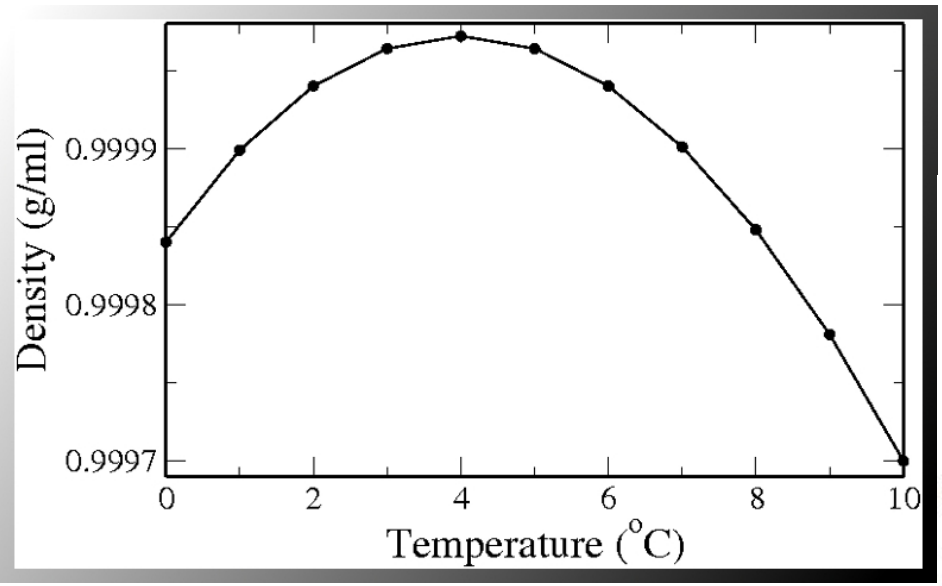
Kell, J. Chem. Eng. Data 20, 97 (75)

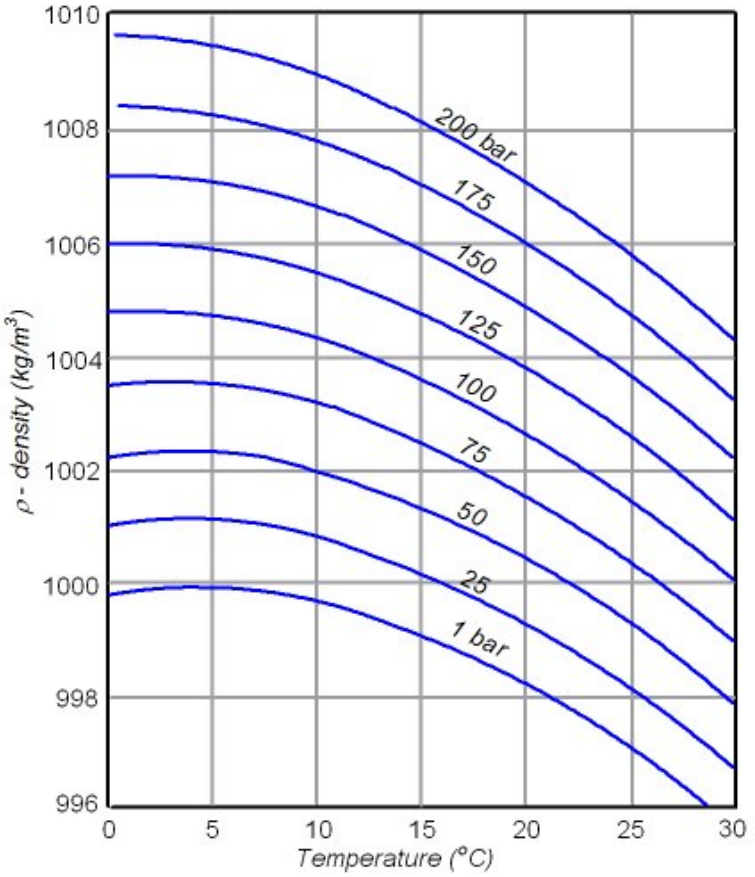
- $\alpha_P = \frac{1}{V}\{\frac{\partial V}{\partial T}\}_P$



Density

Kell, J. Chem. Eng. Data 12, 66 (67)

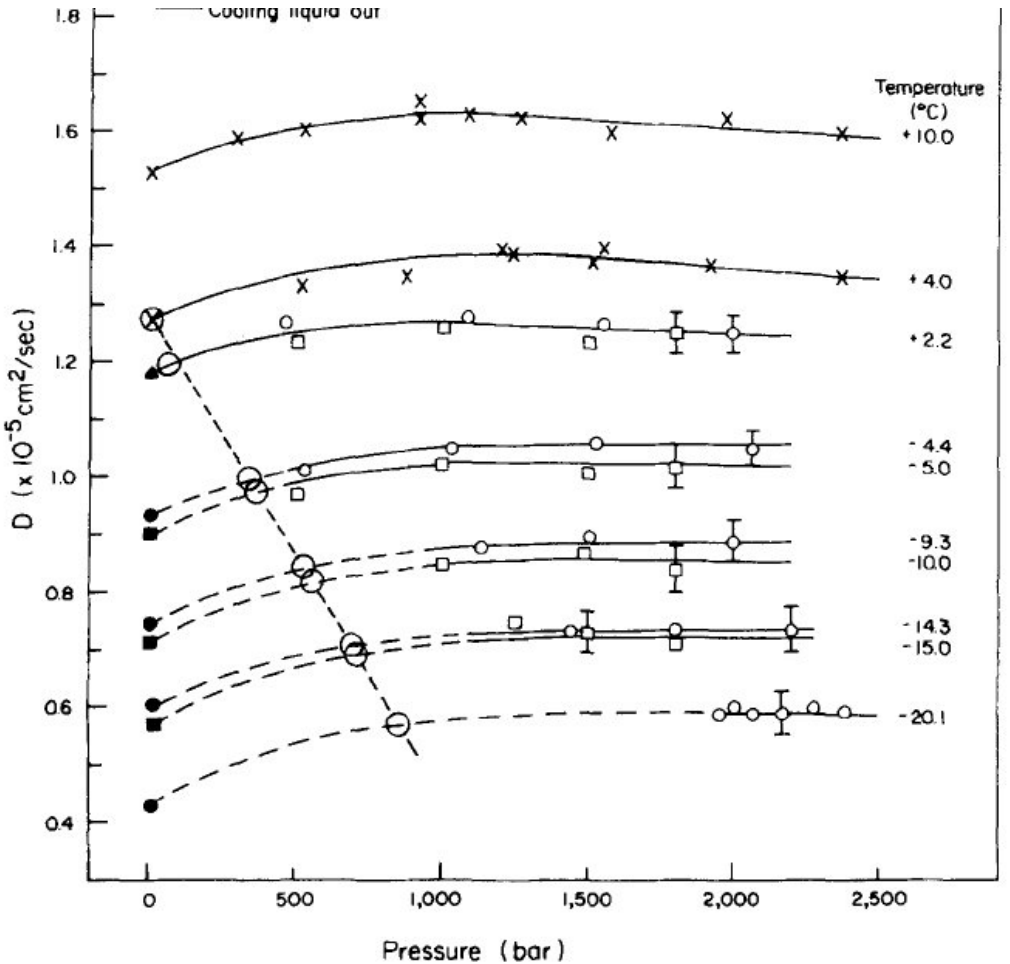




Diffusion

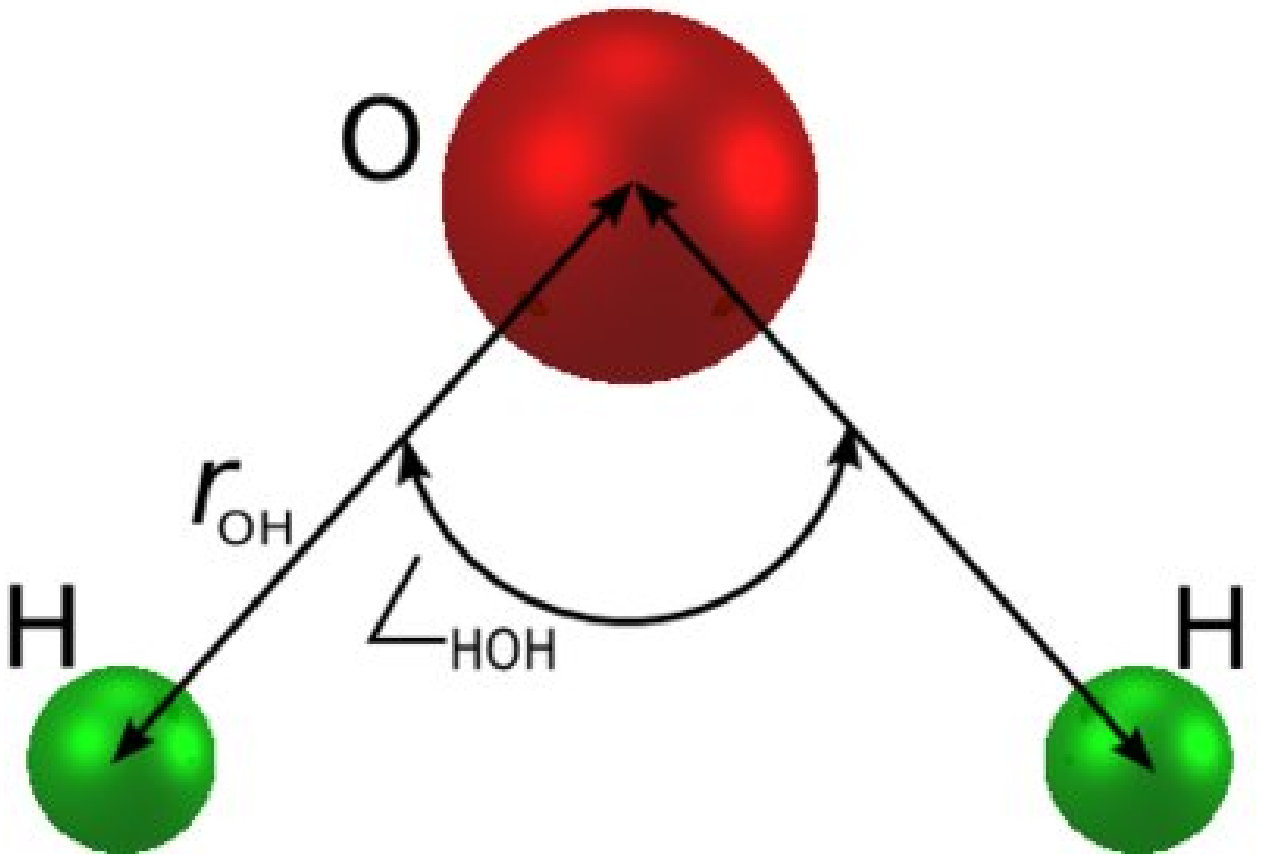
Angell, Finch, Bach 65, 3063 (76)

- $\langle r(t)r(0)\rangle = 6Dt$



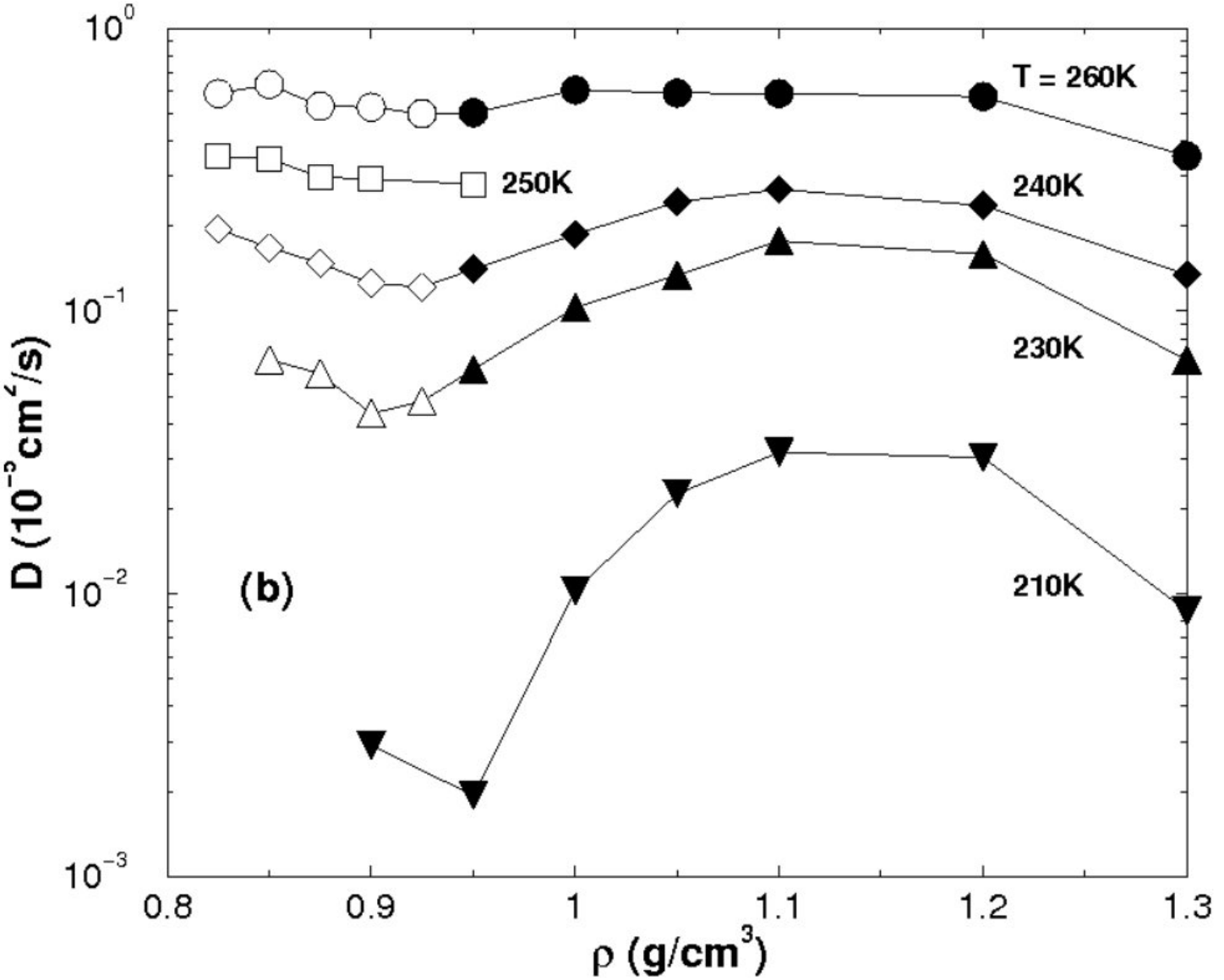
Diffusion - SPC/E

Berendsen, Grigera, Straatsma, JCP 91, 6269 (87)



Diffusion - SPC/E

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

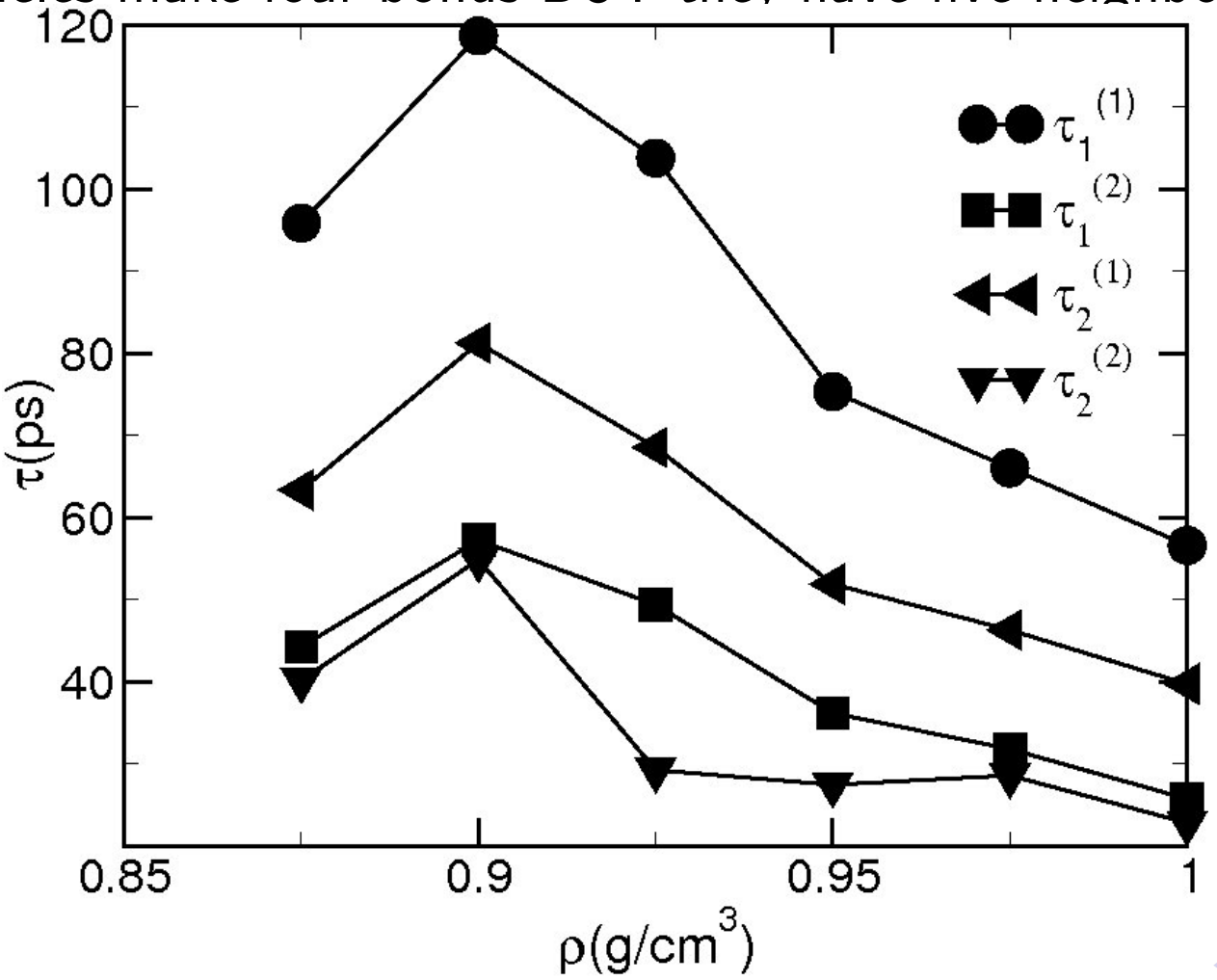


Rotation Diffusion - SPC/E

Netz, Starr, Barbosa, Stanley, JML 101, 159-168 (02)

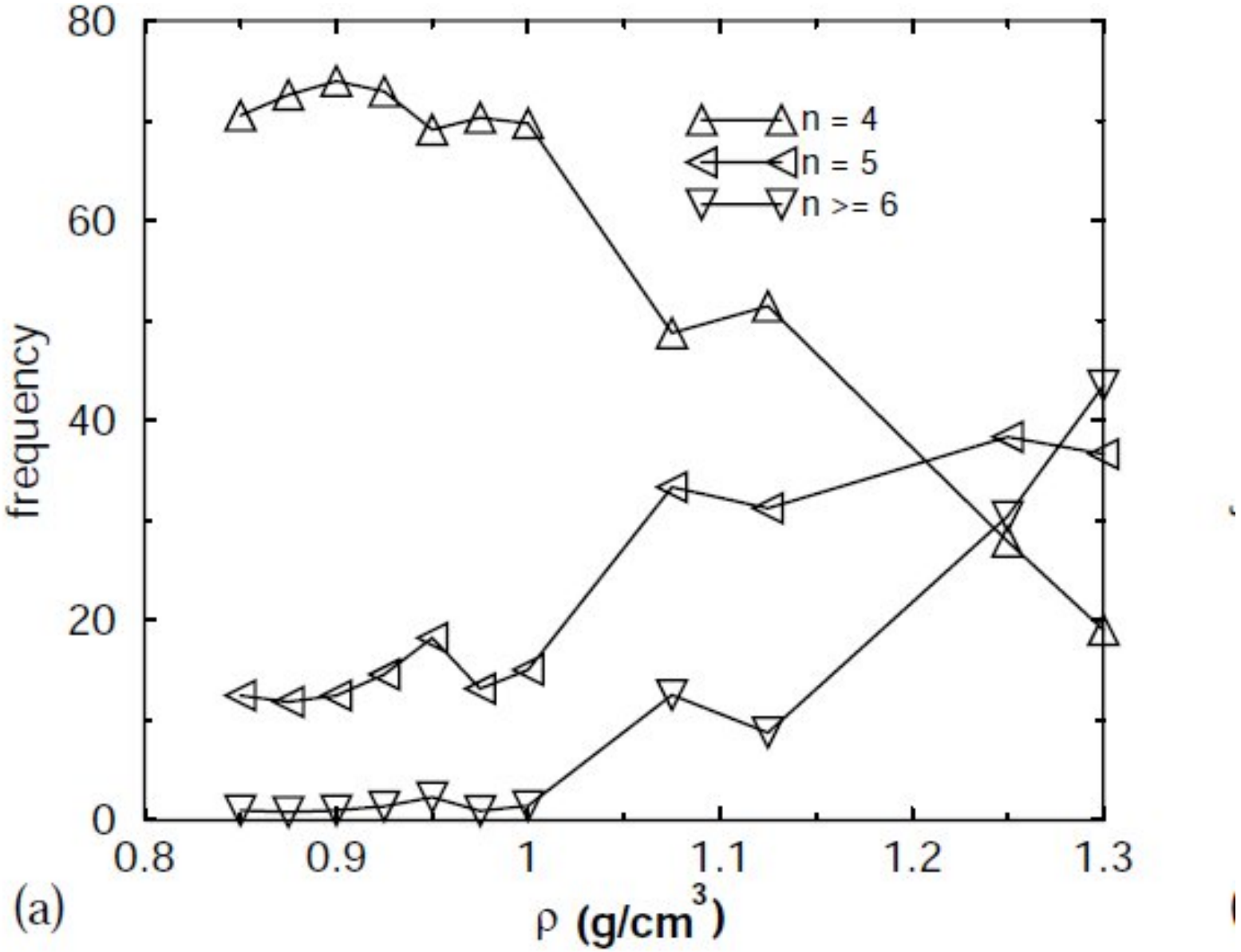
Mazza, Giovanbaptista, Stanley, Starr, PRE 76, 31203 (07)

- Particles make four bonds BUT they have five neighbors!!!



Frequency - SPC/E

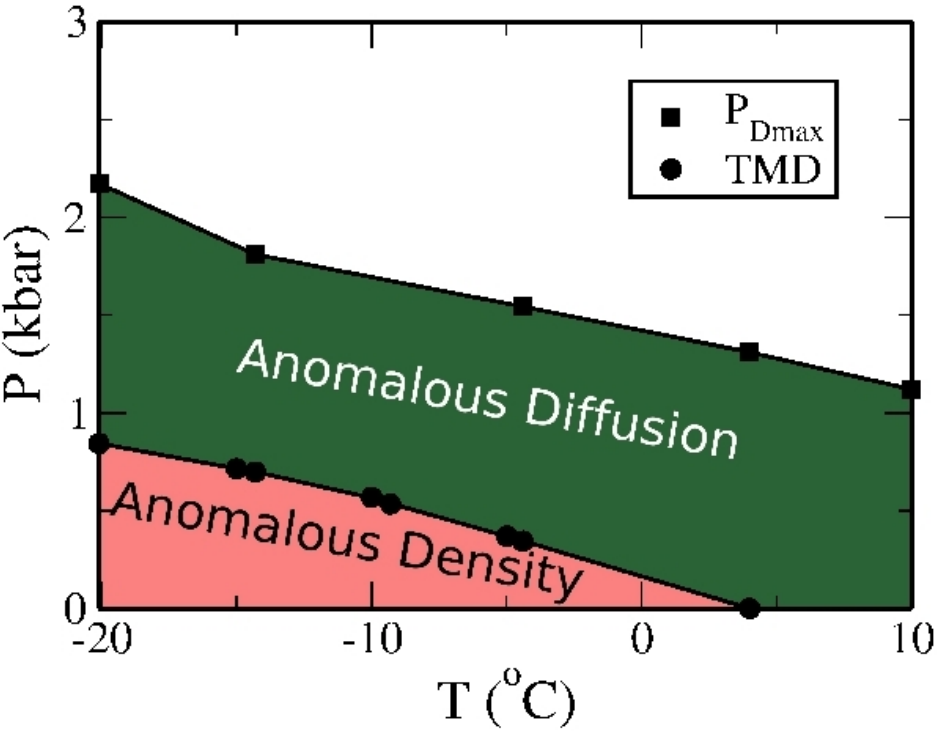
Netz, Starr, Barbosa and Stanley, Physica A 314, 470 (2002)

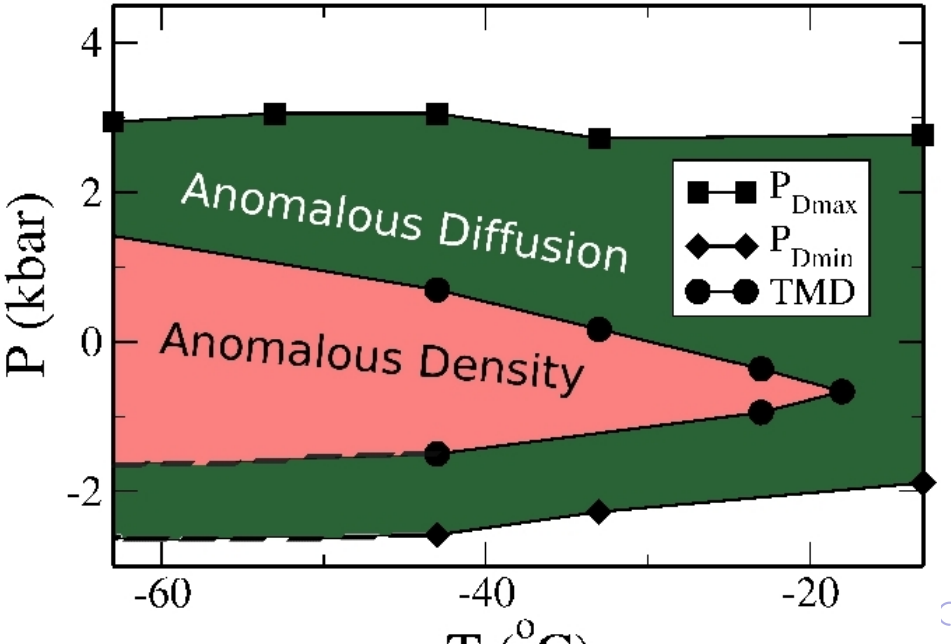


Water SPC/E

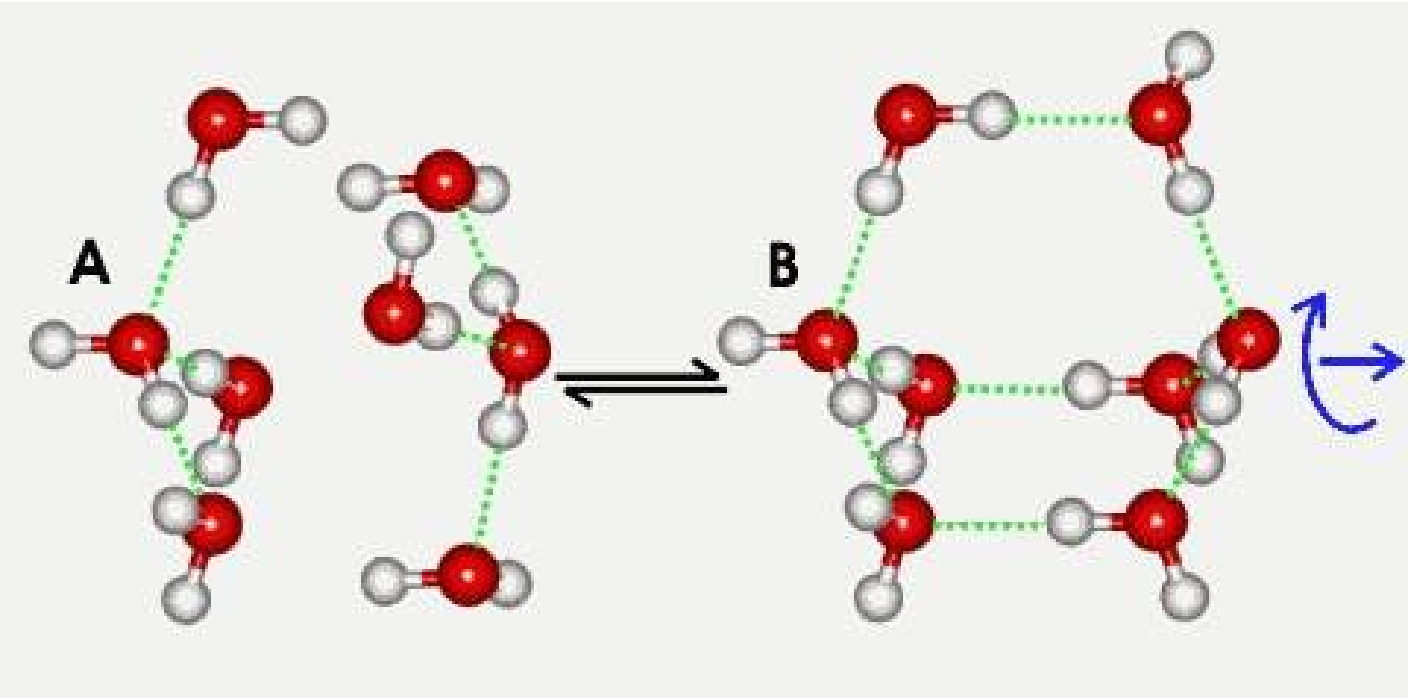
Angell, Finch, Bach 65, 3063 (76)

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

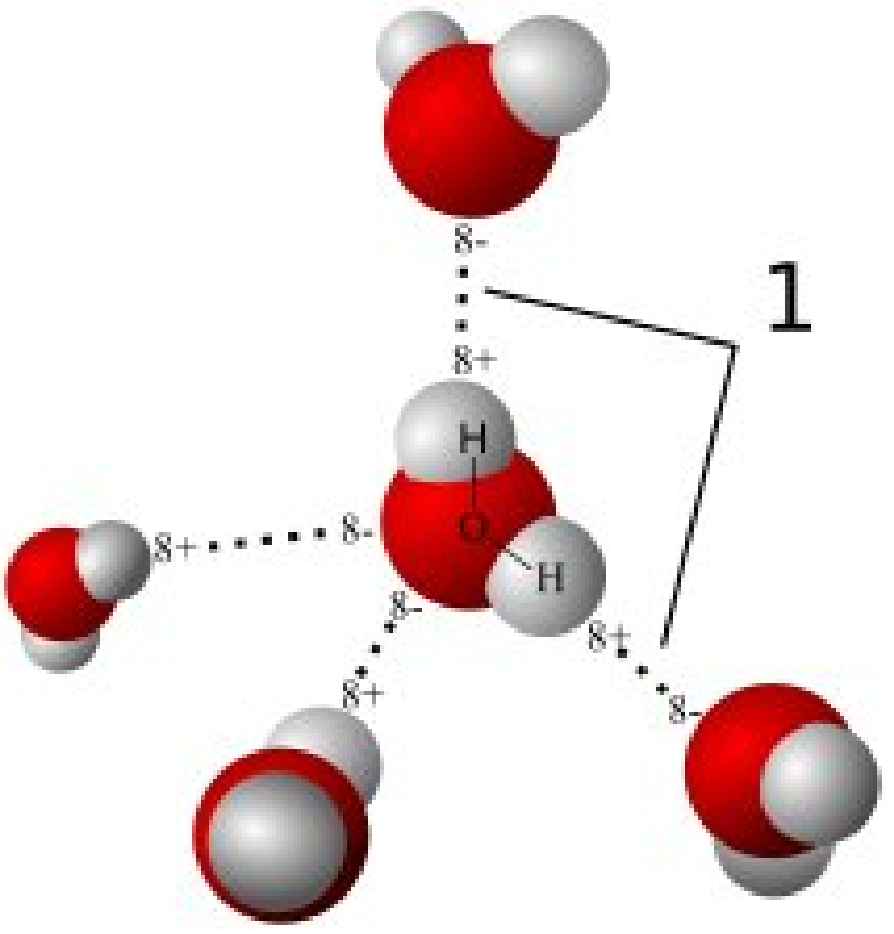




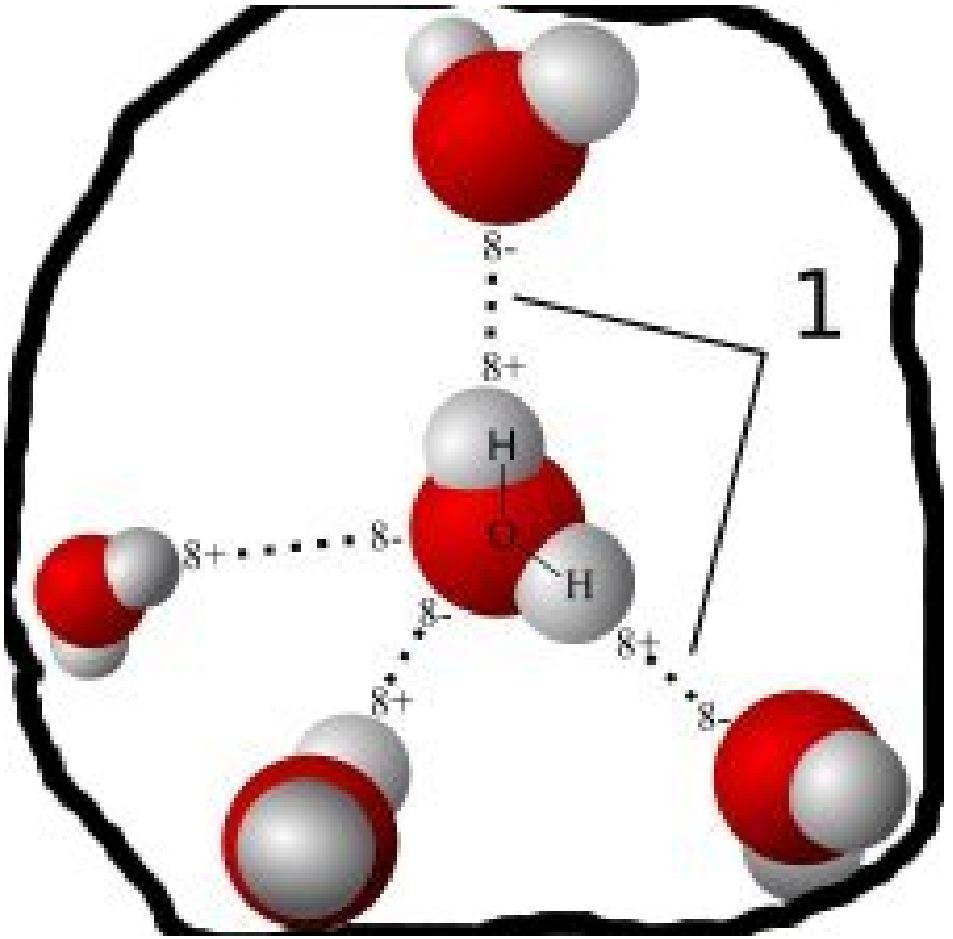
Two Length Scales Potential



Structure

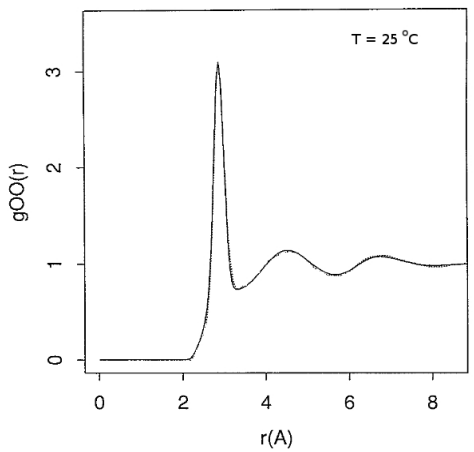


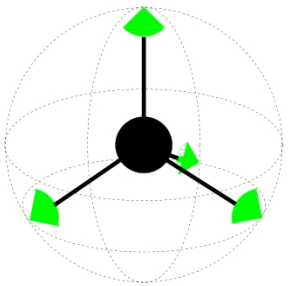
Structure



Effective Potential

- Radial Distribution Function of WATER:





$\sigma_o = 2,86 \times 10^{-10} m$
$\epsilon = 0,006 \frac{kcal}{mol}$

- Ornstein-Zernike Equation:

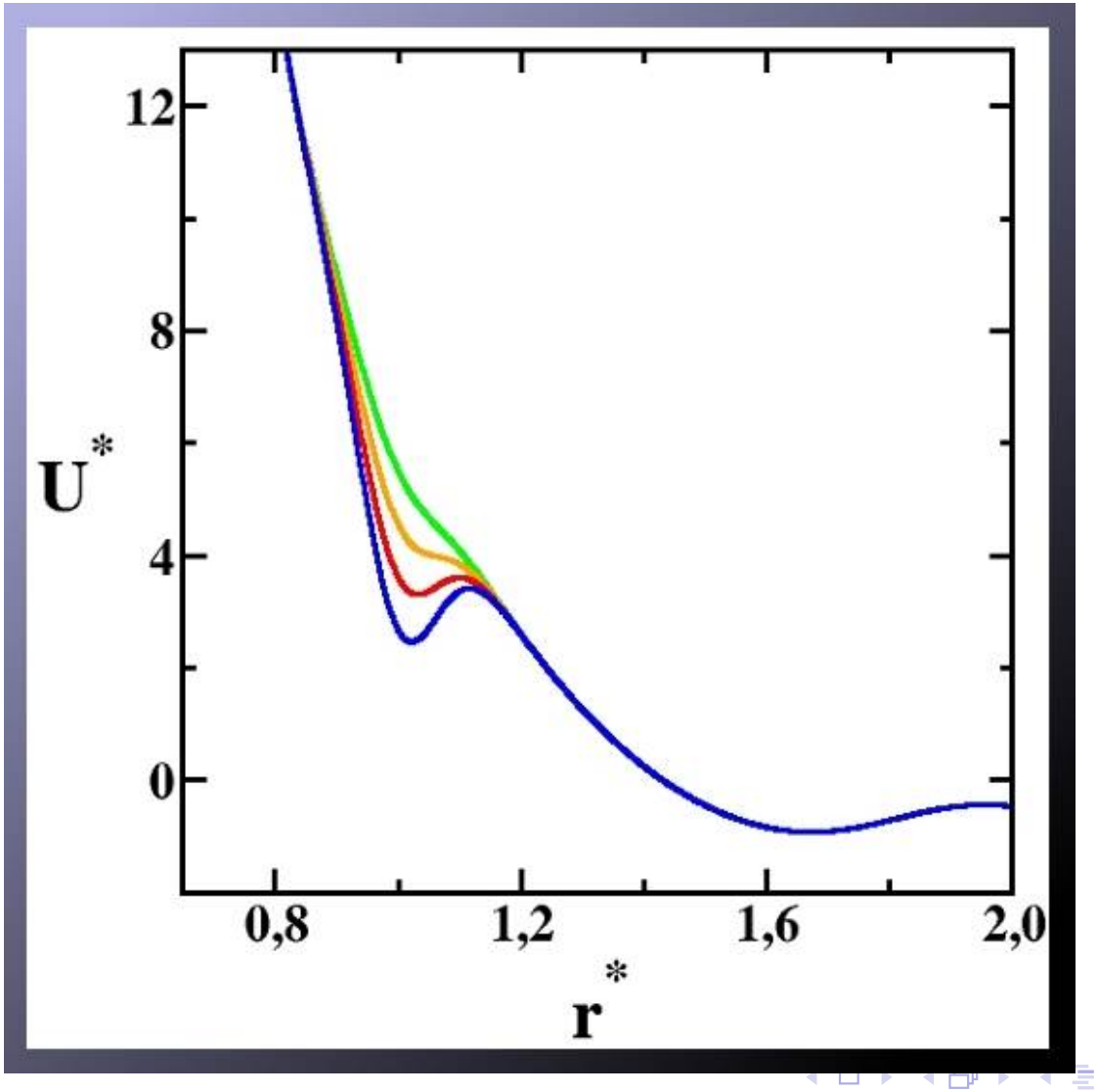
$$h(r) = g(r) - 1 = c(r) + \rho \int c(r - r')h(r')dr'$$

- *Hypernetted Chain Approximation* (HNC):

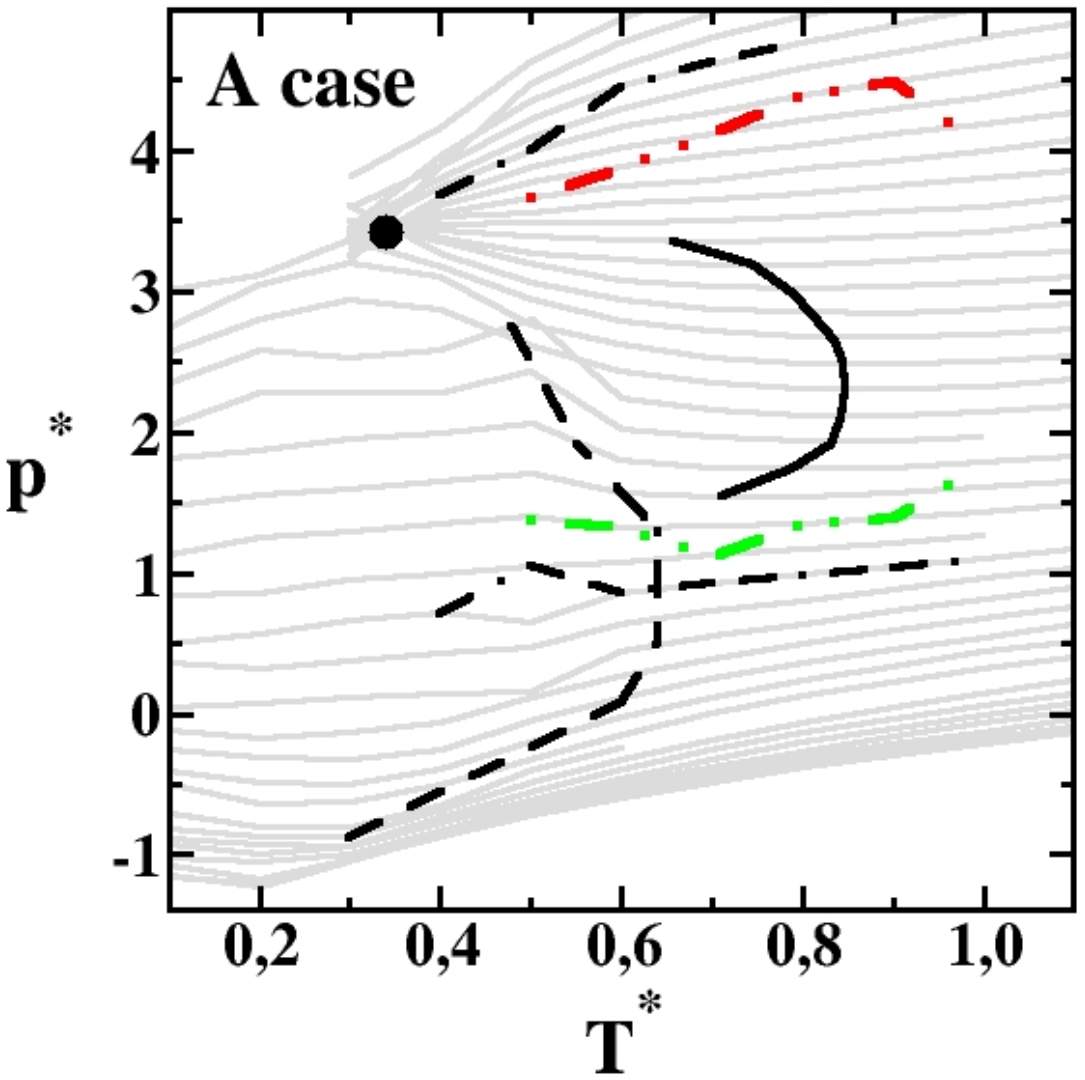
$$U(r) = k_B T\{g(r) - 1 - \ln[g(r)] - c(r)\}$$

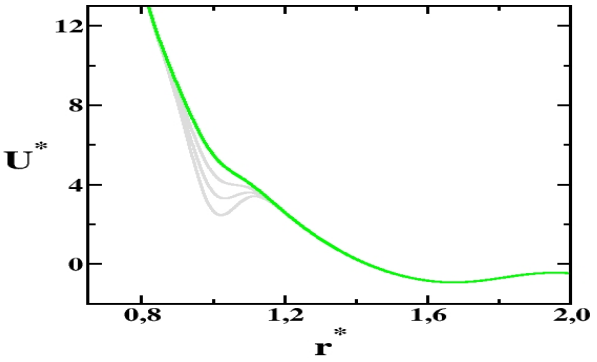
Effective Potential

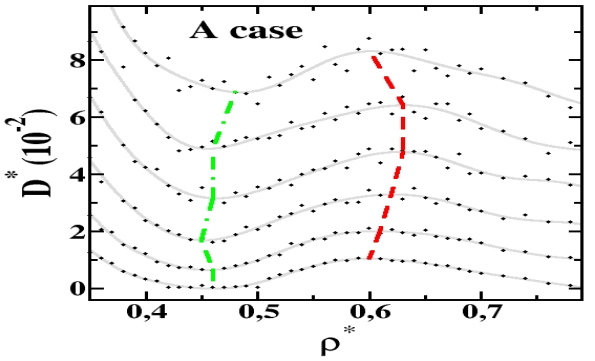
Barraz, Salcedo, Barbosa, JCP 131, 094504 (09)

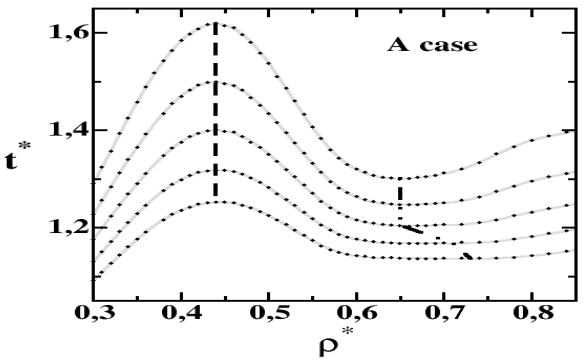


Phase Diagram

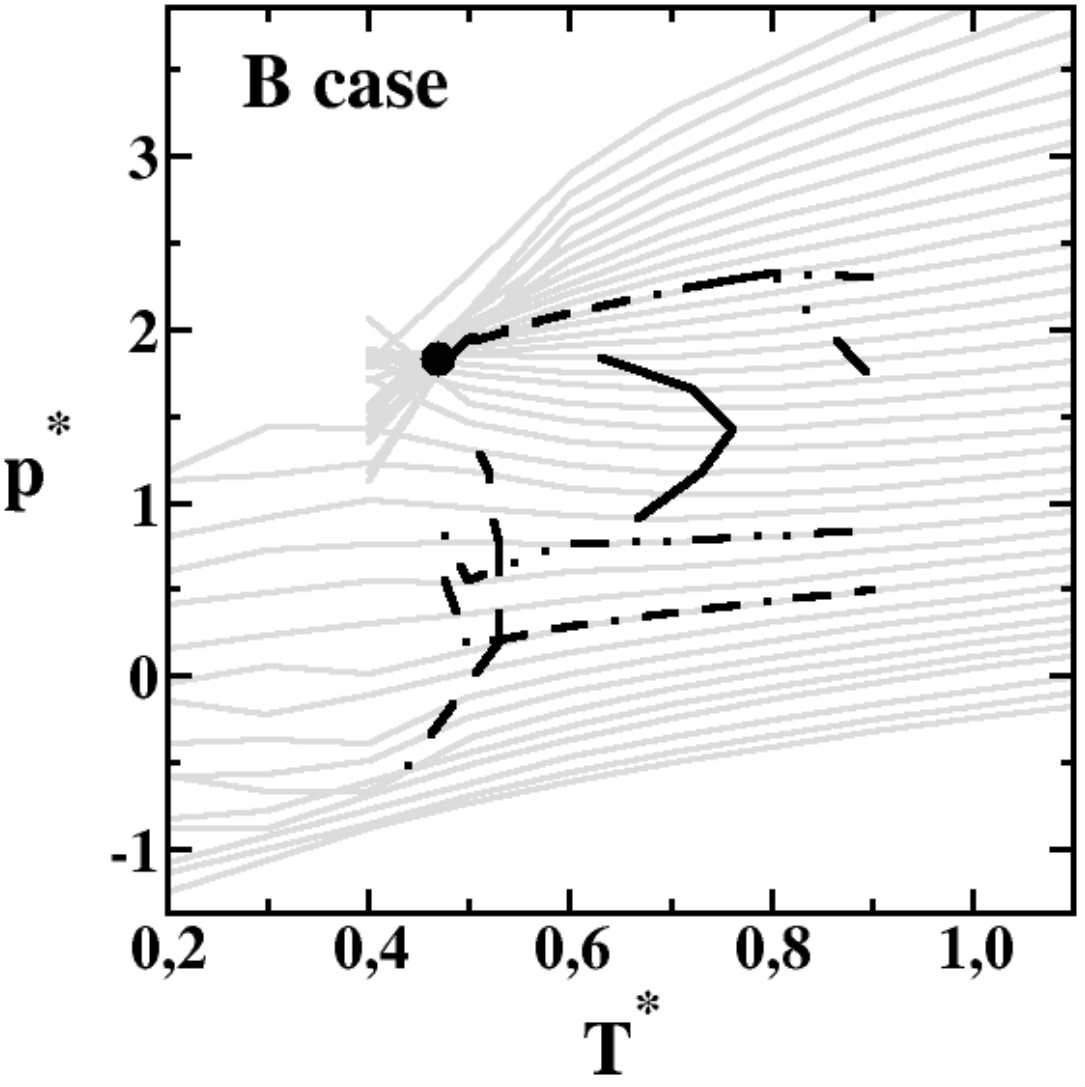


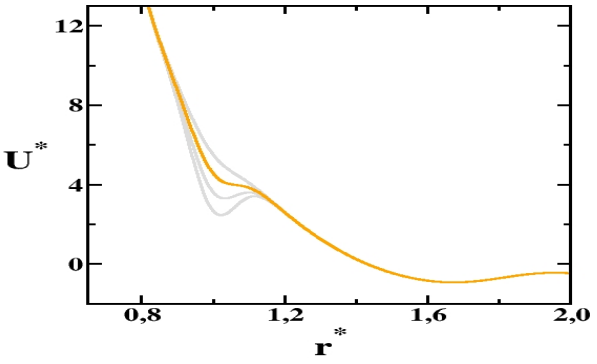


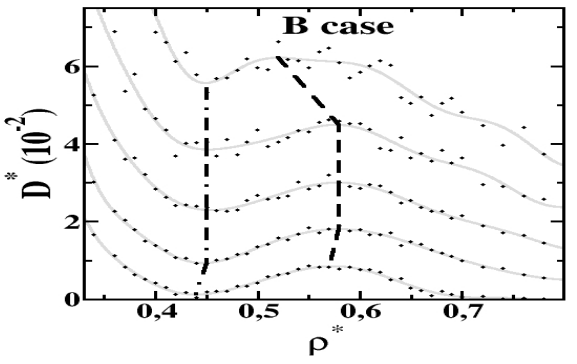


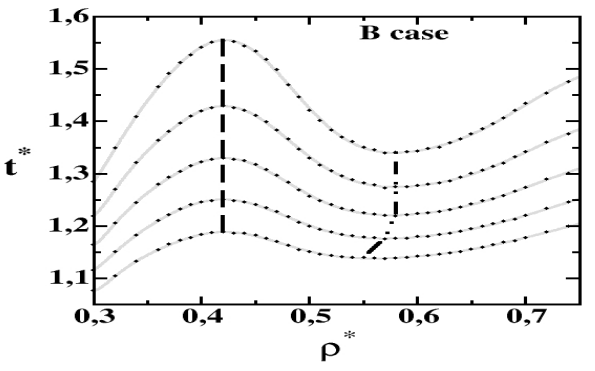


Phase Diagram

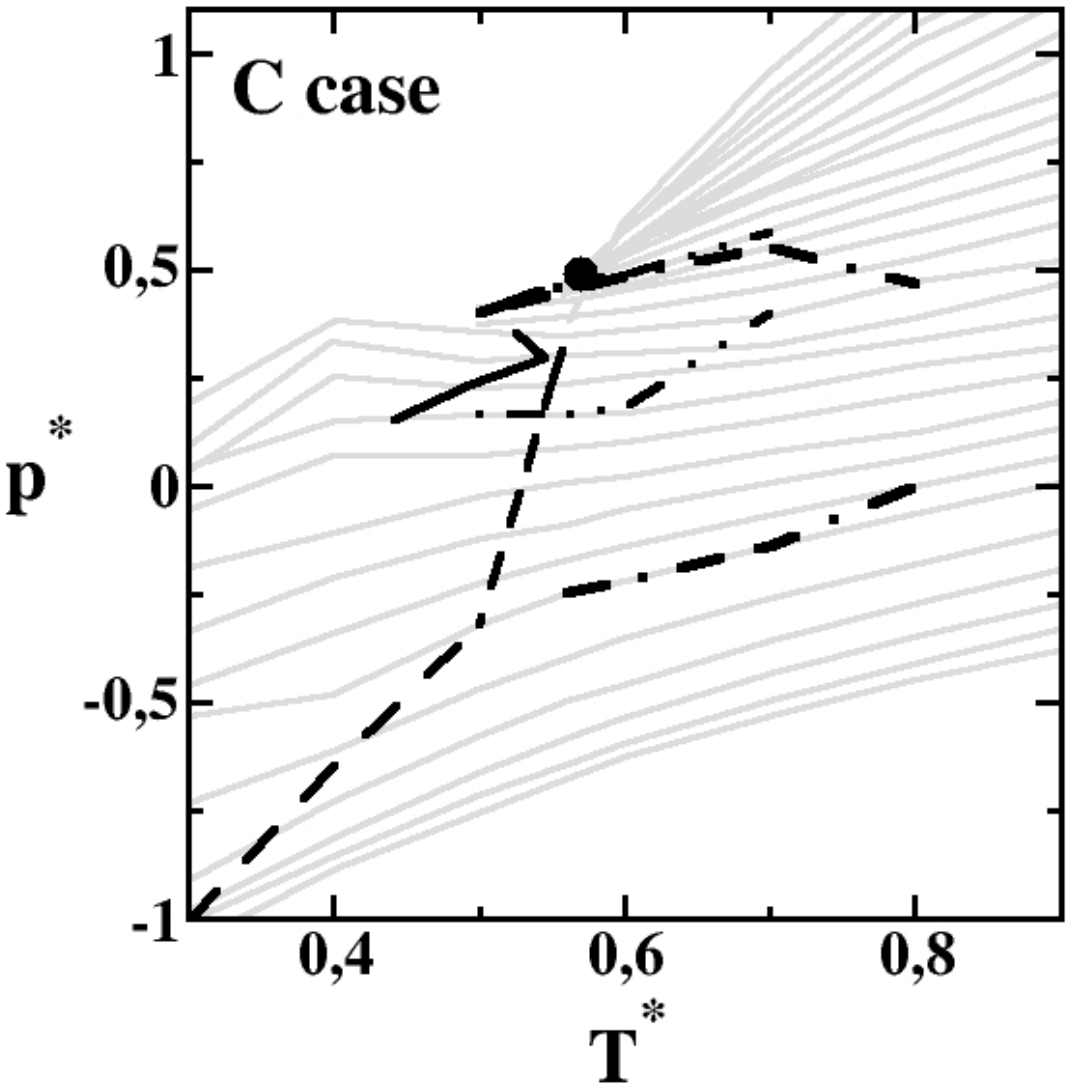


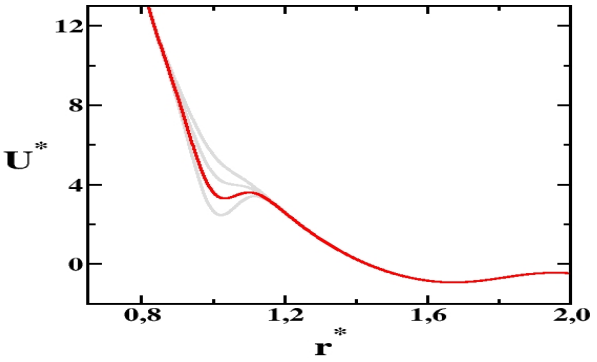


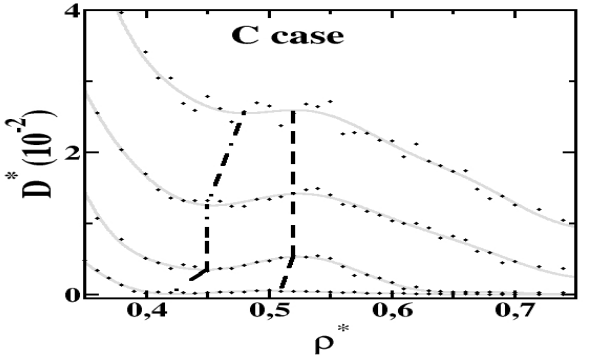


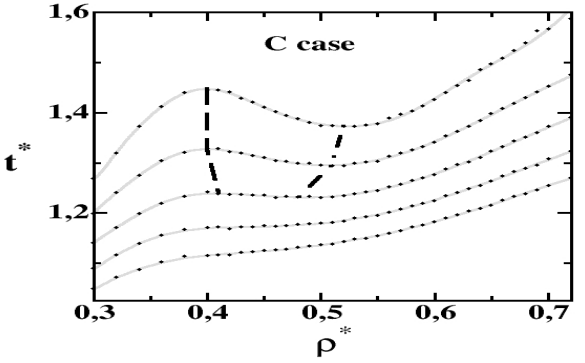


Phase Diagram

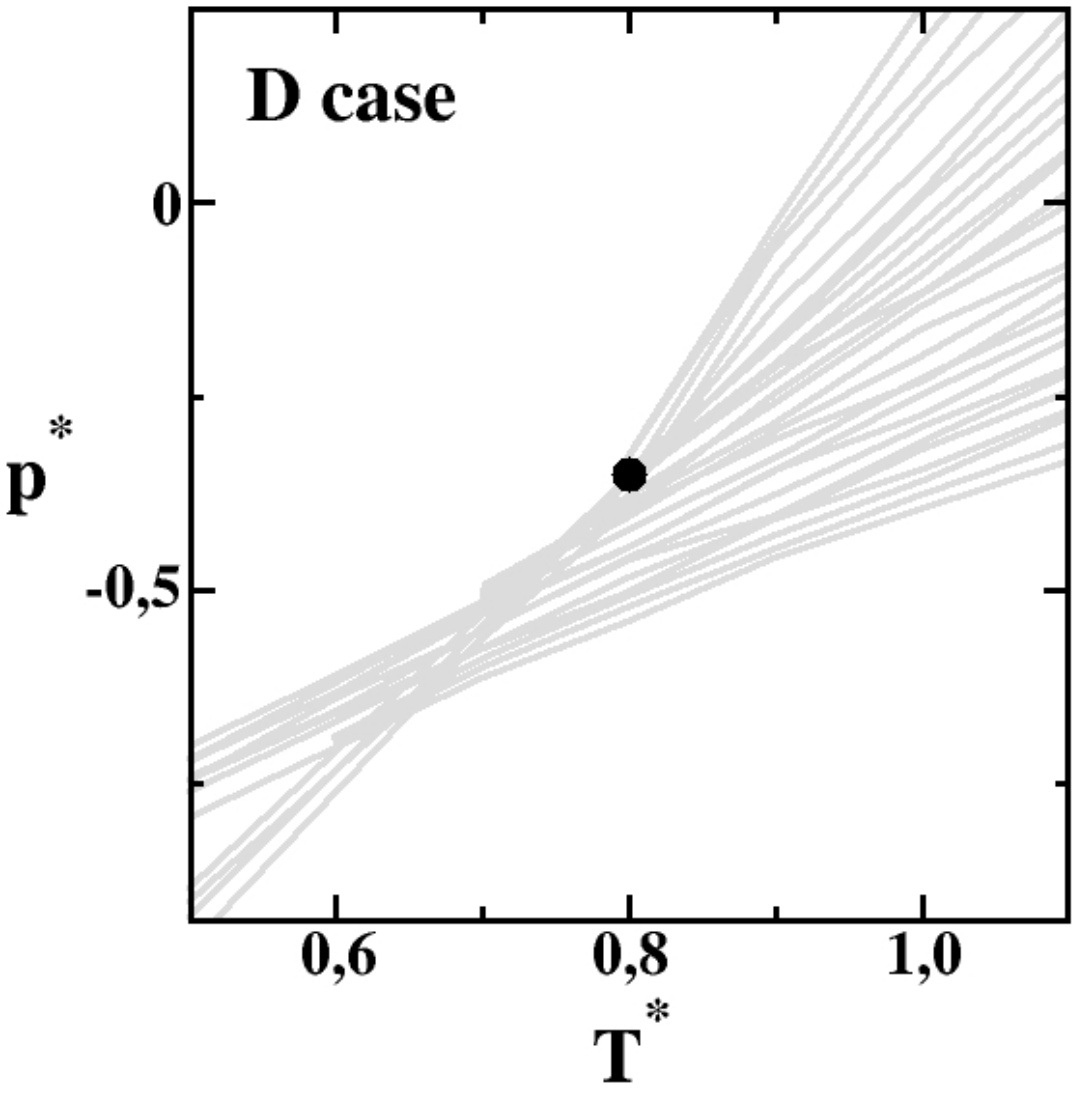


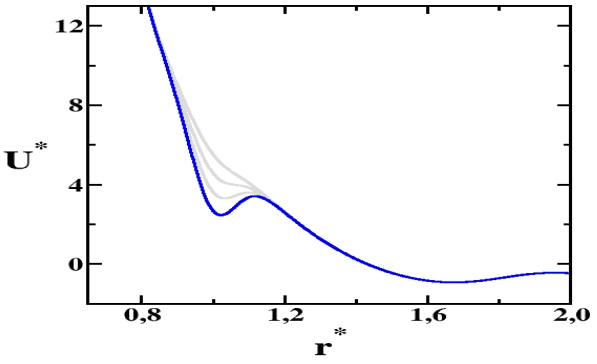


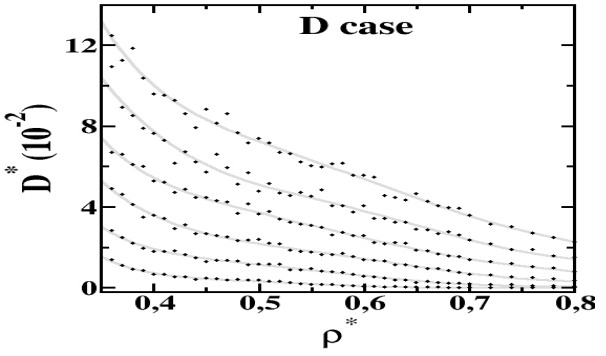


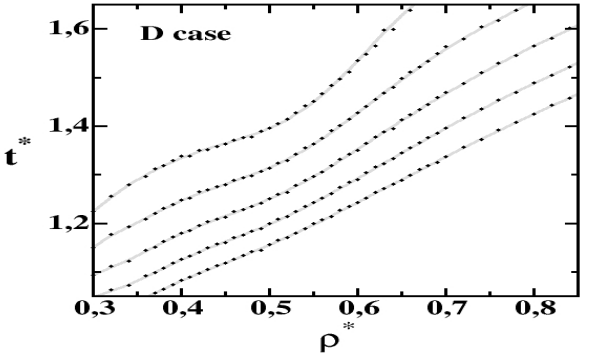


Phase Diagram

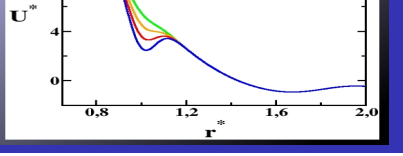


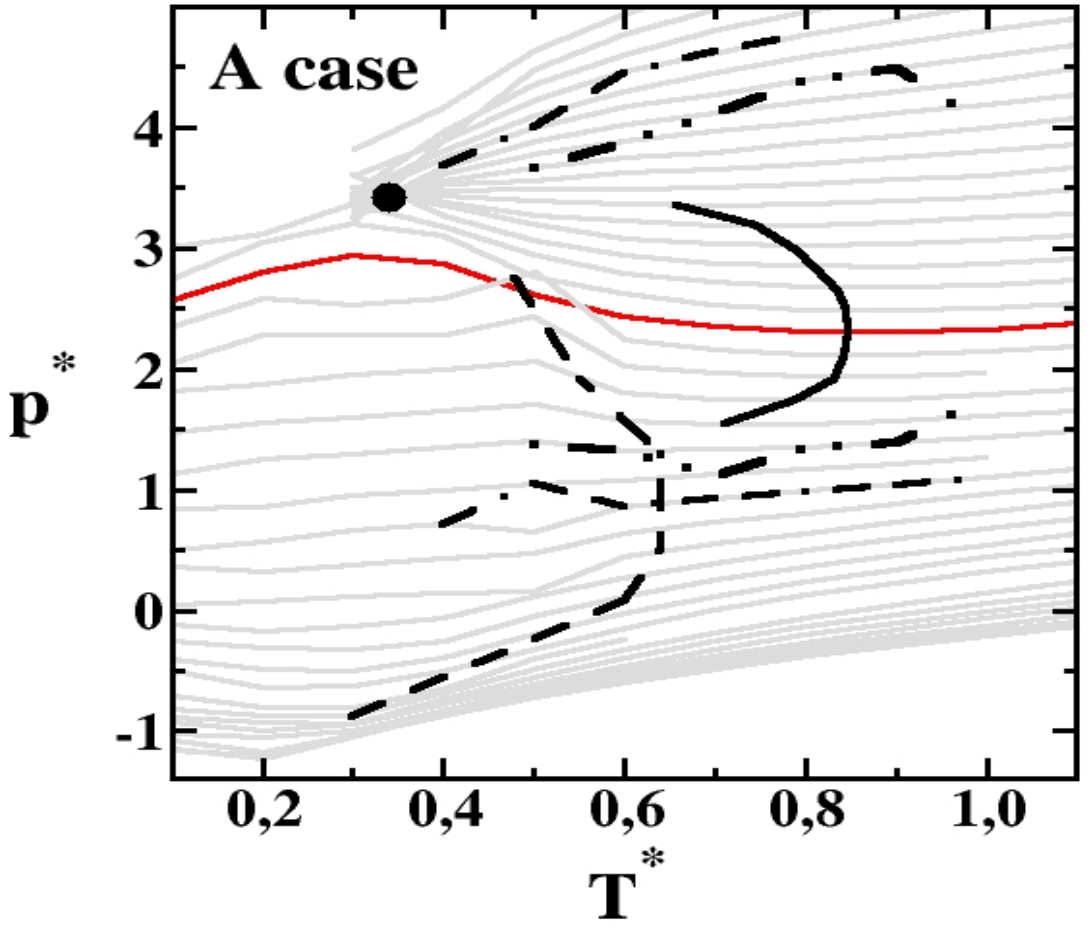






Radial Distribution Function





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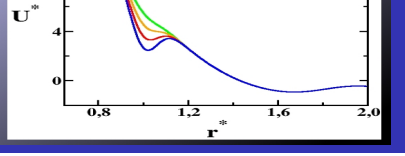
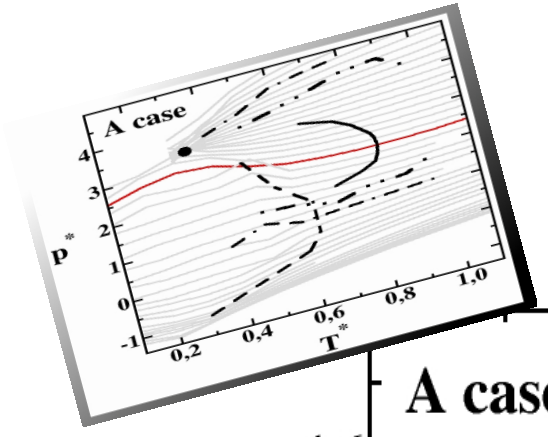
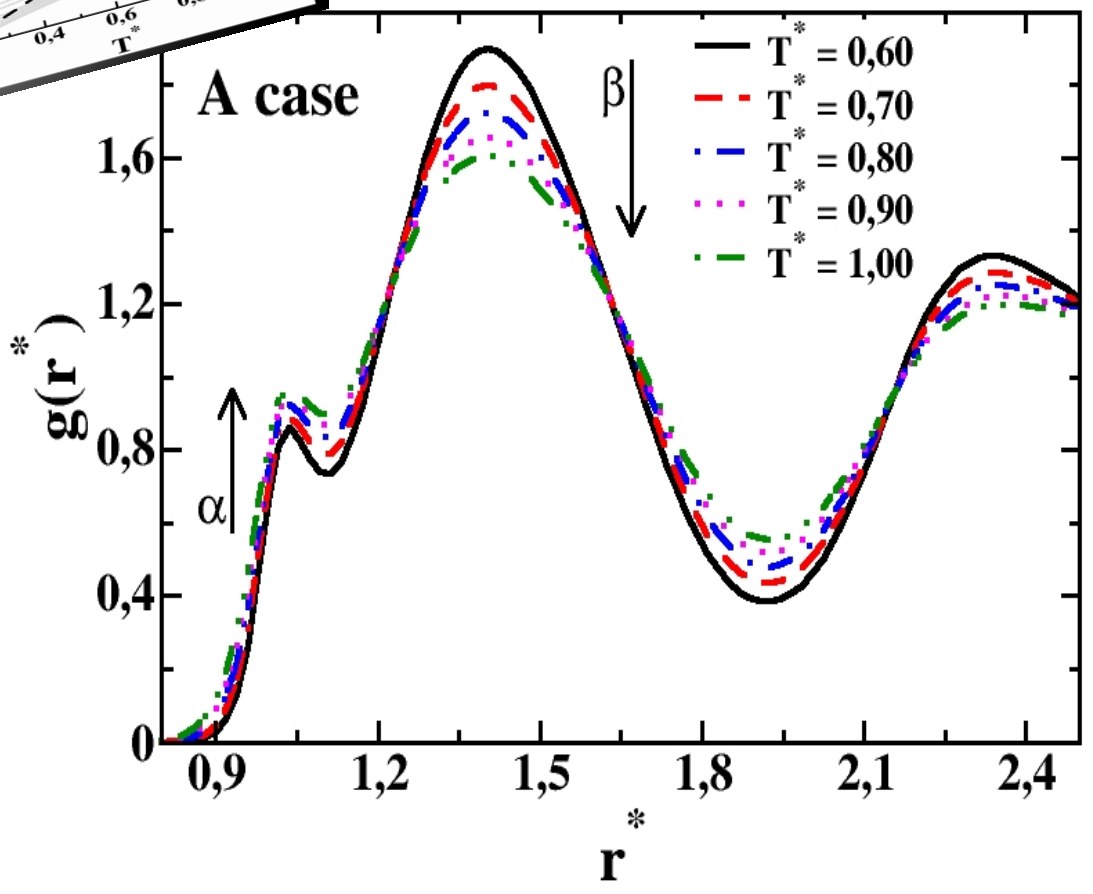
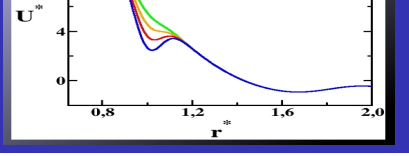
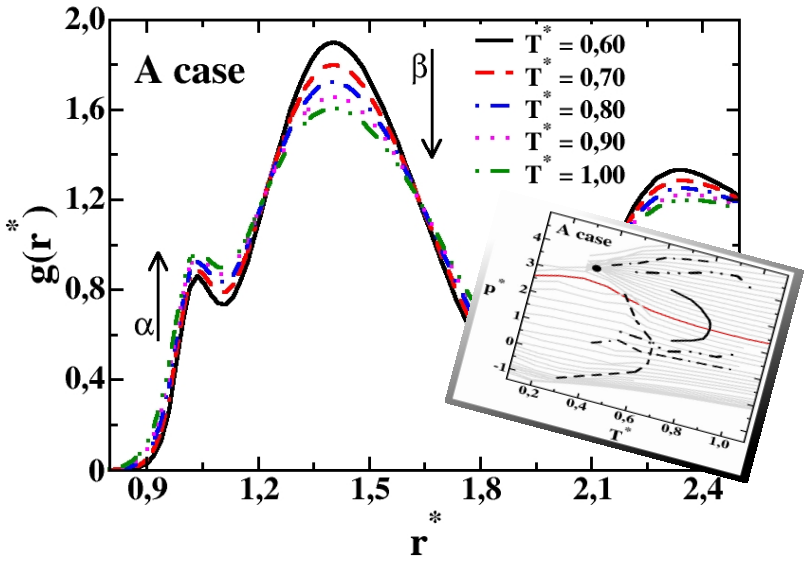


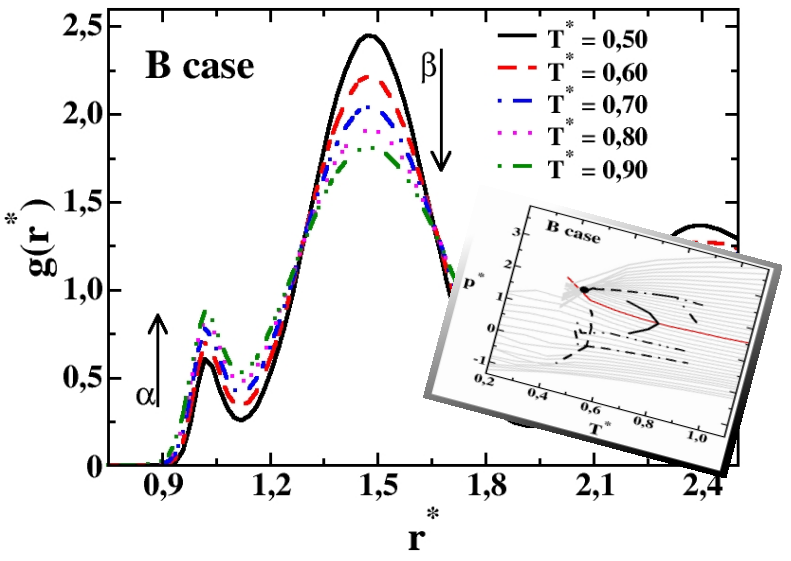


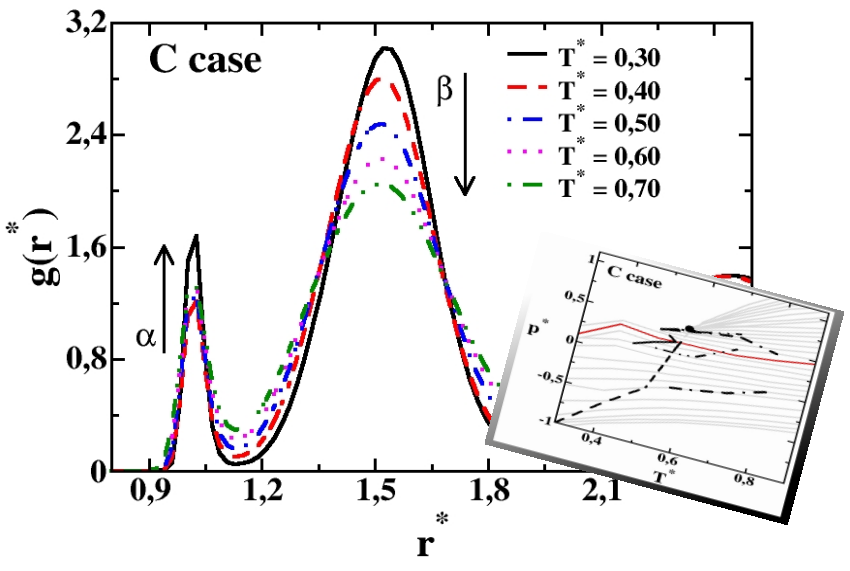


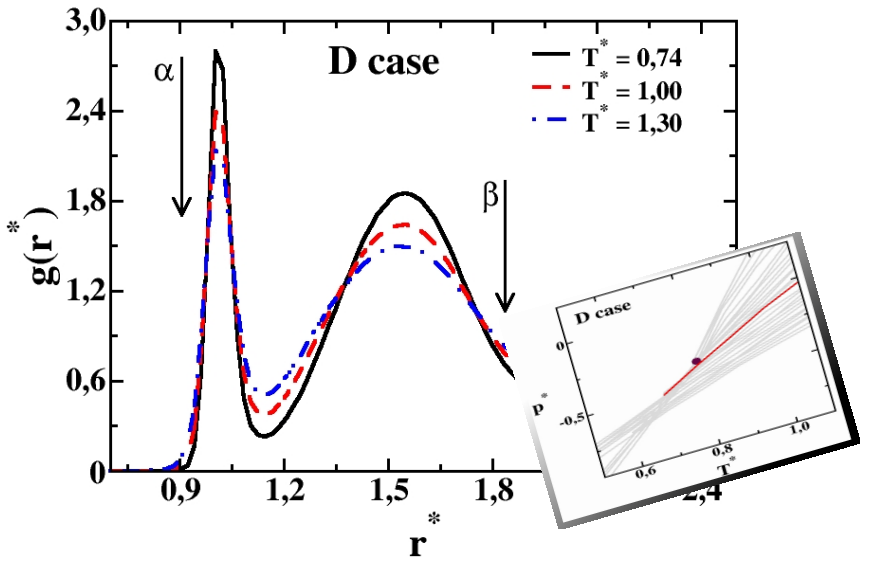
Radial Distribution Function





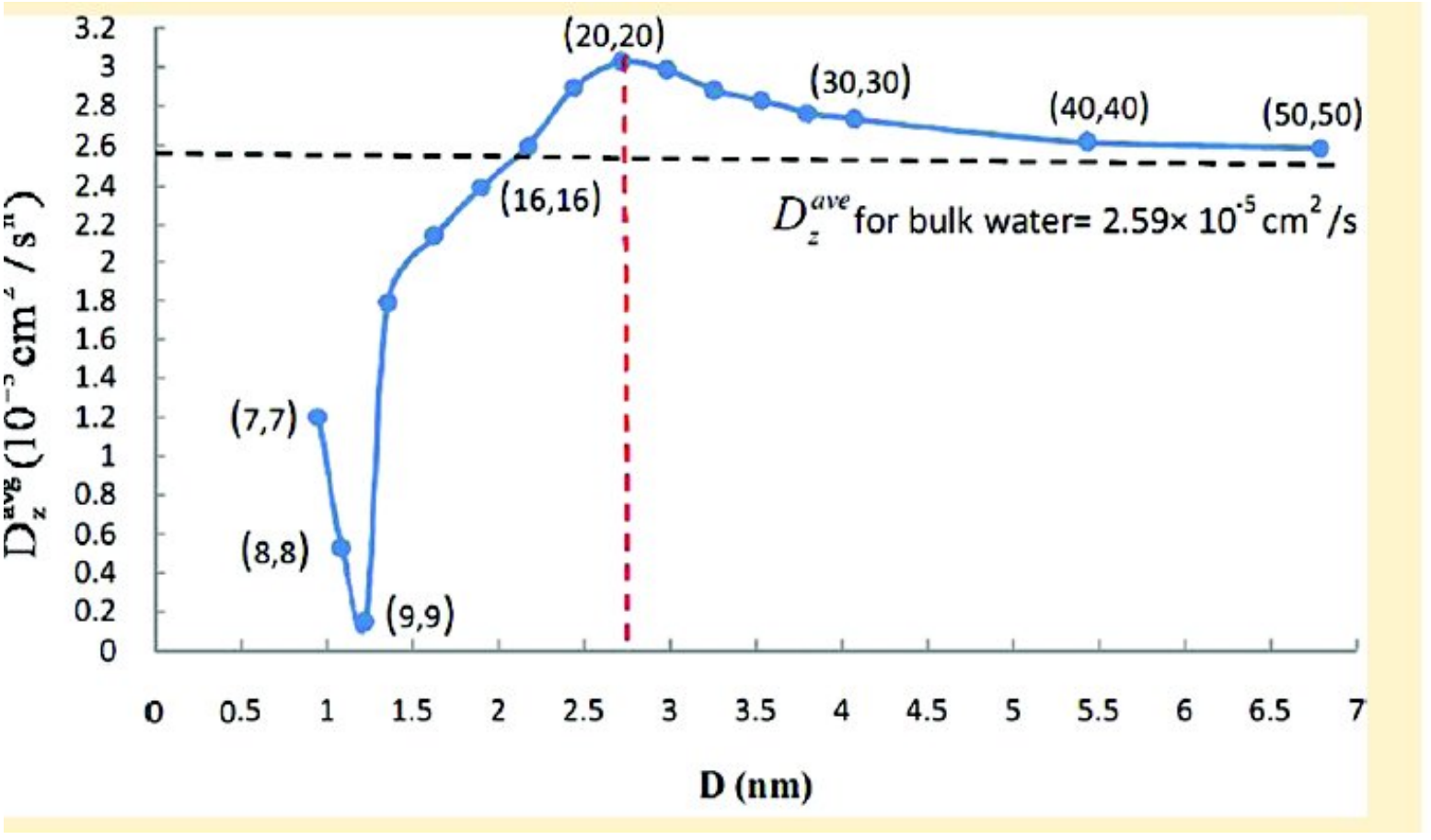






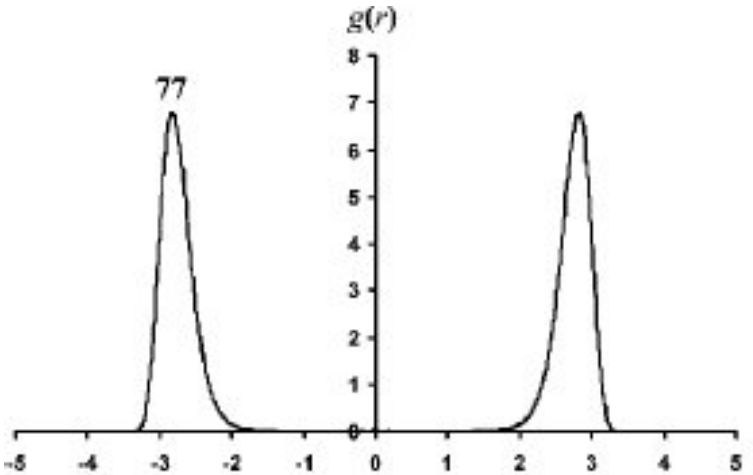
Diffusion in Nanotubes

A.B. Farinami, JPCB 115, 12145 (2012)-SPC/E

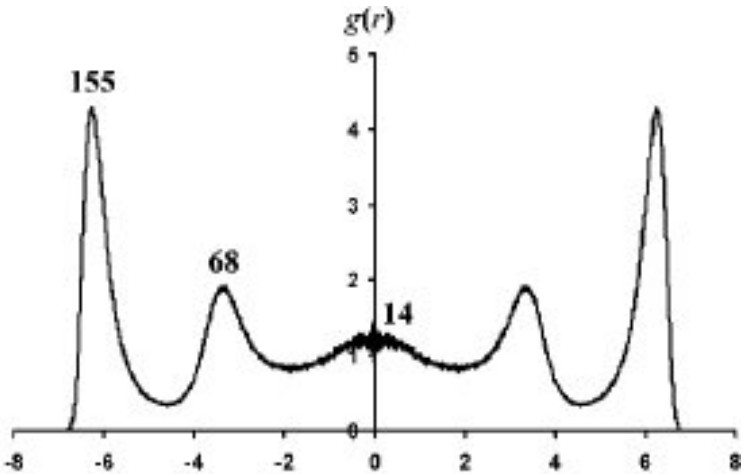


Distribution in Nanotubes - Simulations

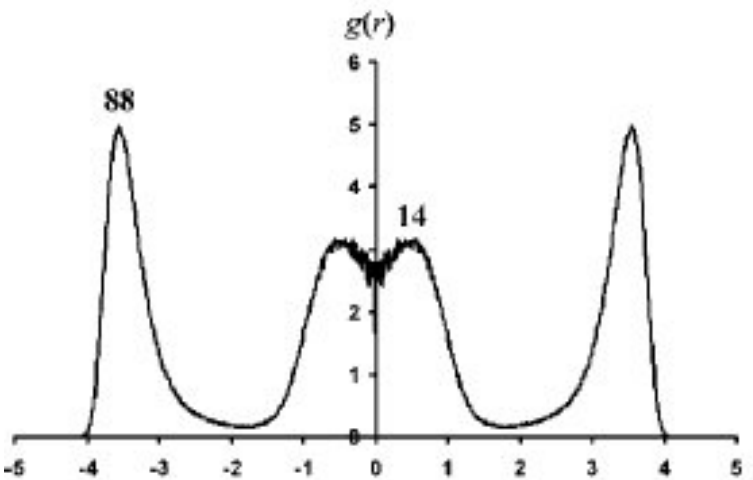
T. Nanok, JCPA 113, 2103 (2009) - SPC/E



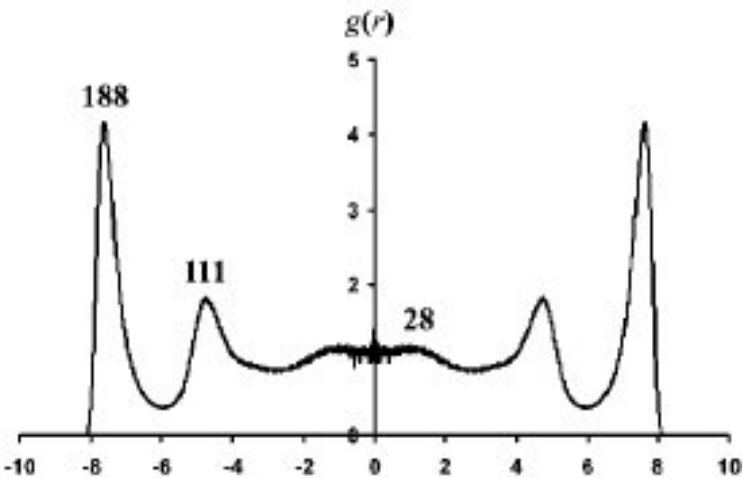
(9,9)-SWBNNT



(14,14)-SWBNNT



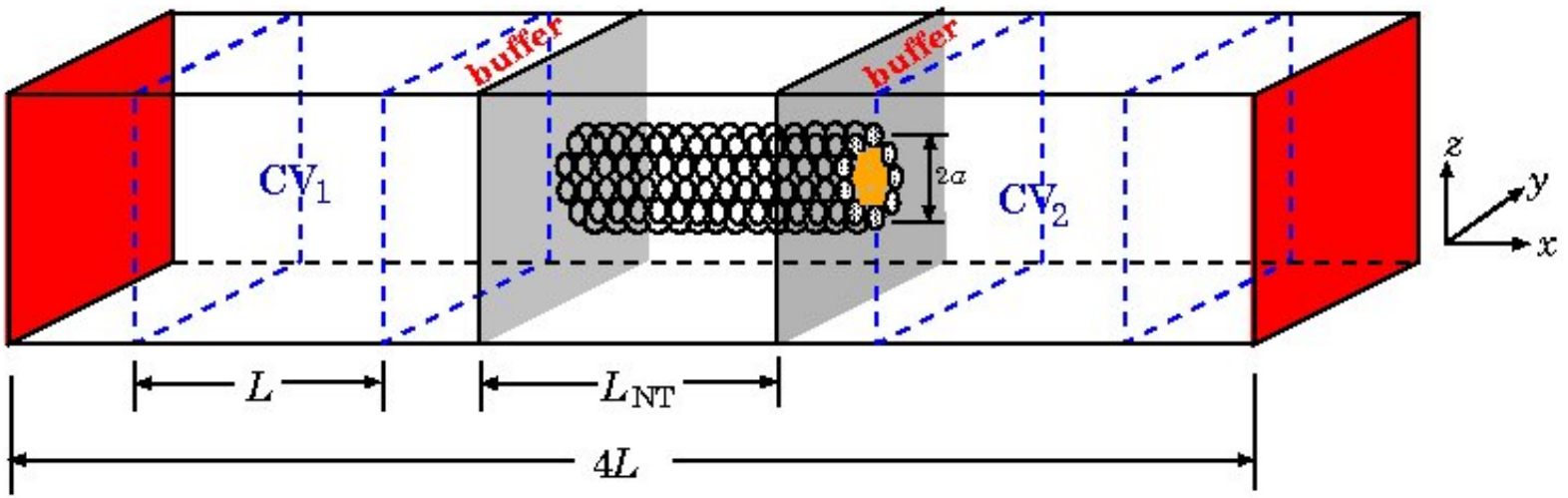
(10,10)-SWBNNT



(16,16)-SWBNNT

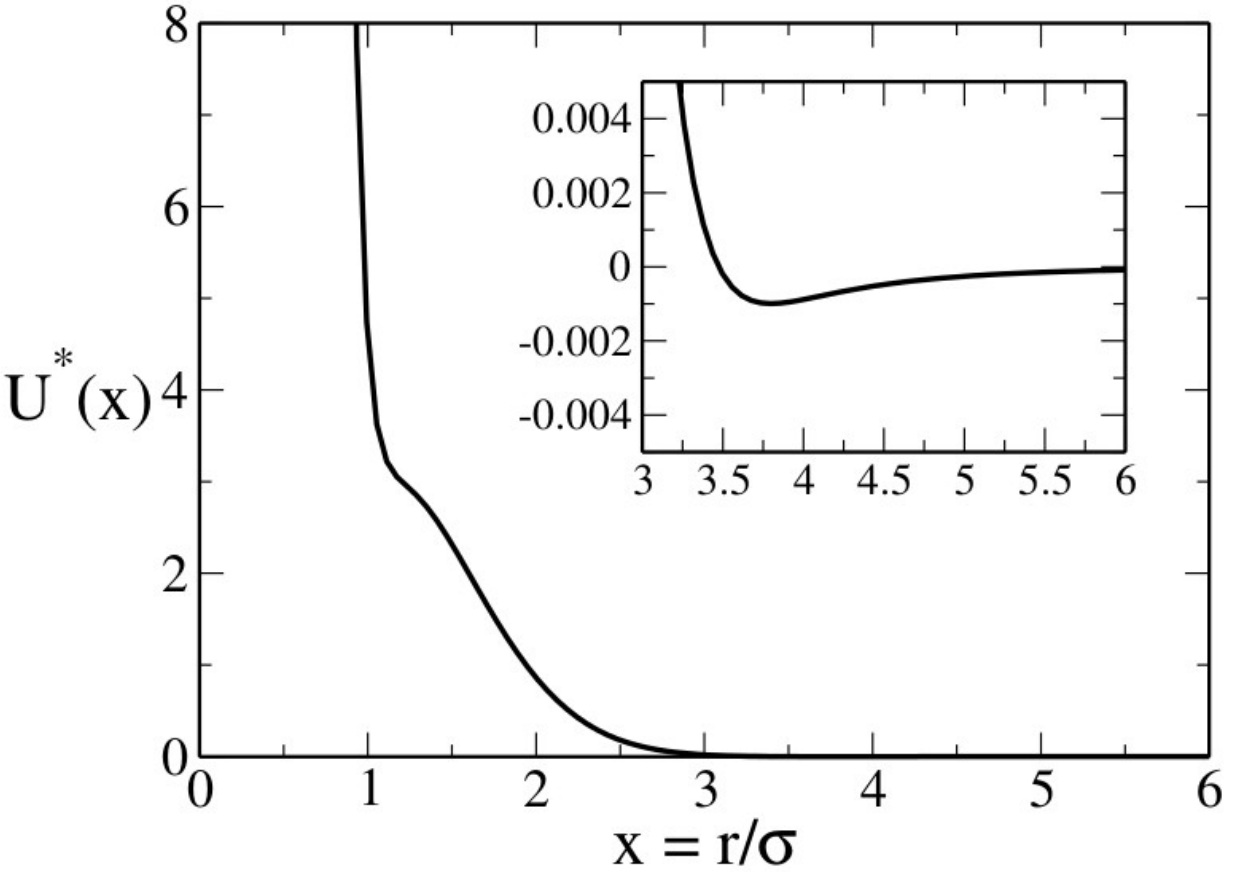
Model for Confining

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

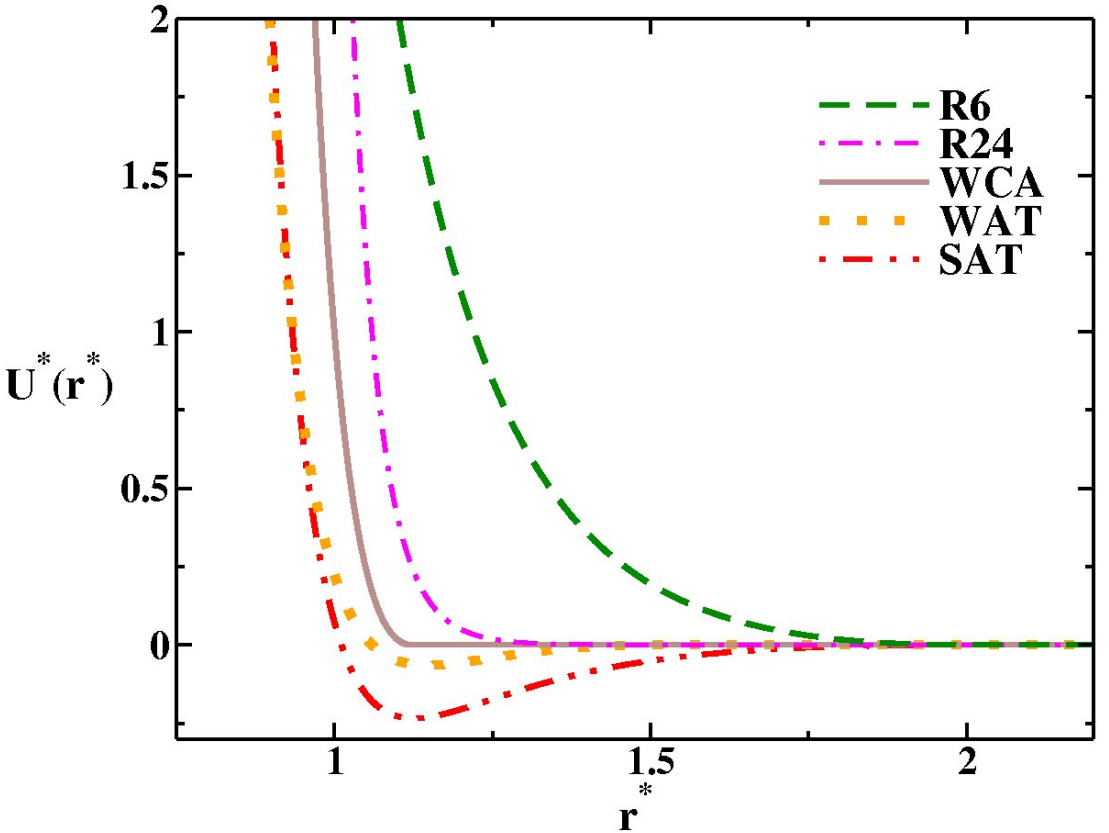


Fluid-Fluid Effective Potential

A. B. de Oliveira, P. Netz and Barbosa JCP124, 84505 (2006)

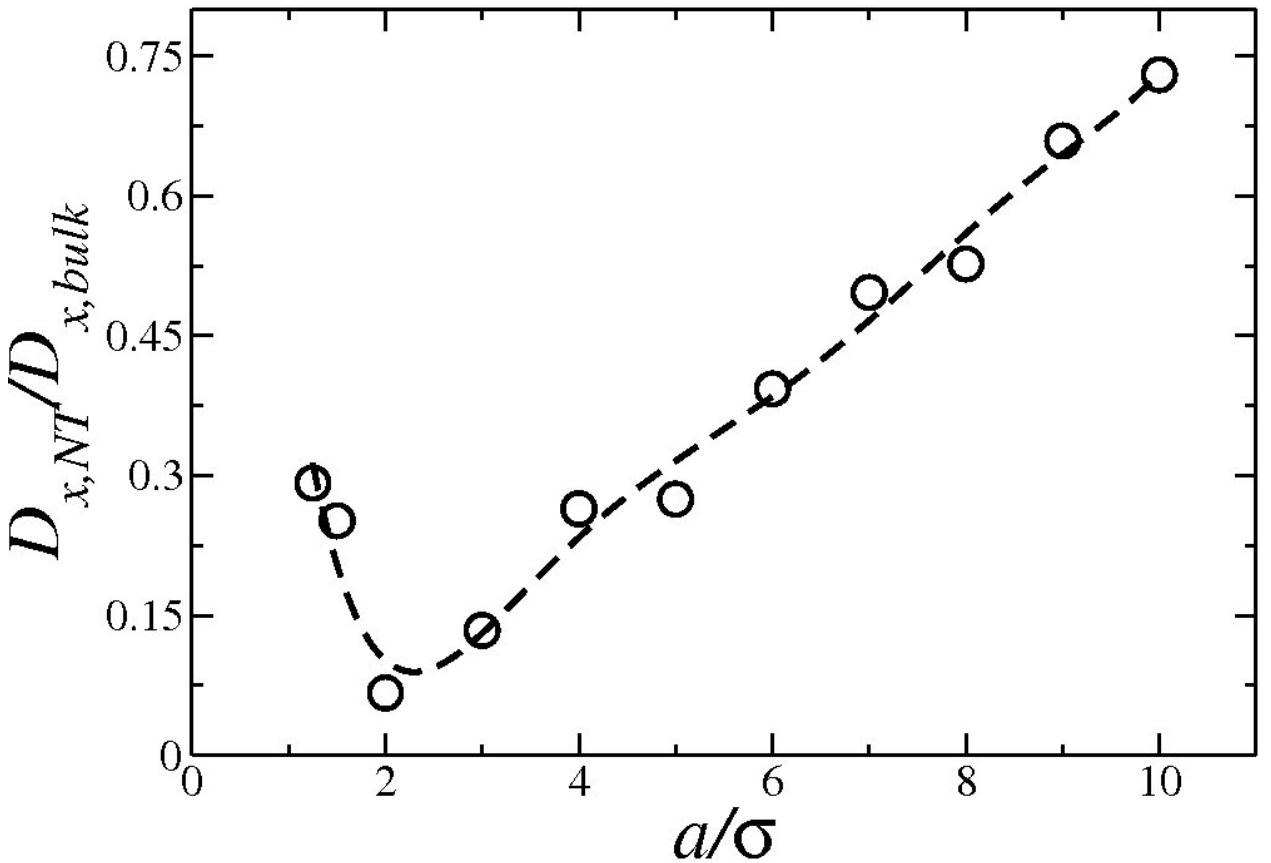


Fluid-Wall Effective Potential



Diffusion

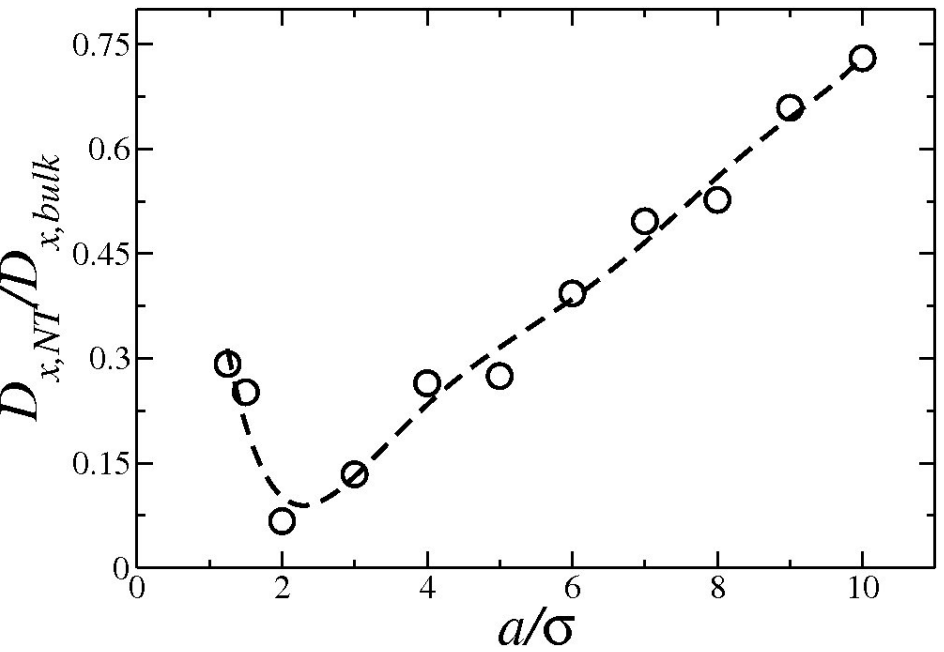
J. R. Bordin, A. B. de Oliveira, A. Diehl and Barbosa, JCP 137, 084504 (2012)

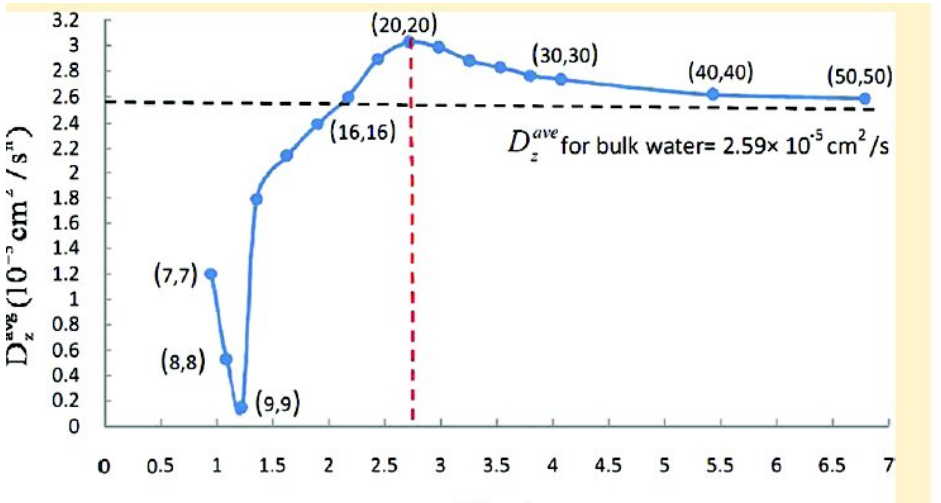


Diffusion

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

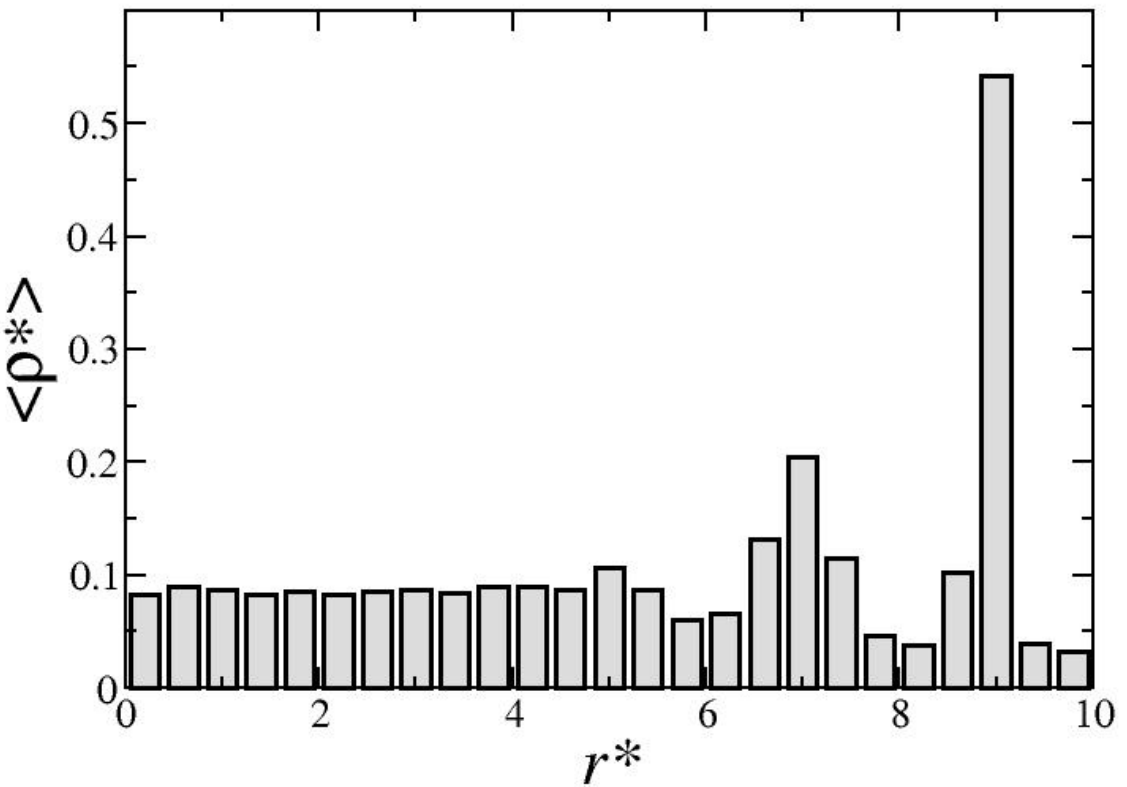
J. R. Bordin, A. B. de Oliveira, A. Diehl and Barbosa, JCP 137, 084504 (2012)



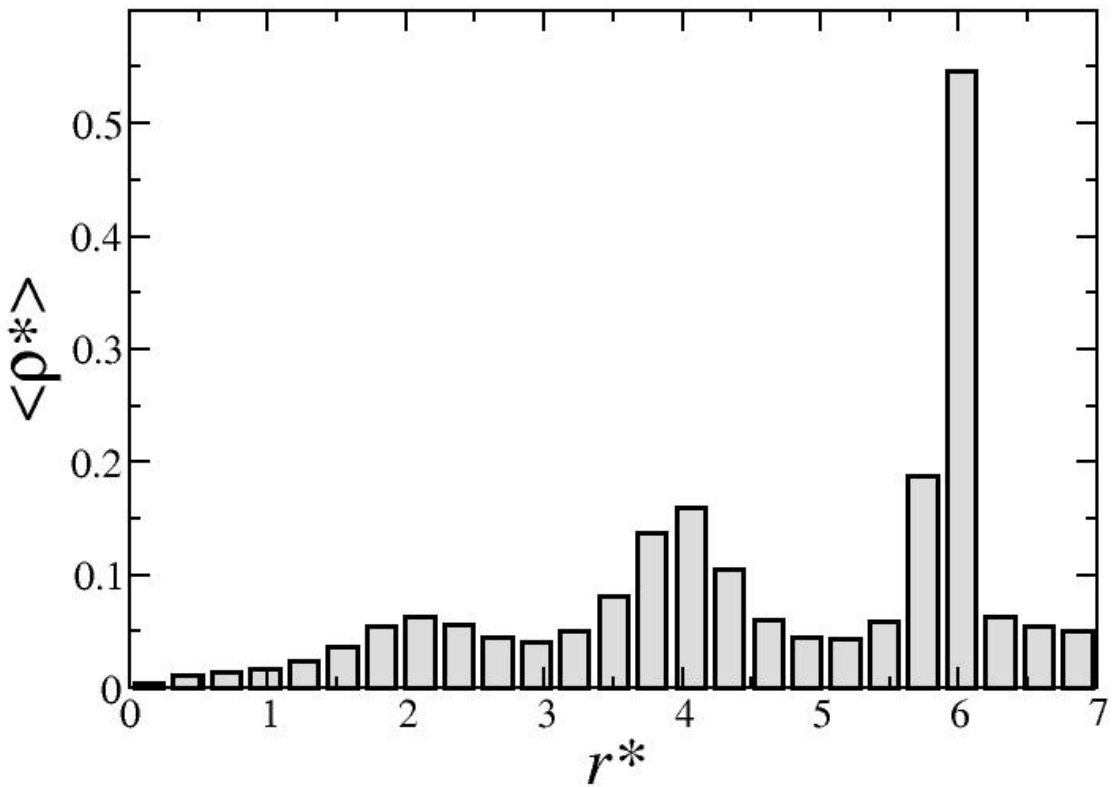


Density vs. r - a=10

J. R. Bordin, A. B. de Oliveira, A. Diehl and Barbosa, JCP 137, 084504 (2012)

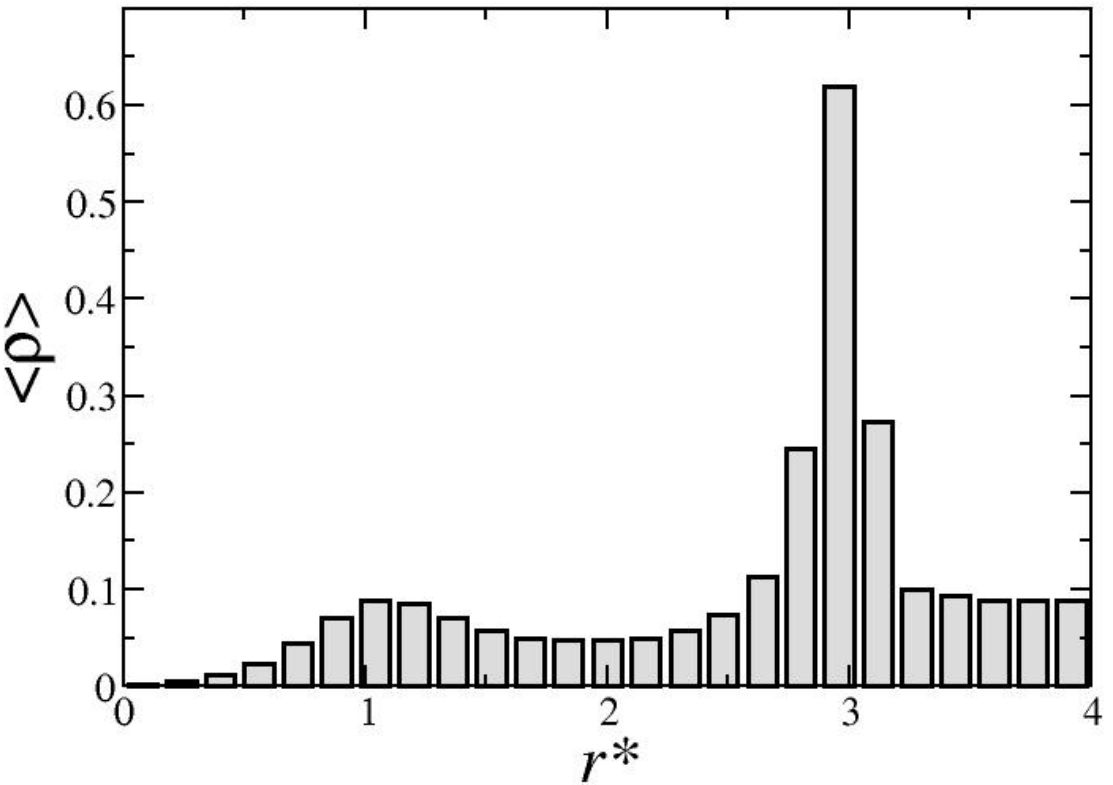


Density vs. r - a=7



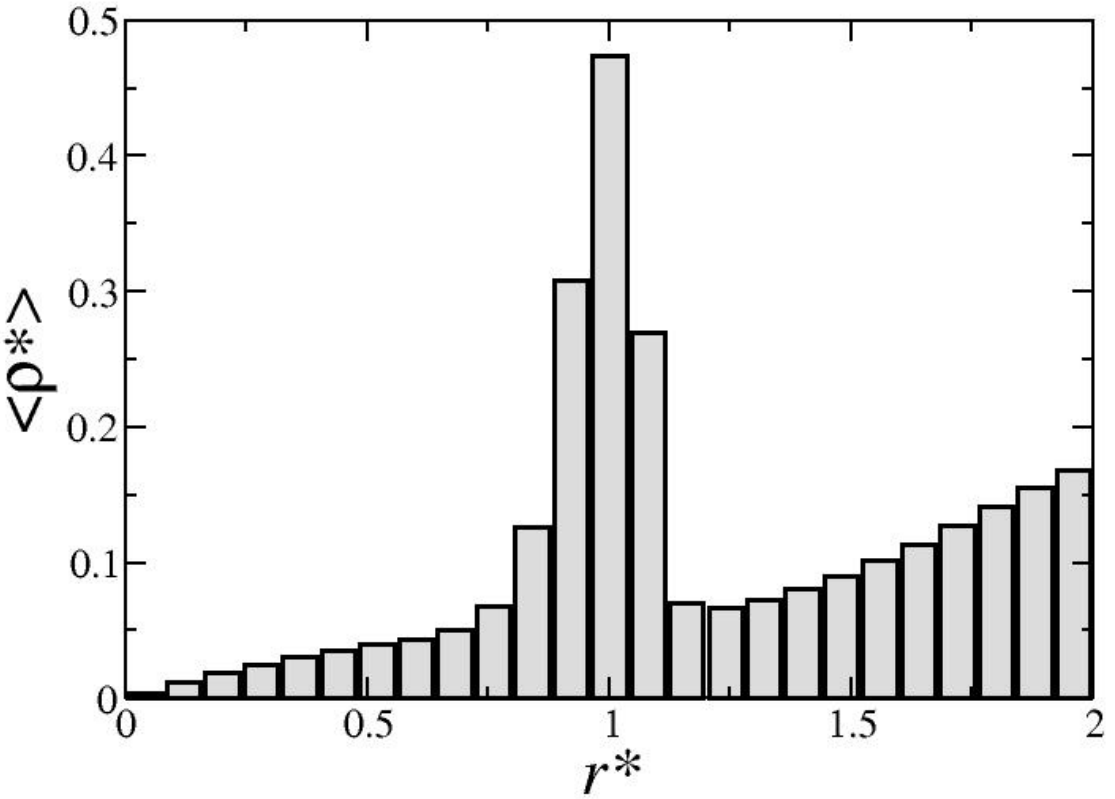
Density vs. r - a=4

J. R. Bordin, A. Diehl and Barbosa, PRE (2013)



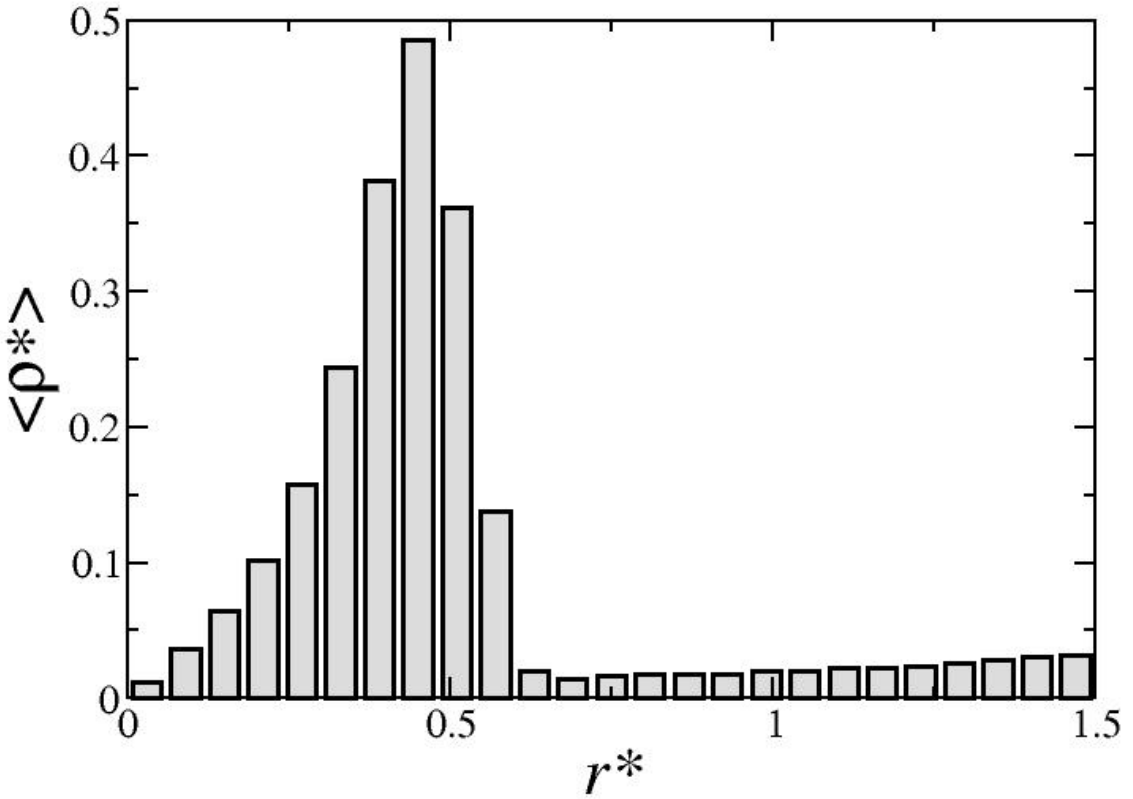
Density vs. r - a=2

J. R. Bordin, A. Diehl and Barbosa, PRE (2013)



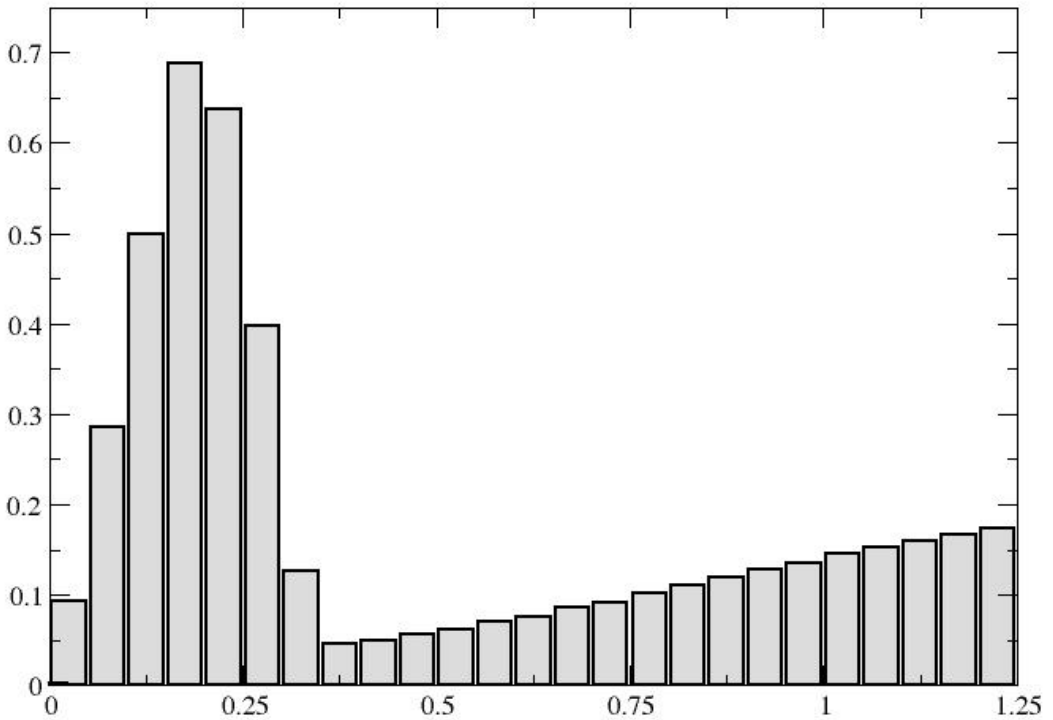
Density vs. r - a=1.5

J. R. Bordin, A. Diehl and Barbosa, PRE (2013)



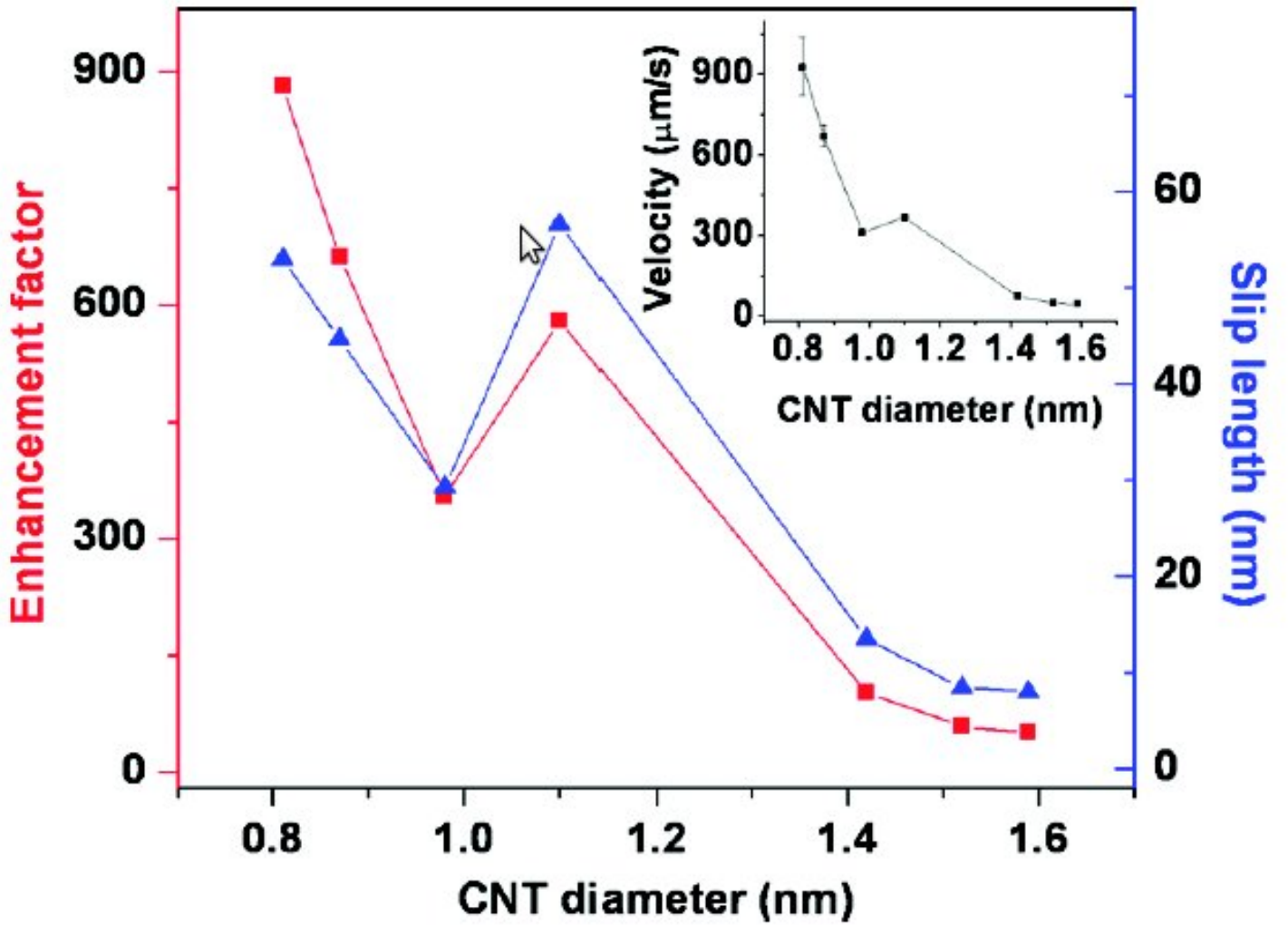
Density vs. r - a=1.25

J. R. Bordin, A. Diehl and Barbosa, PRE (2013)



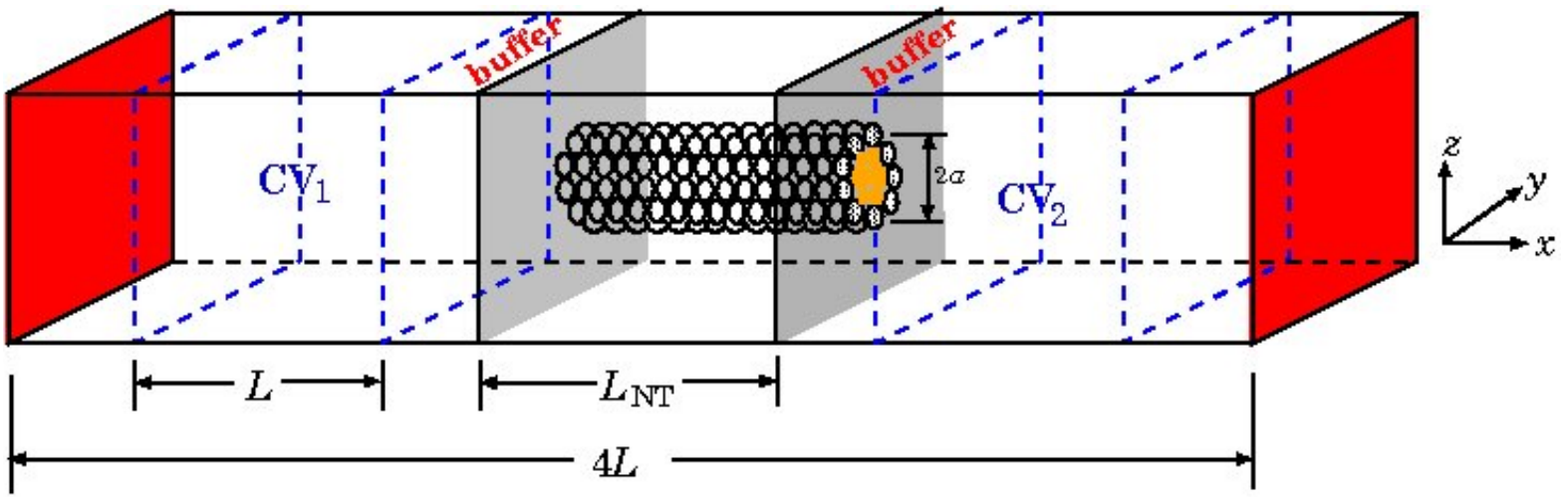
Flux in Nanotubes

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



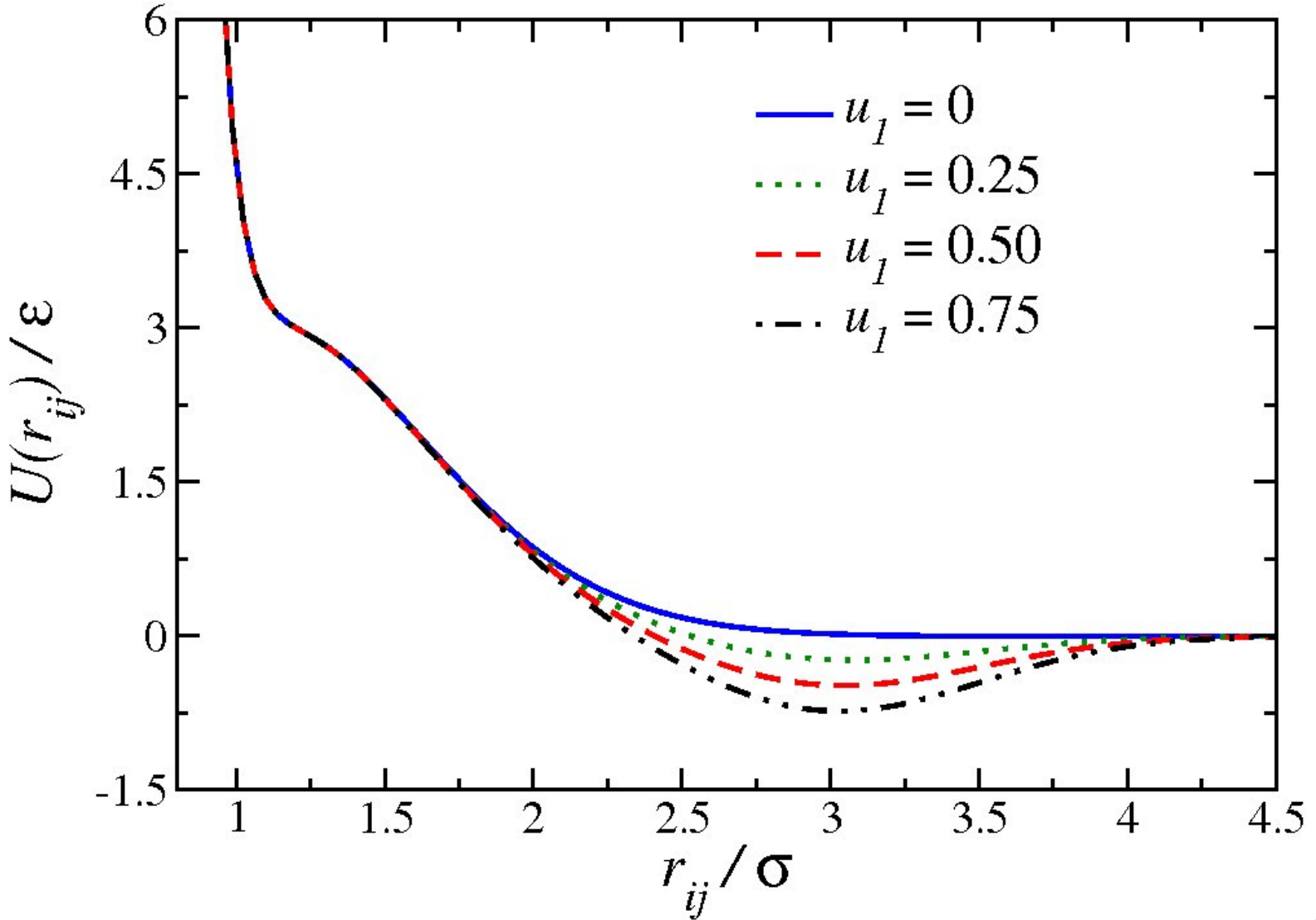
Model for Nanotubes

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



Fluid-Fluid Effective Potential

J. da Silva and Barbosa, JCP 133, 244506 (2010)



Enhancement Flow

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

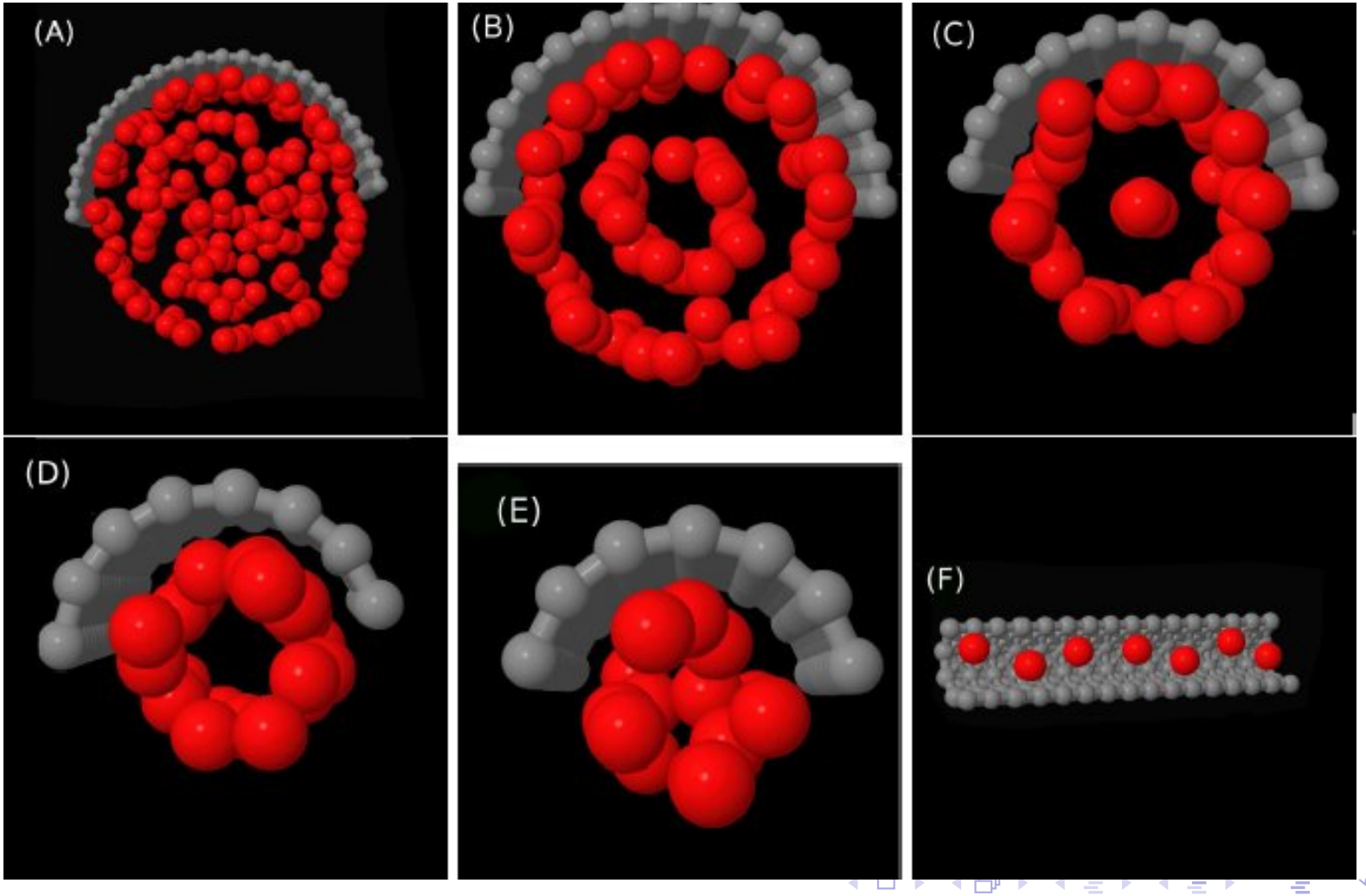
$$\begin{aligned} \langle v_x \rangle &= \gamma_{HP} \frac{\Delta p}{L_{NT}} \\ \gamma_{HP} &= \frac{a^2}{8\eta} \\ \eta &= \frac{k_B T}{3\pi\sigma D_x} \end{aligned}$$

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

$$\epsilon = \frac{\gamma_{MD}}{\gamma_{HP}} \tag{1}$$

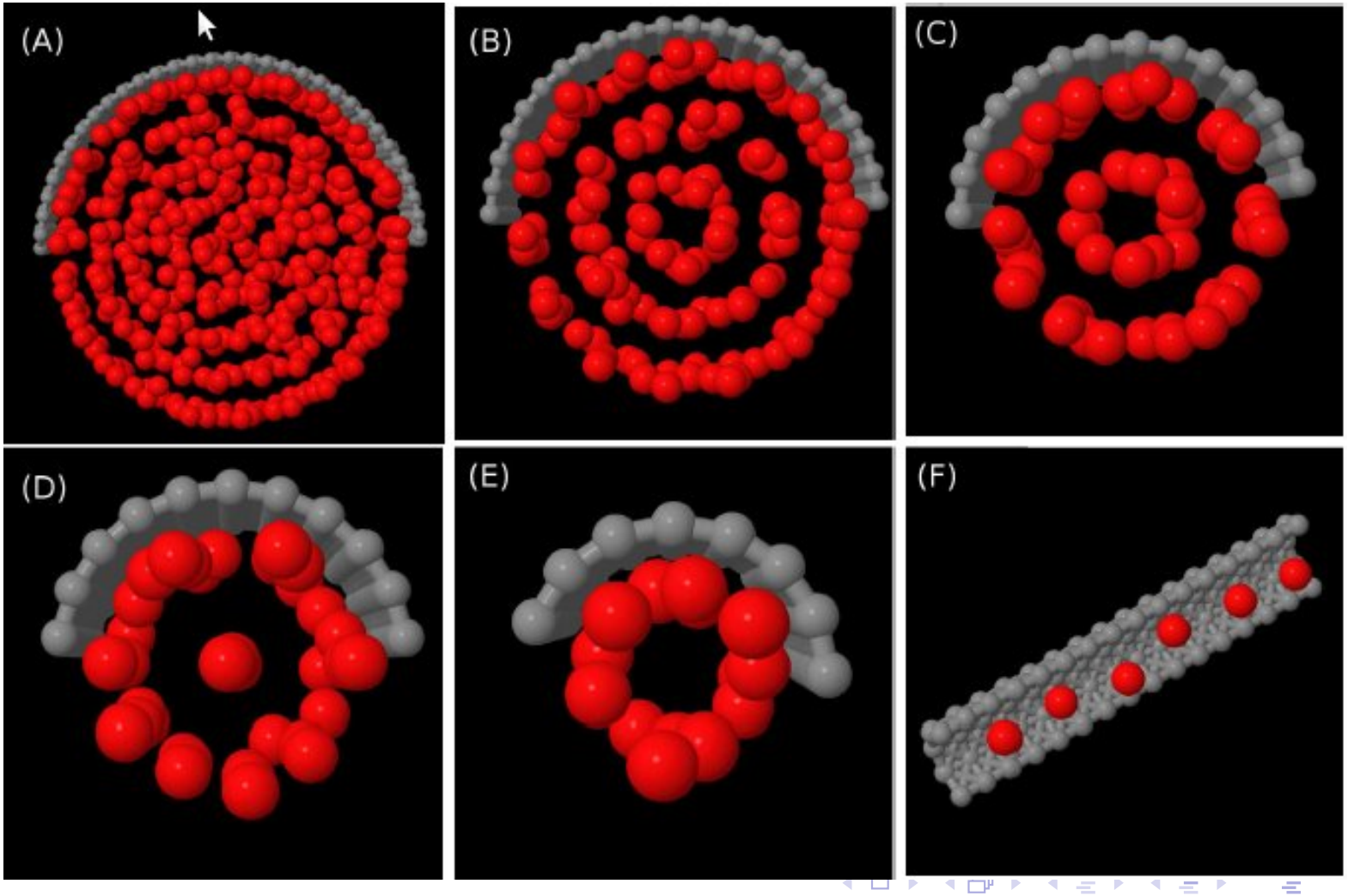
Layers - Attractive

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



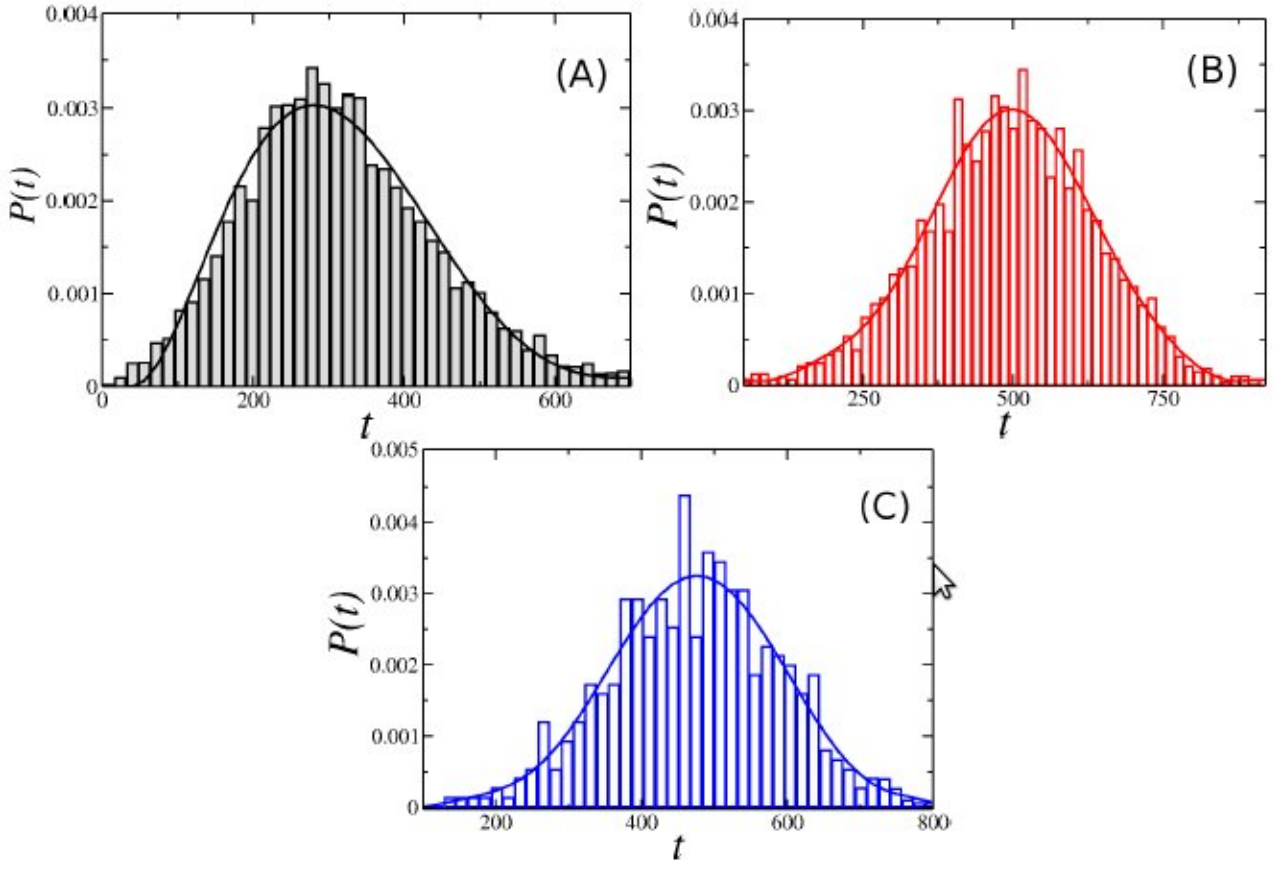
Layers - Repulsive

J. R. Bordin, A. Diehl and Barbosa, JPCB (2013)



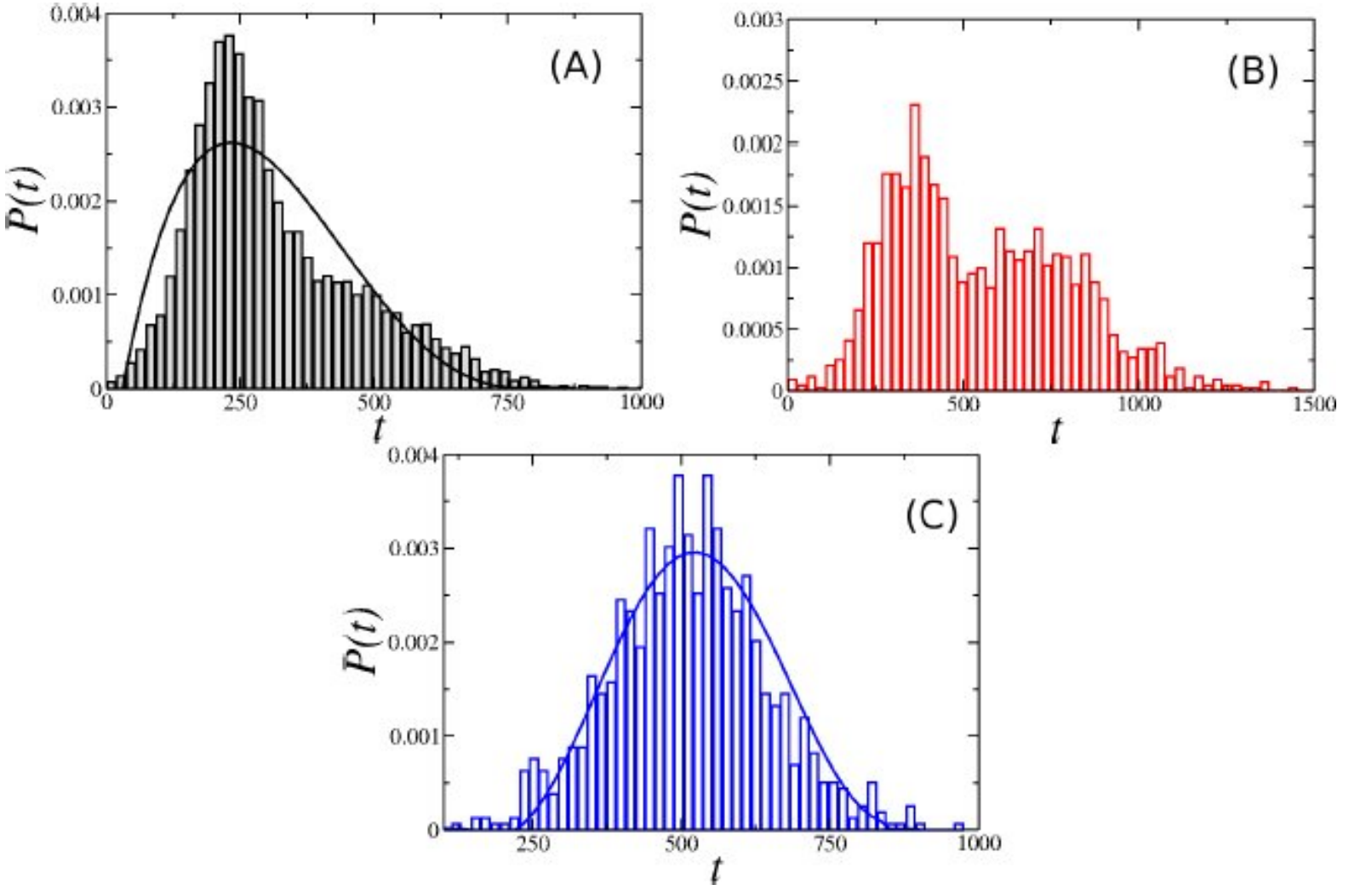
Distribution - Attractive

J. R. Bordin, A. Diehl and Barbosa, JPCB (2013)



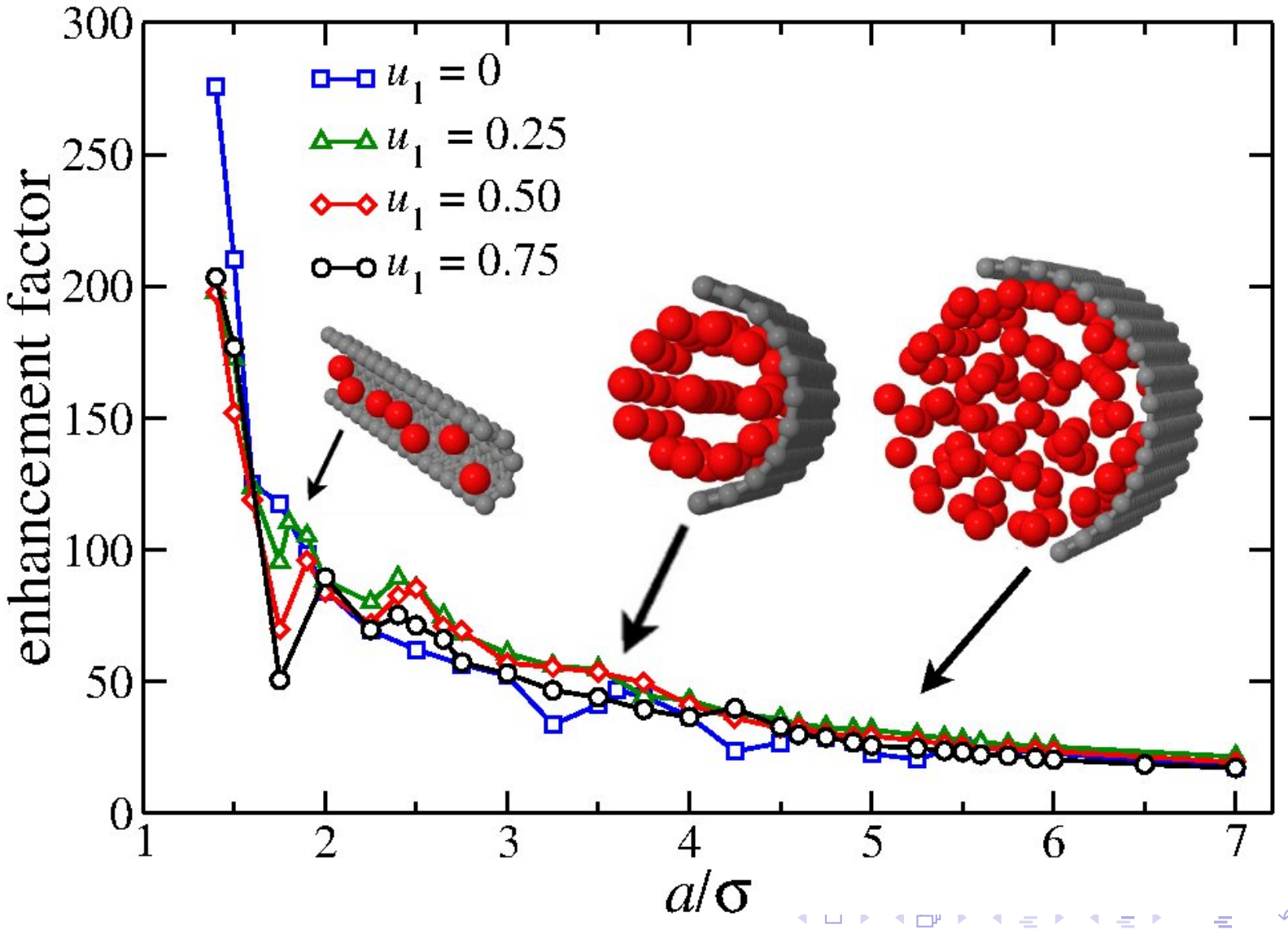
Distribution - Repulsive

J. R. Bordin, A. Diehl and Barbosa, JPCB (2013)



Enhancement Flow

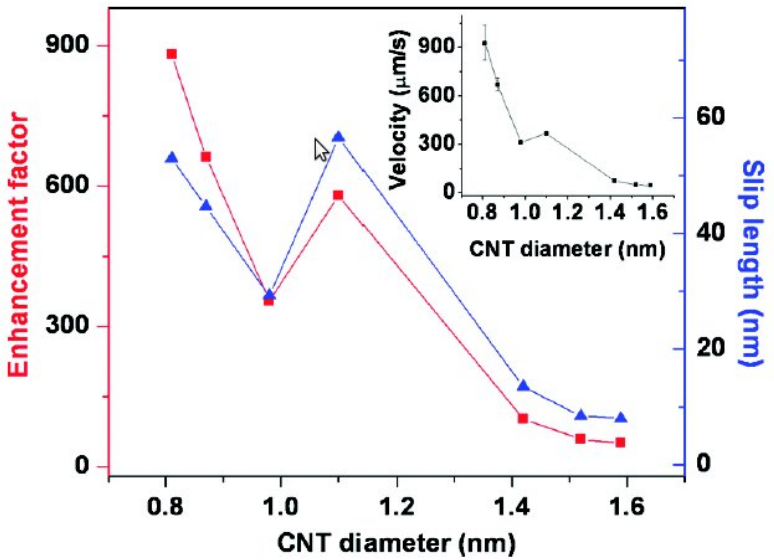
J. R. Bordin, A. Diehl and Barbosa, JPCB 117, 7047(2013)

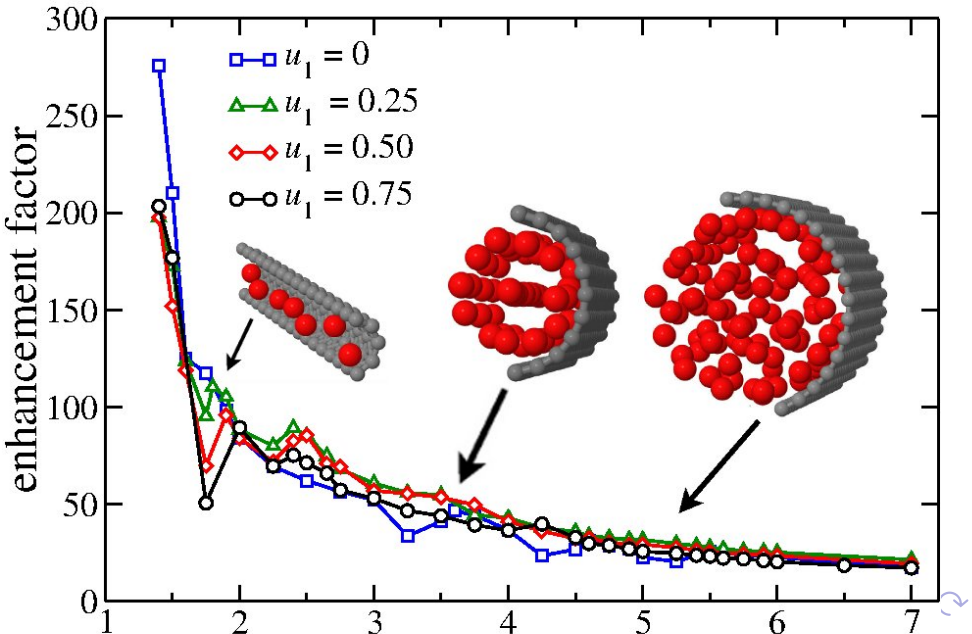


Enhancement Flow

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

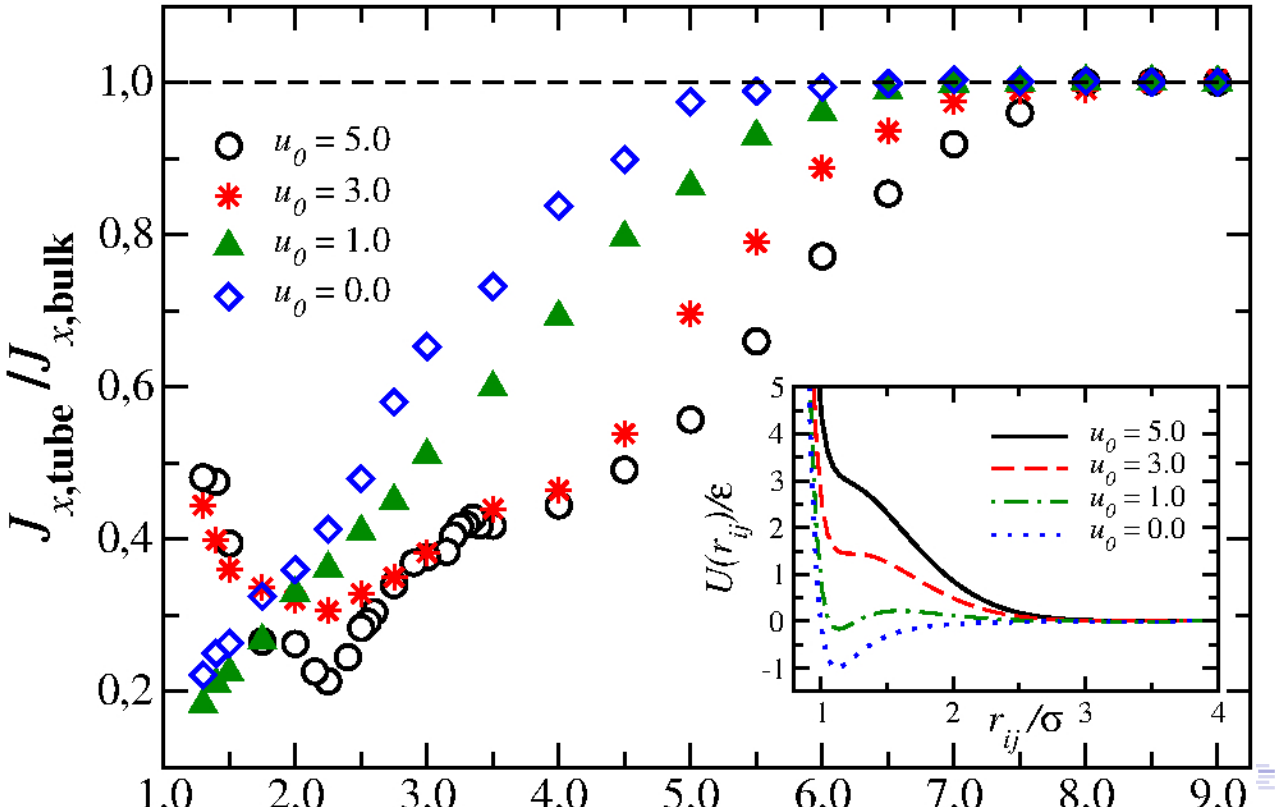
J. R. Bordin, A. Diehl and Barbosa, JPCB 117, 7047(2013





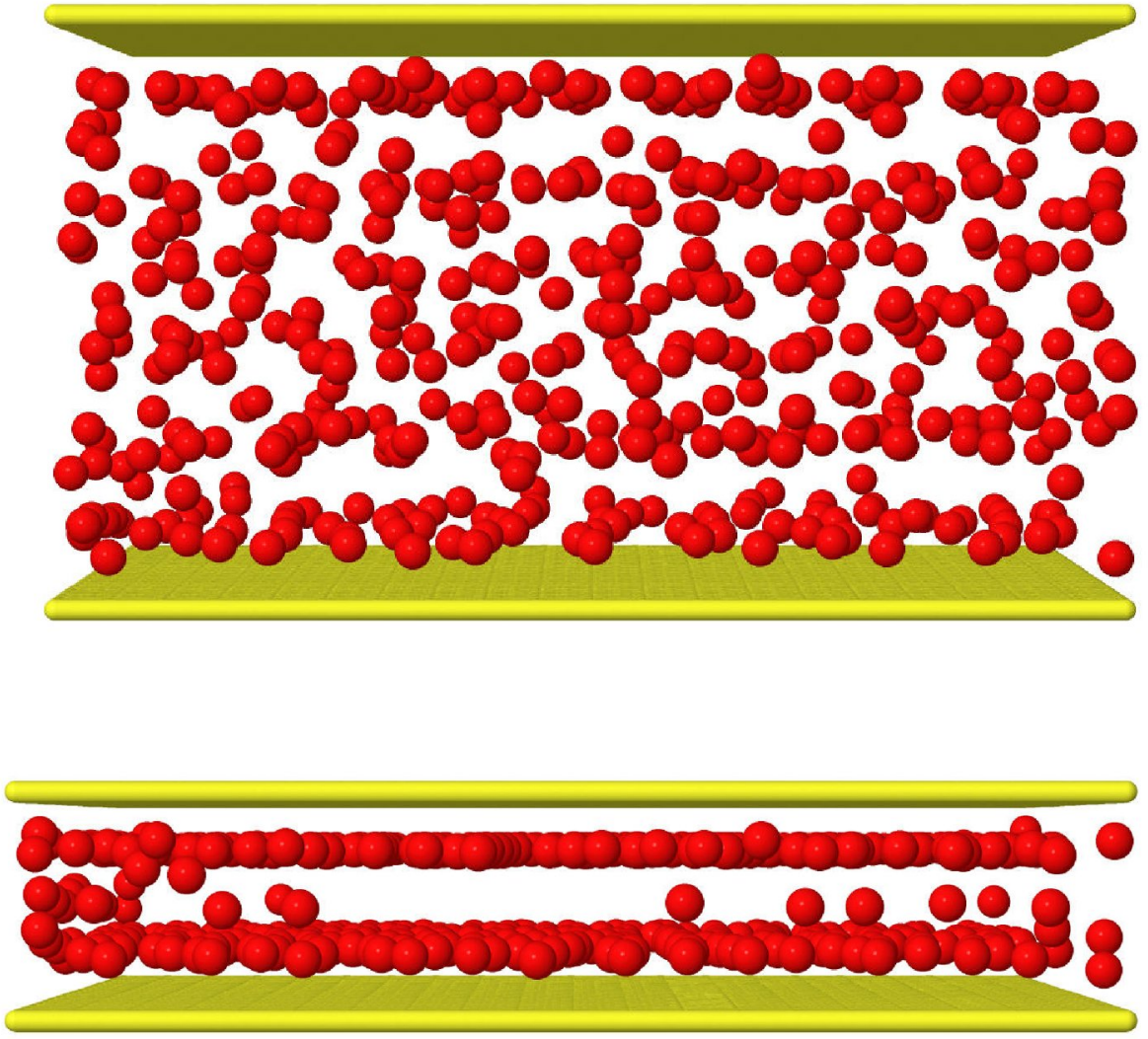
Flux increases is only for two length scales?

J. R. Bordin, A. Diehl, J. S. Andrade, Barbosa, J. of Chem. Phys. 140 194504 (2014)



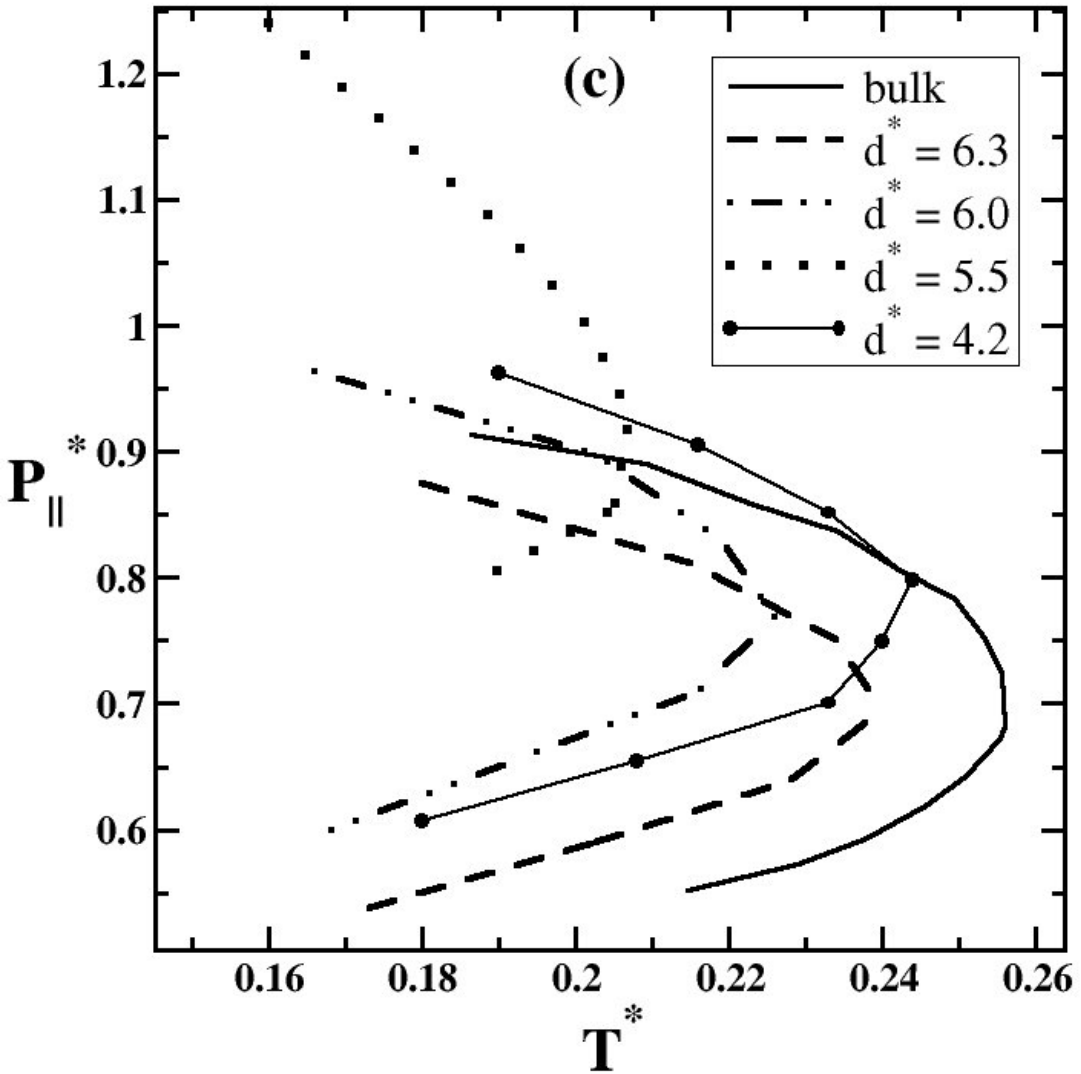
What might happen at the wall?

L.B. Krott and Barbosa PRE 89 012110 (2014)

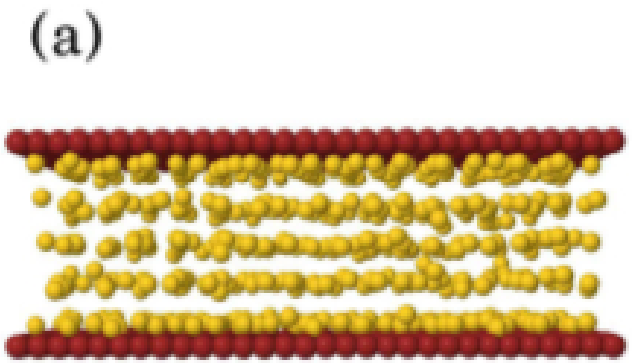


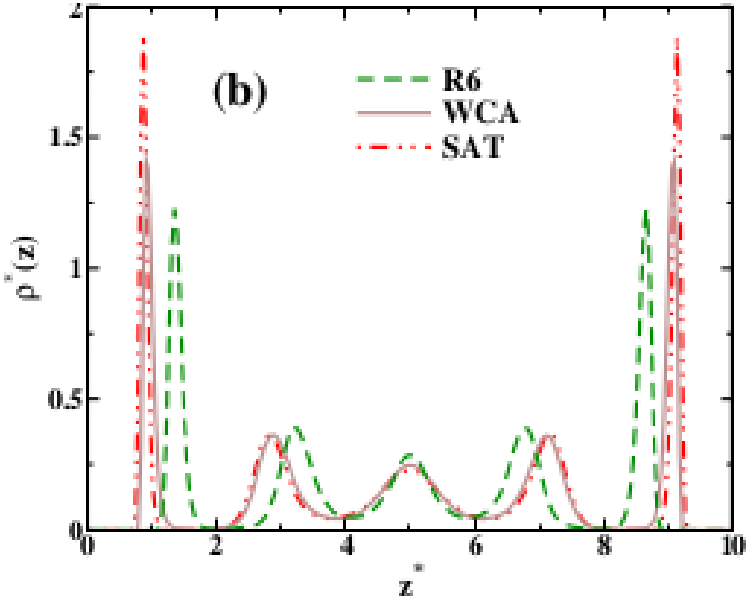
Rigid Plates - Density Anomaly

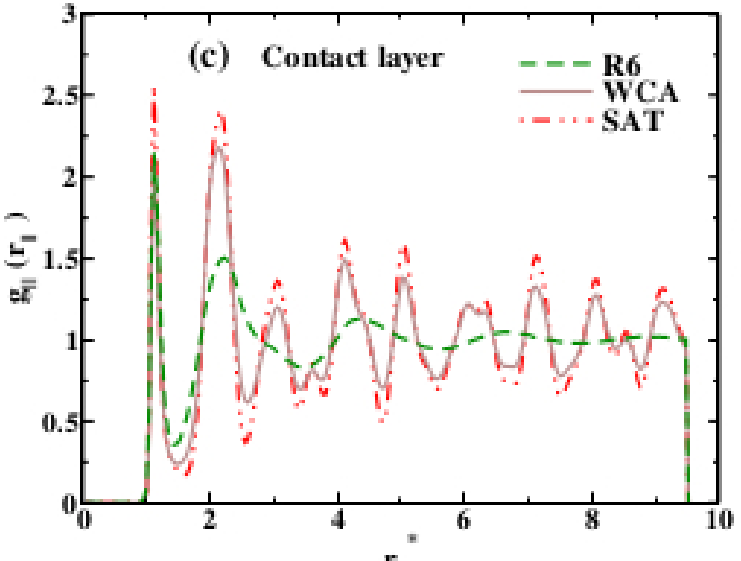
L.B. Krott and Barbosa PRE 89 012110 (2014)

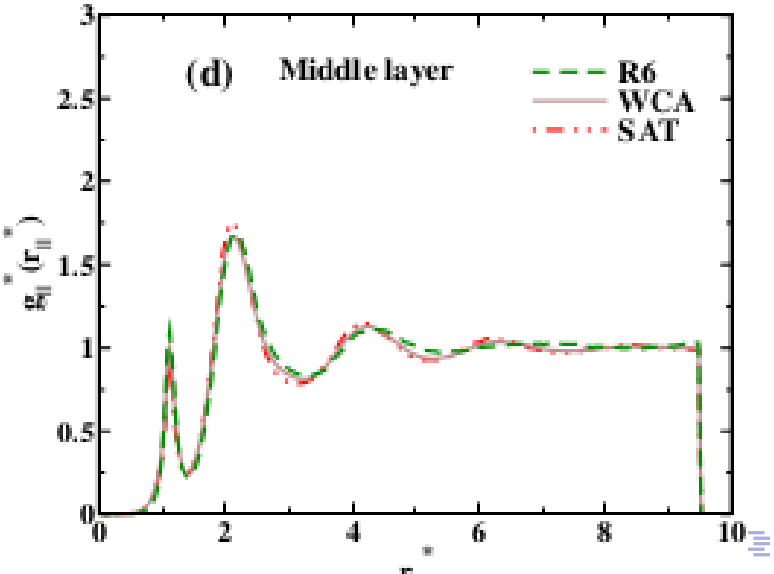


Many Layers

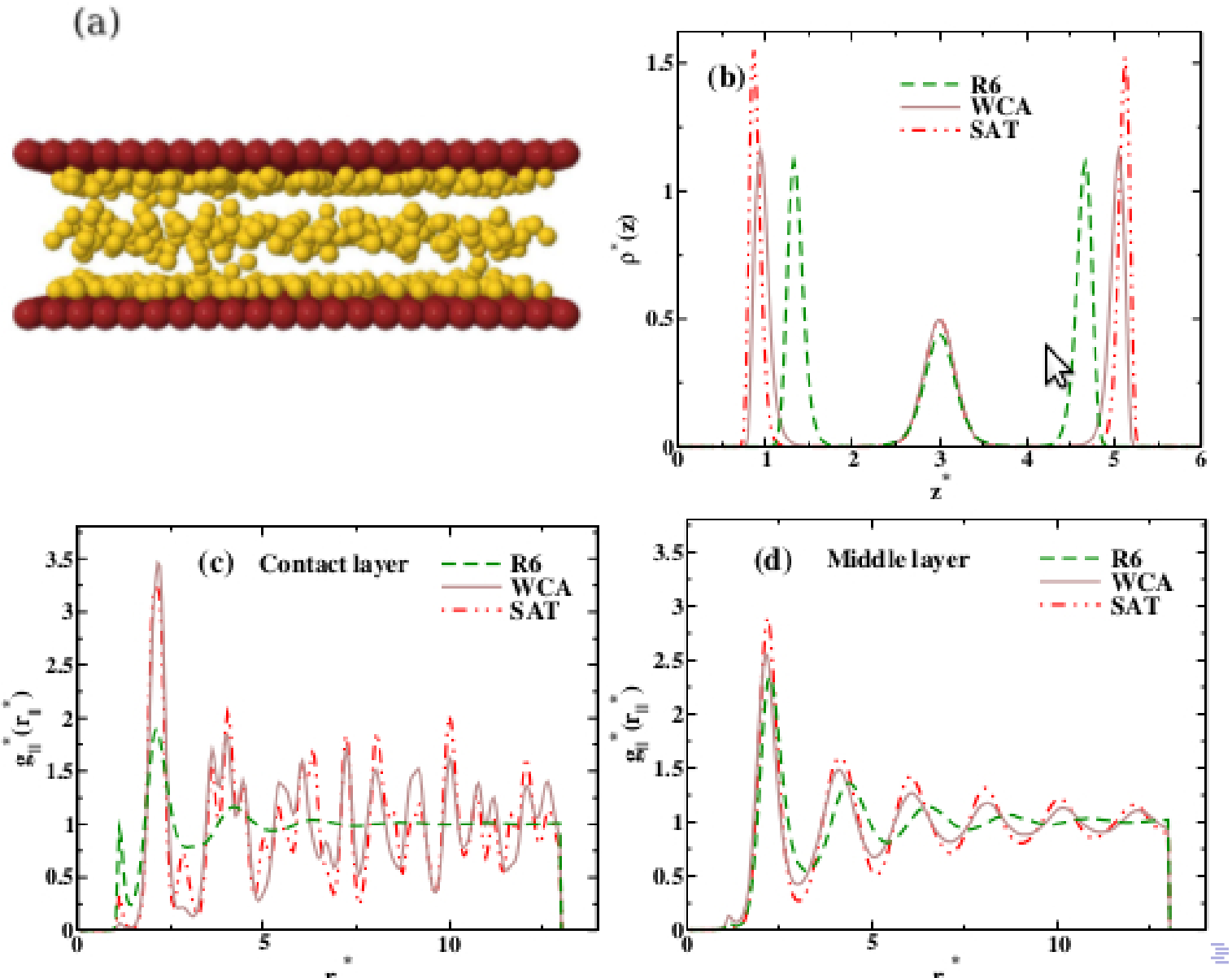

(a)


(b)
R6
WCA
SAT
ρ*(z)
z*
0
0.5
1
1.5
2
4
6
8
10

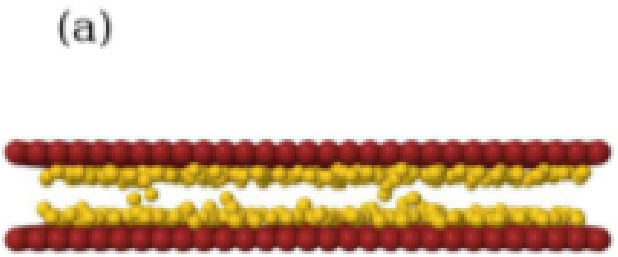

(c) Contact layer
R6
WCA
SAT
g*∥(r*∥)
0
0.5
1
1.5
2
2.5
3
2
4
6
8
10

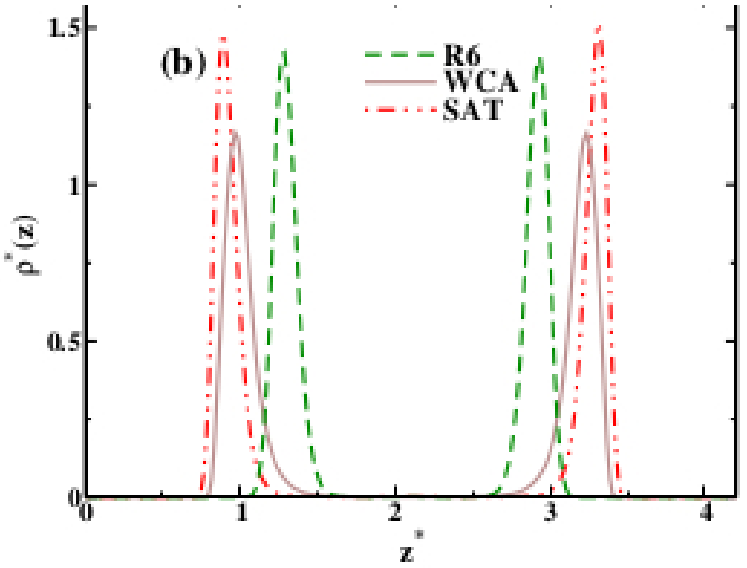

(d) Middle layer
R6
WCA
SAT
g*∥(r*∥)
0
0.5
1
1.5
2
2.5
3
2
4
6
8
10

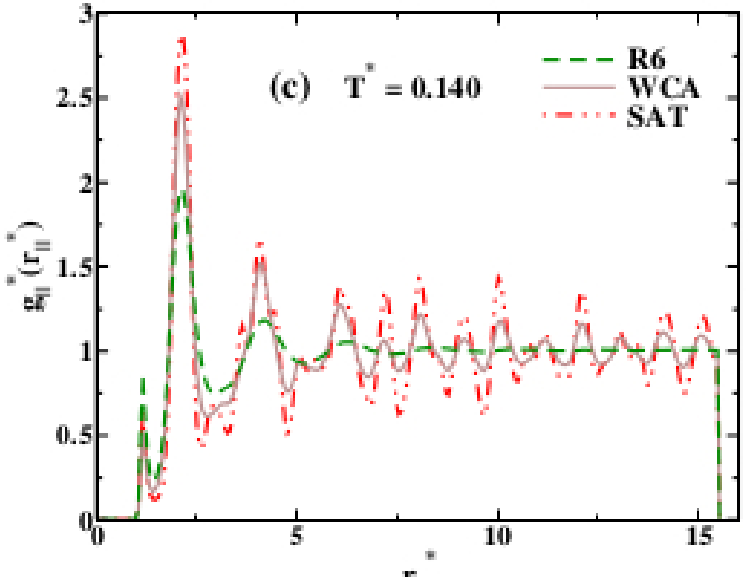
Three Layers

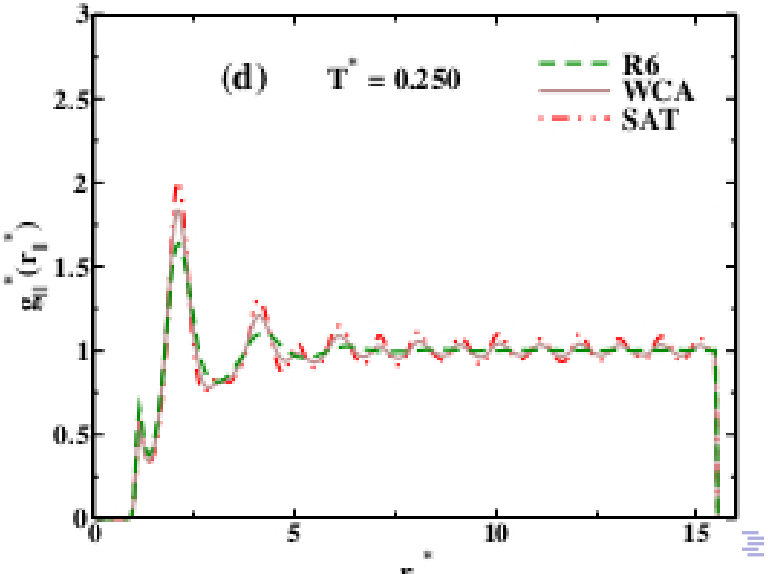


Two Layers

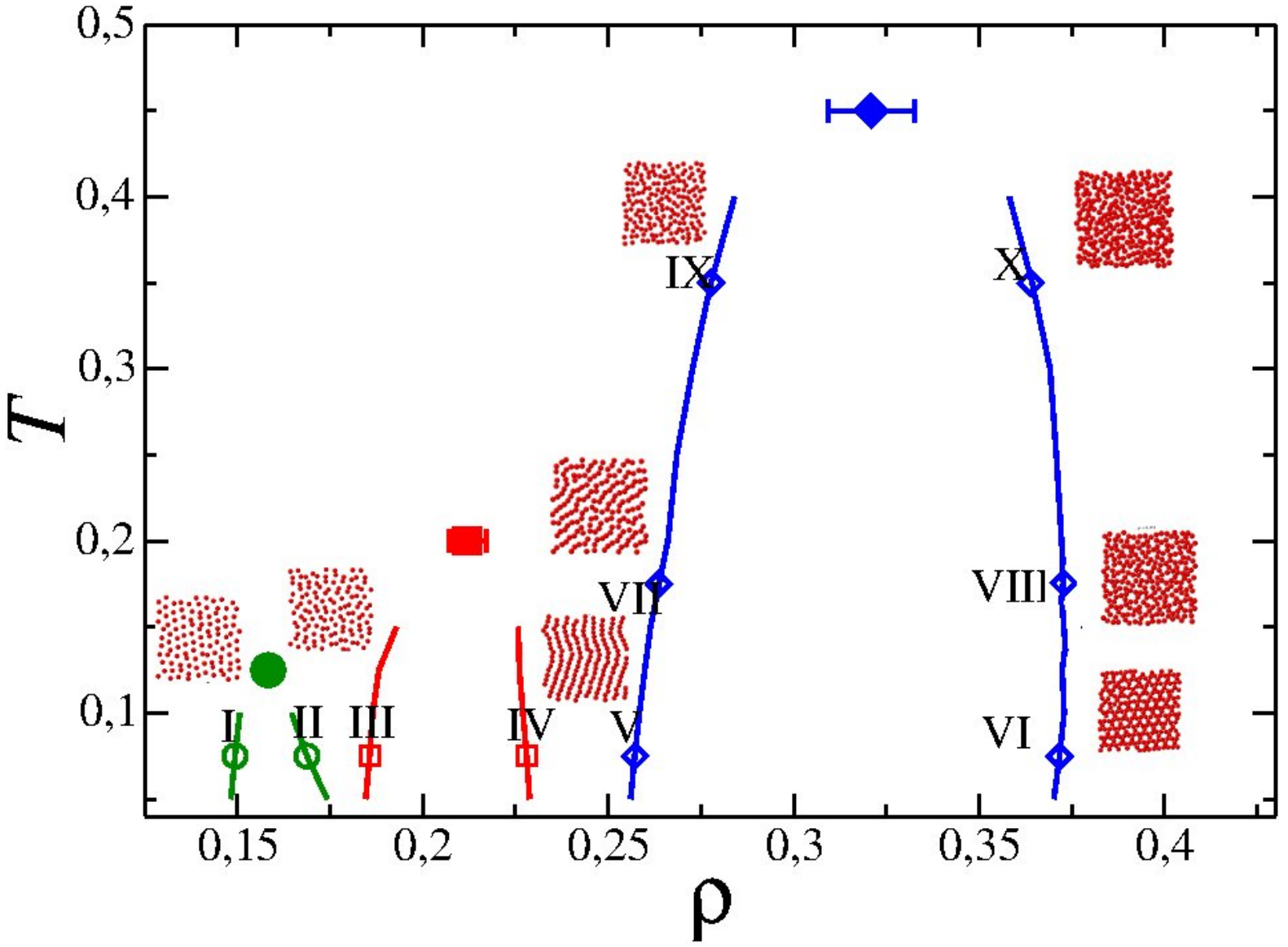

(a)


(b)
R6
WCA
SAT
ρ*(z)
z*
0
0.5
1
1.5
1
2
3
4


(c) T* = 0.140
R6
WCA
SAT
g_II*(r_II*)
r_II*
0
0.5
1
1.5
2
2.5
3
5
10
15


(d) T* = 0.250
R6
WCA
SAT
g_II*(r_II*)
r_II*
0
0.5
1
1.5
2
2.5
3
5
10
15

T vs. Density



Conclusions

- Diffusion increases
- Enhancement Flow
- Ordering at the wall