

Superflow of Nanoconfined Water



What is the mystery?

Two Length Scales Bulk Water

Nanotubes

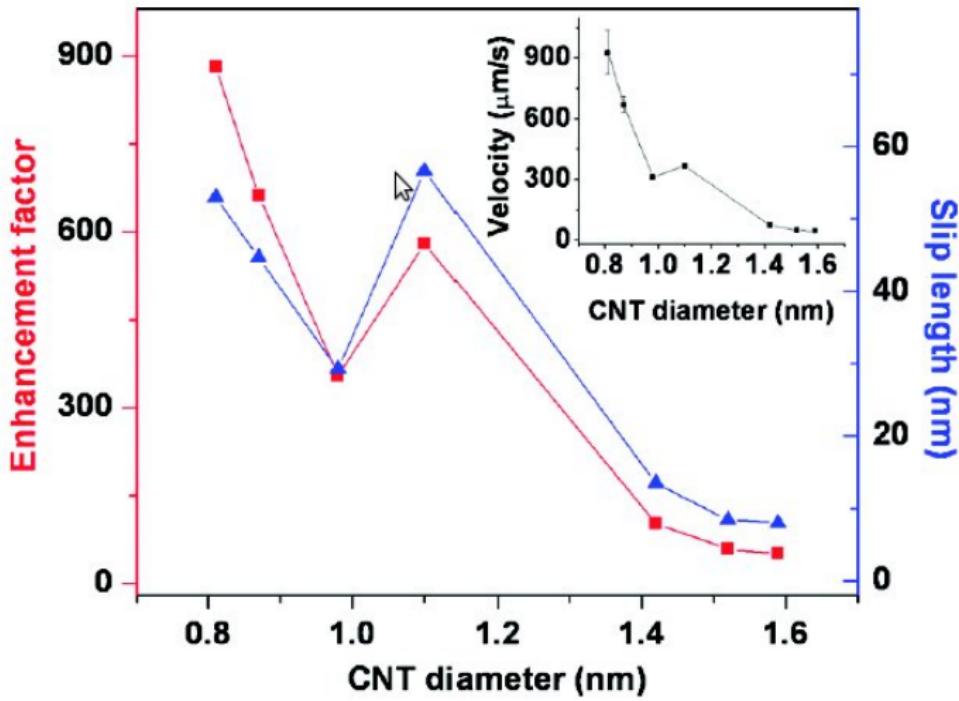
Conclusions

Our Group



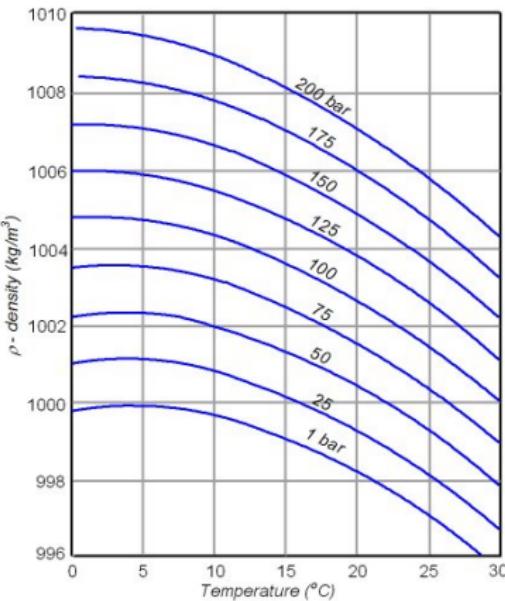
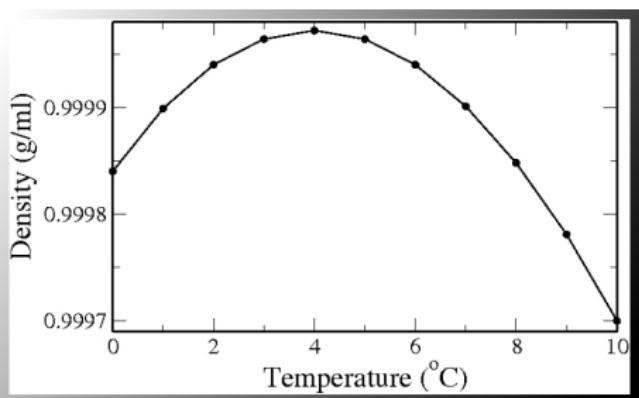
What is the mystery?

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



Density

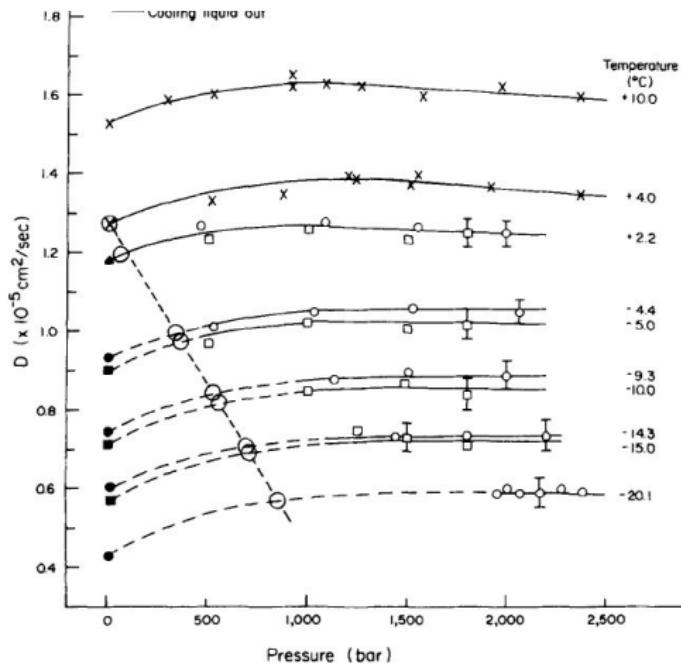
Kell, J. Chem. Eng. Data 12, 66 (67)



Diffusion

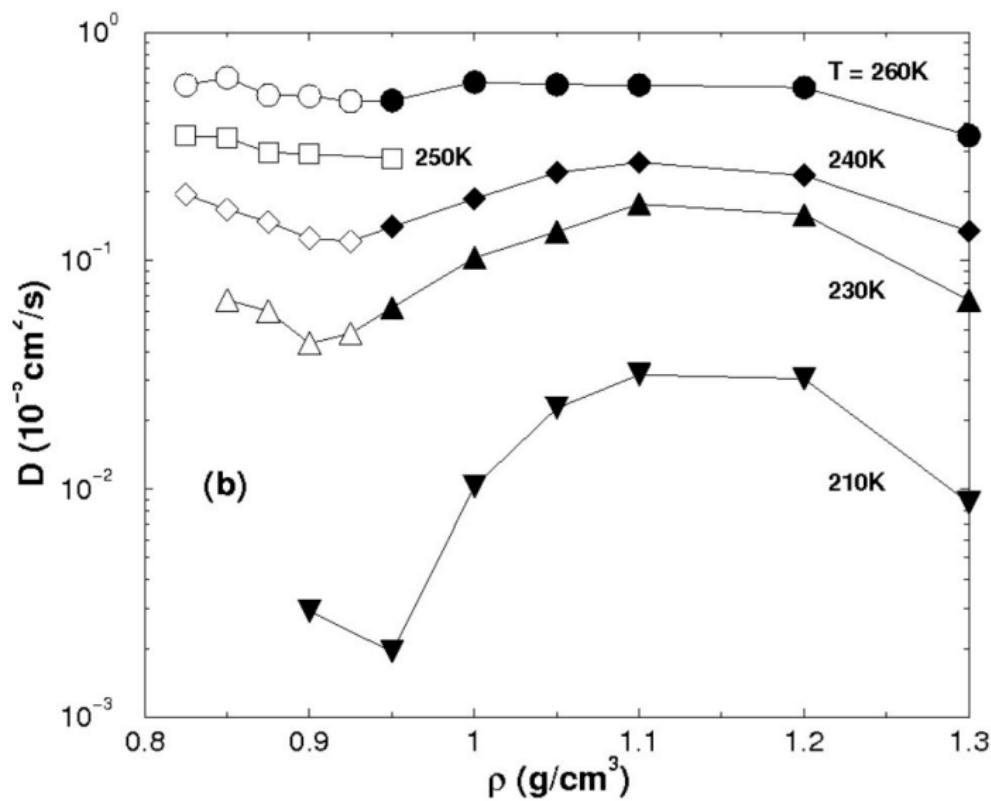
Angell, Finch, Bach 65, 3063 (76)

► $\langle r(t)r(0) \rangle = 6Dt$



Diffusion - SPC/E

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

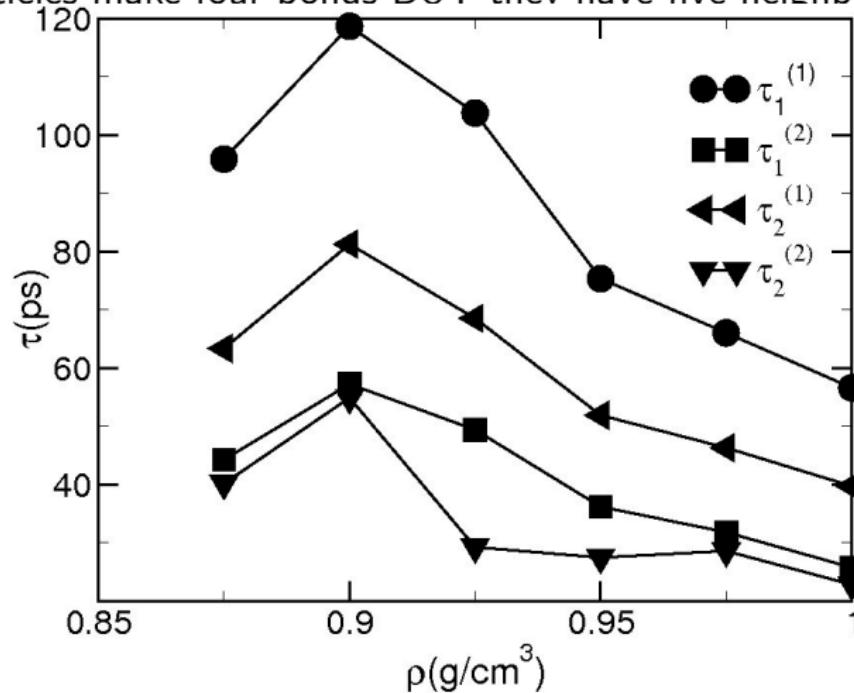


Rotation Diffusion - SPC/E

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

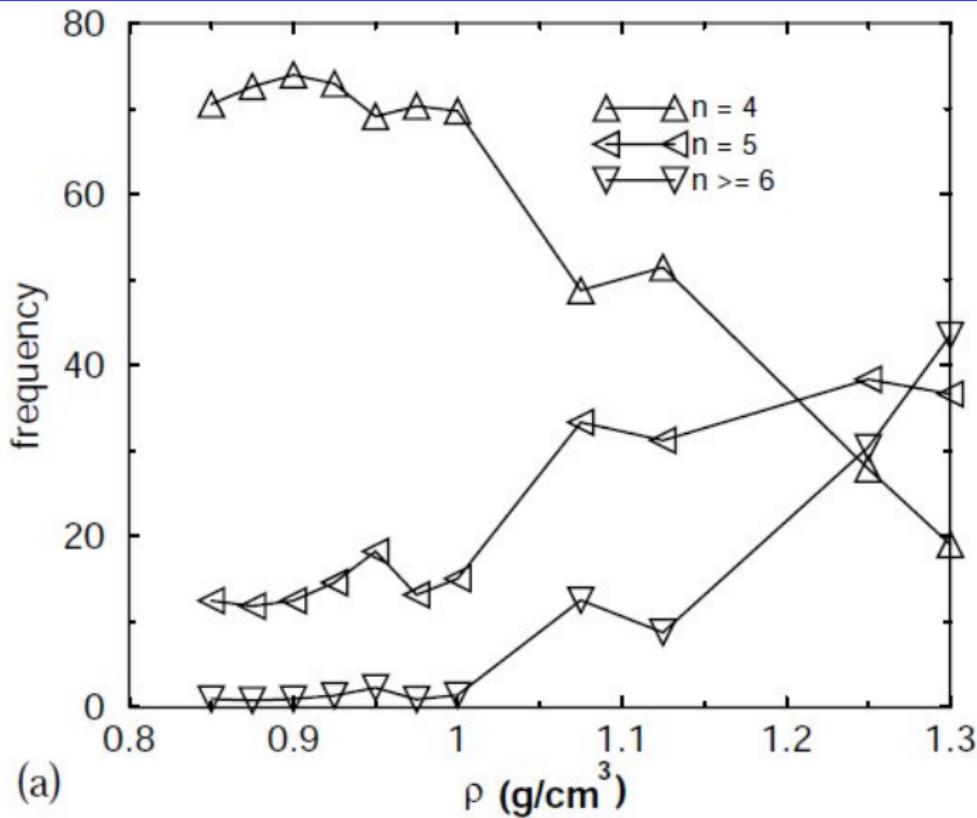
Mazza, Giovanbaptista, Stanley, Starr, PRE 76, 31203 (07)

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

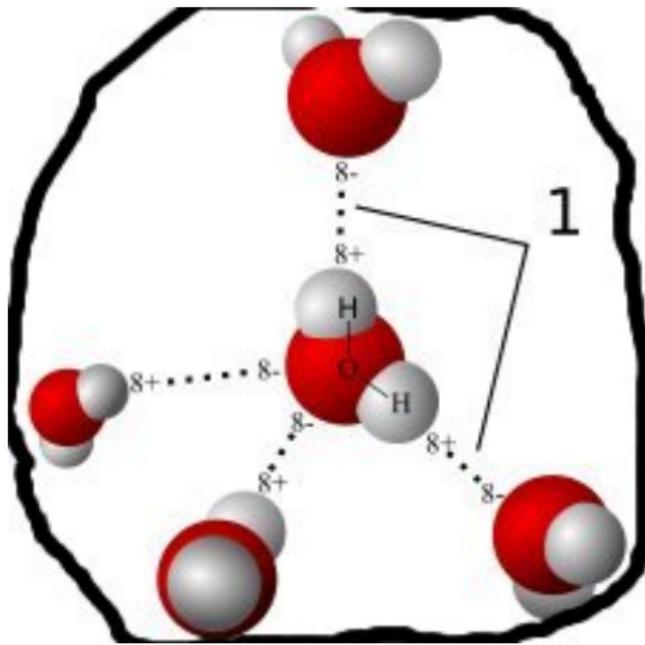


Frequency - SPC/E

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

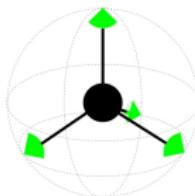
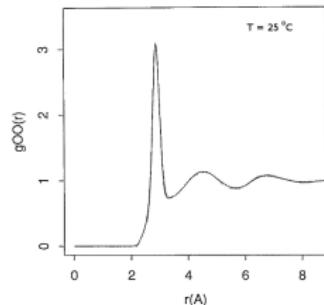


Structure



Effective Potential

- Radial Distribution Function of WATER:



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

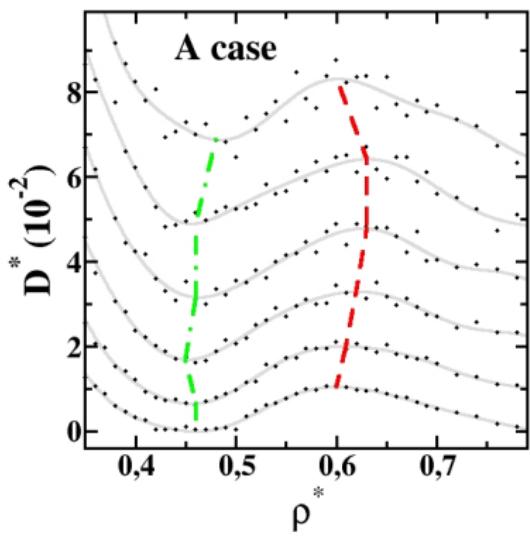
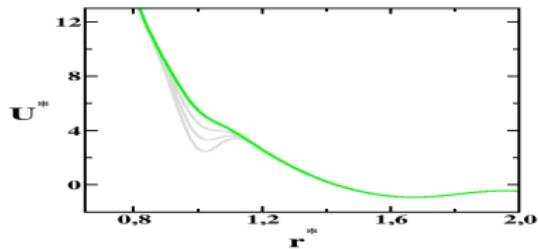
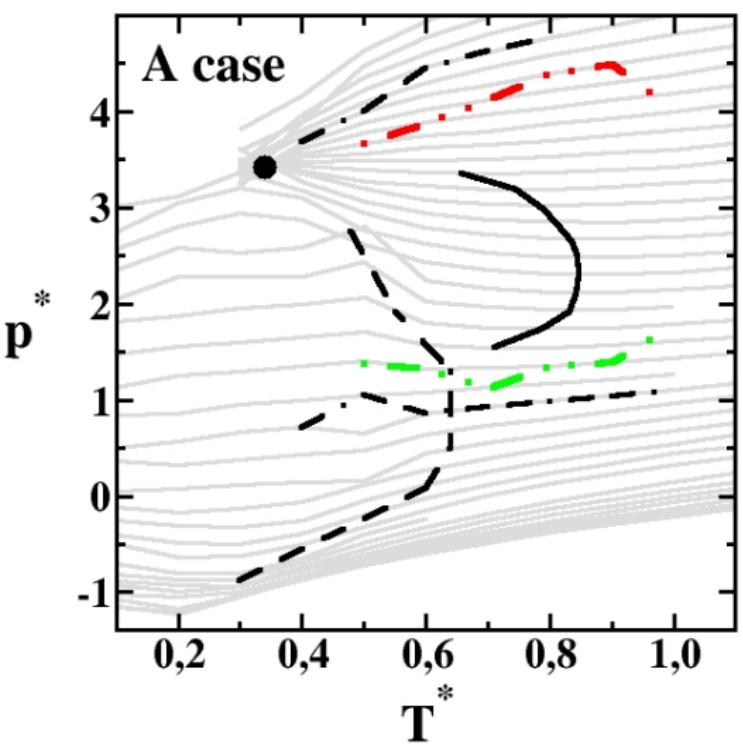
- Ornstein-Zernike Equation:

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

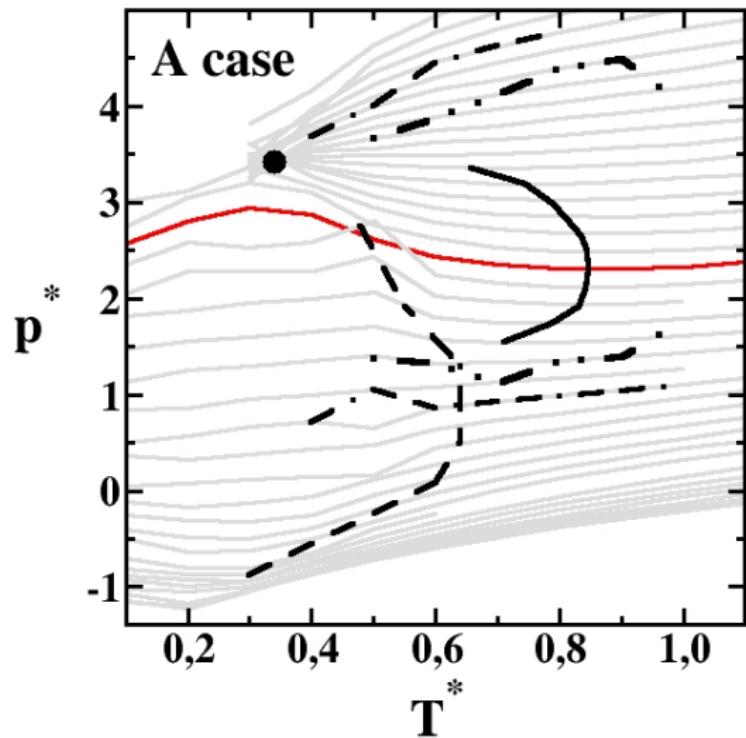
- Hypernetted Chain Approximation (HNC):

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

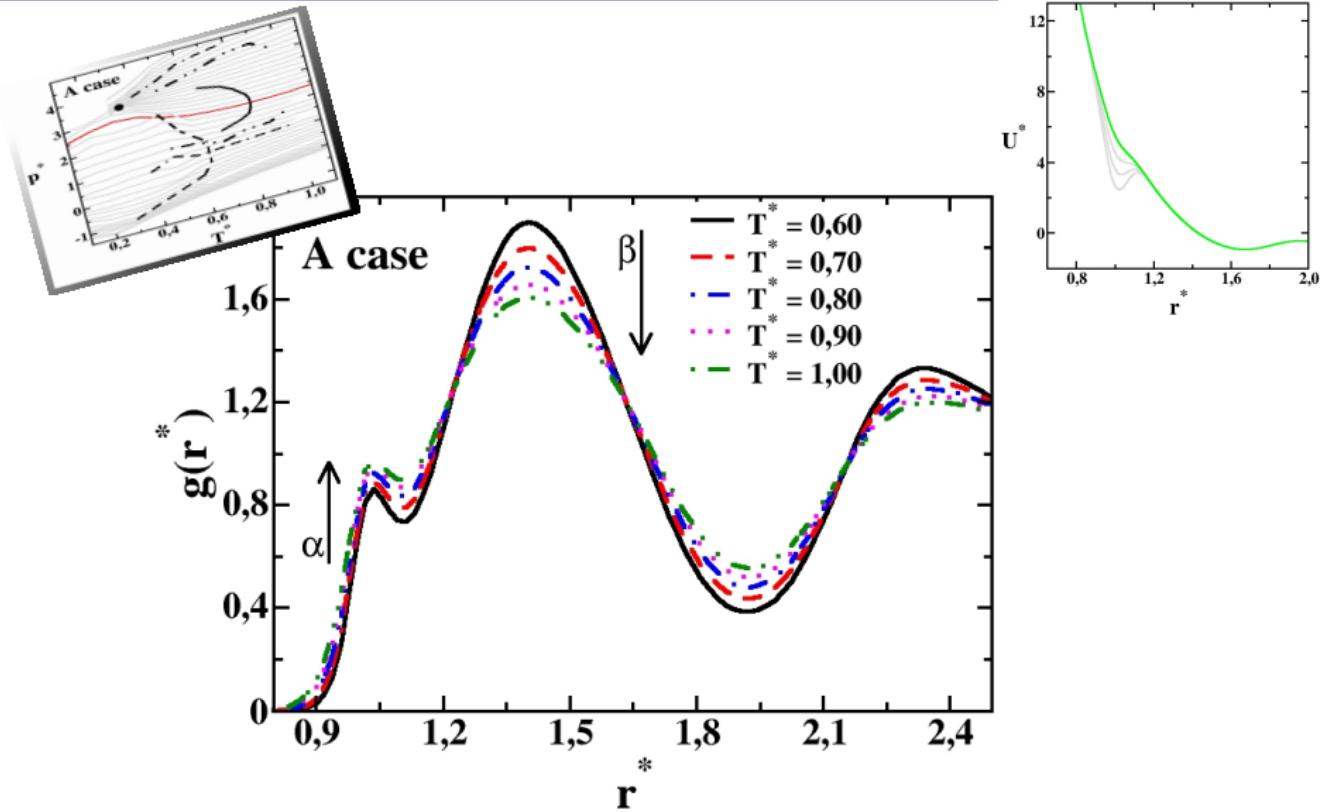
Phase Diagram



Radial Distribution Function

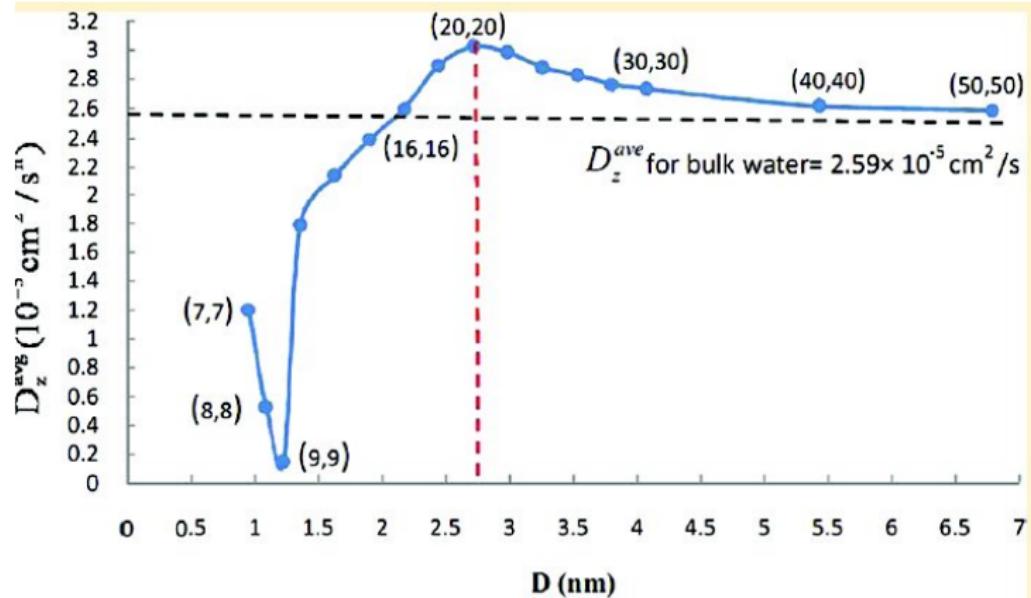


Radial Distribution Function



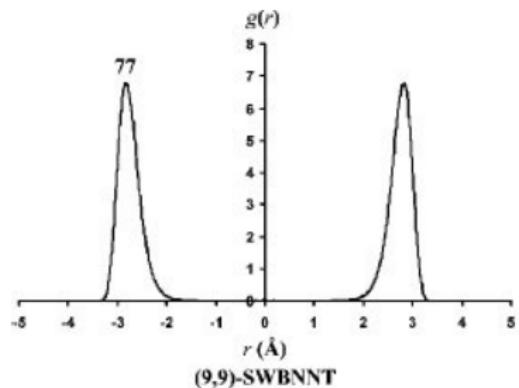
Diffusion in Nanotubes

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

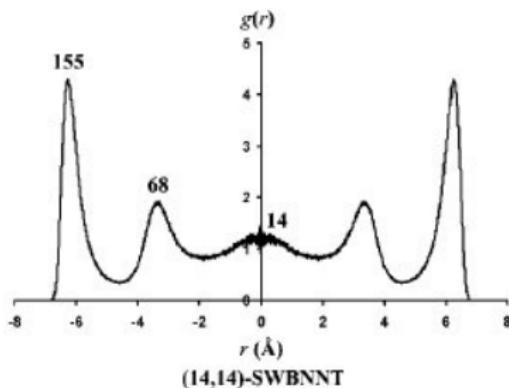


Distribution in Nanotubes - Simulations

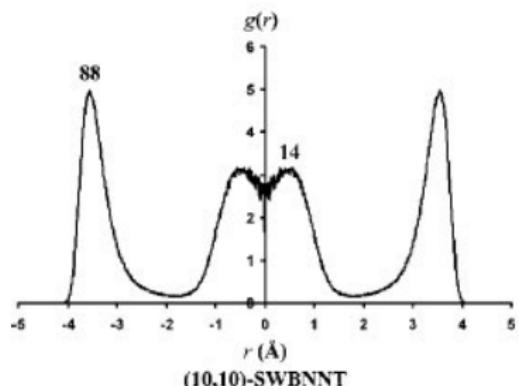
T. Nanok, JCPA 113, 2103 (2009) - SPC/E



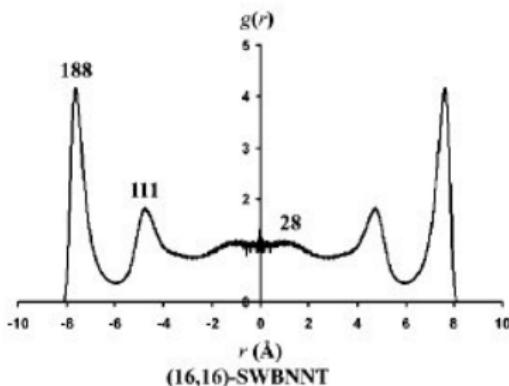
(9,9)-SWBNNT



(14,14)-SWBNNT



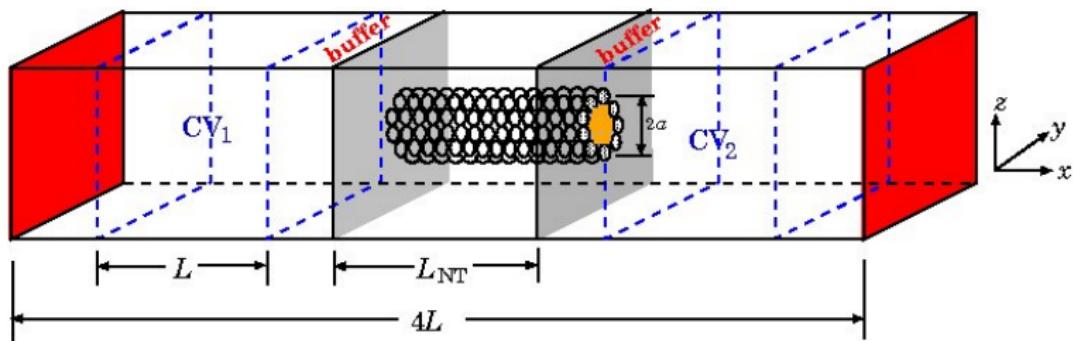
(10,10)-SWBNNT



(16,16)-SWBNNT

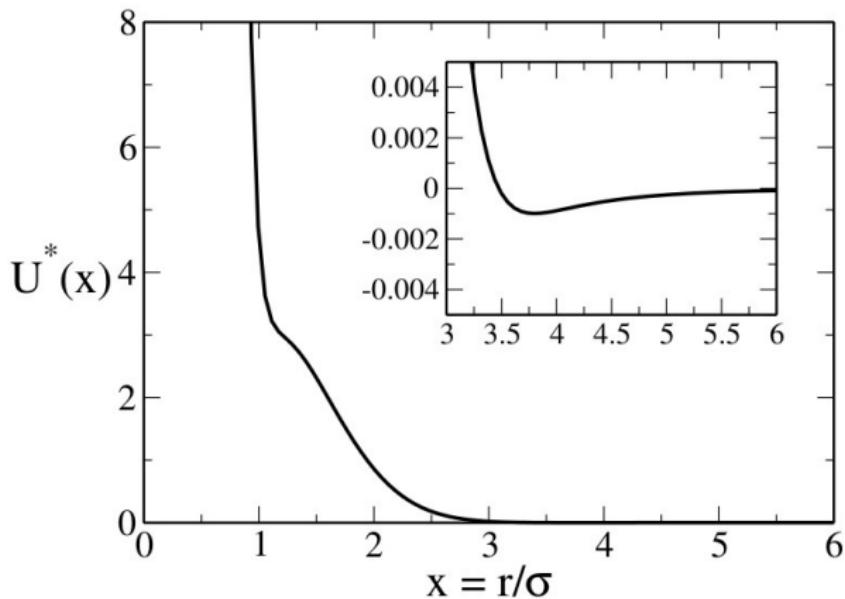
Model for Confining

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

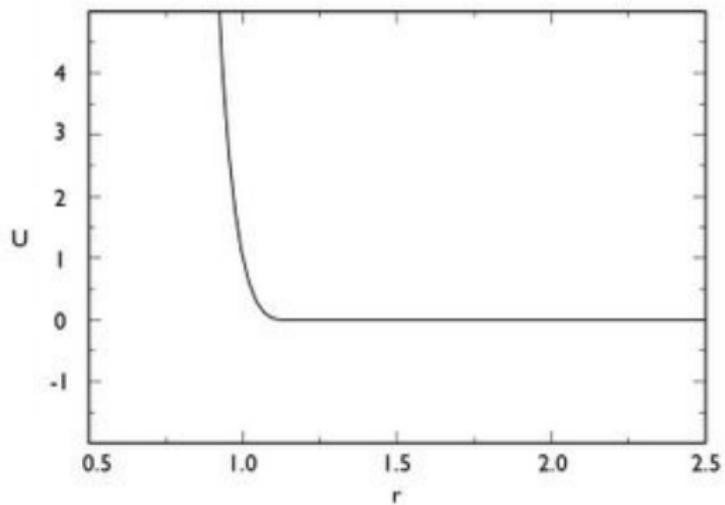


Fluid-Fluid Effective Potential

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

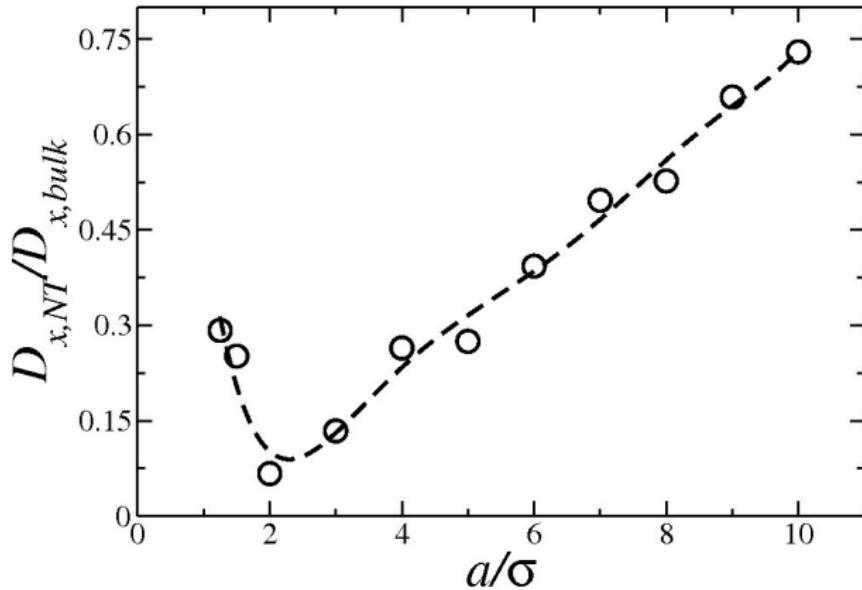


Fluid-Wall Effective Potential



Diffusion

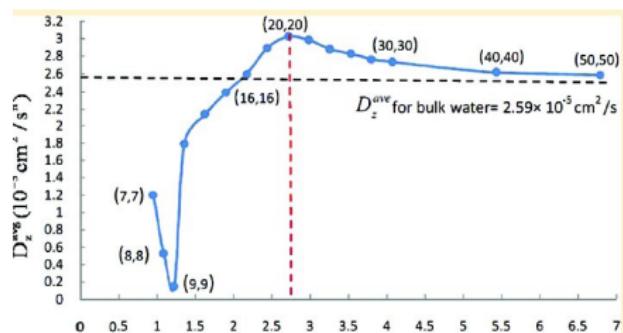
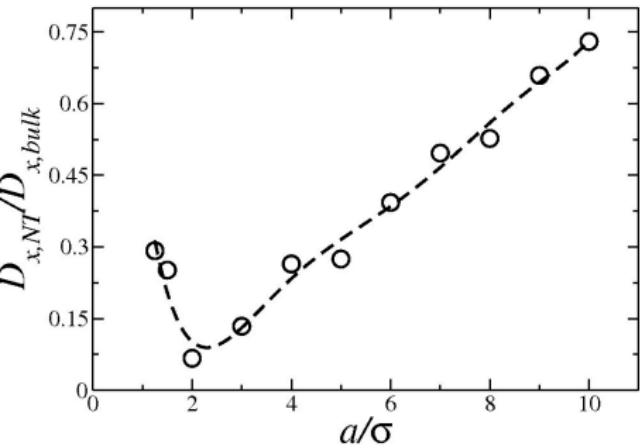
J. R. Bordin, A. B. de Oliveira, A. Diehl and MCB, JCP 137, 084504 (2012)



Diffusion

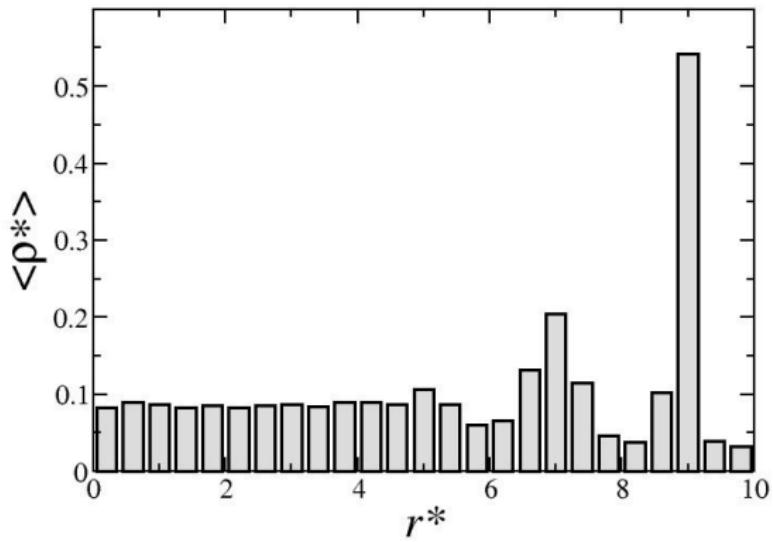
A.B. Farinami, JPCB 115, 12145 (2012)

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

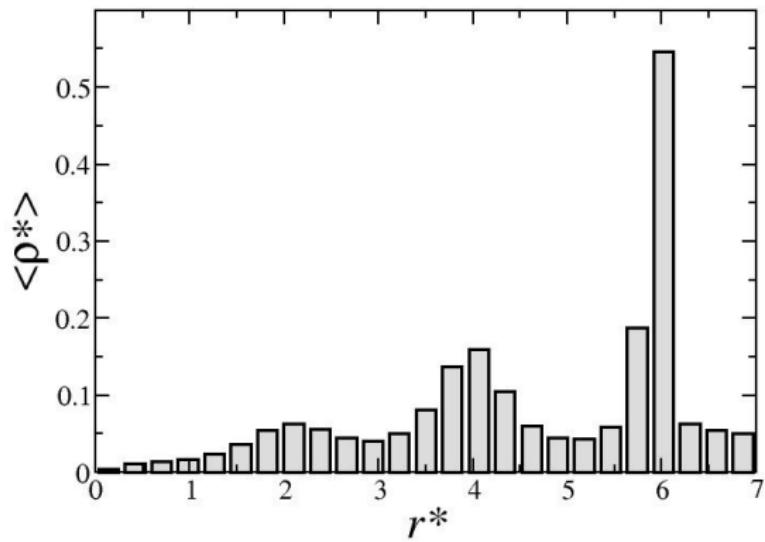


Density vs. r - $a=10$

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

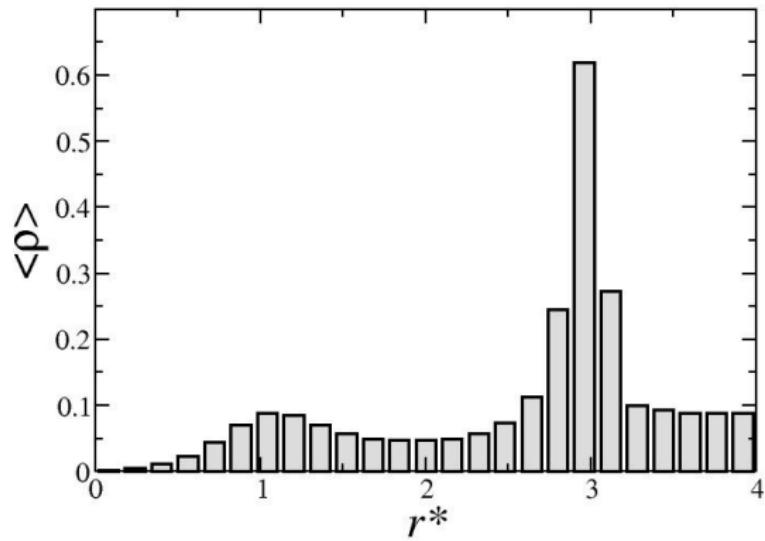


Density vs. r - $a=7$



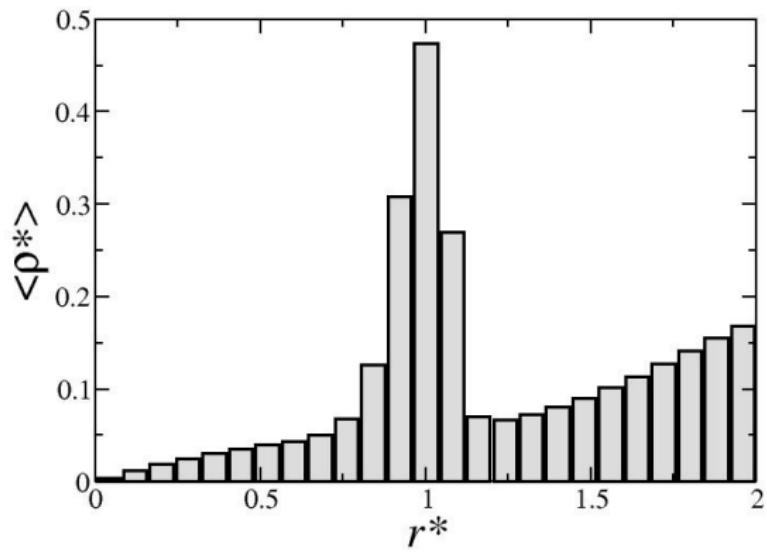
Density vs. $r - a=4$

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



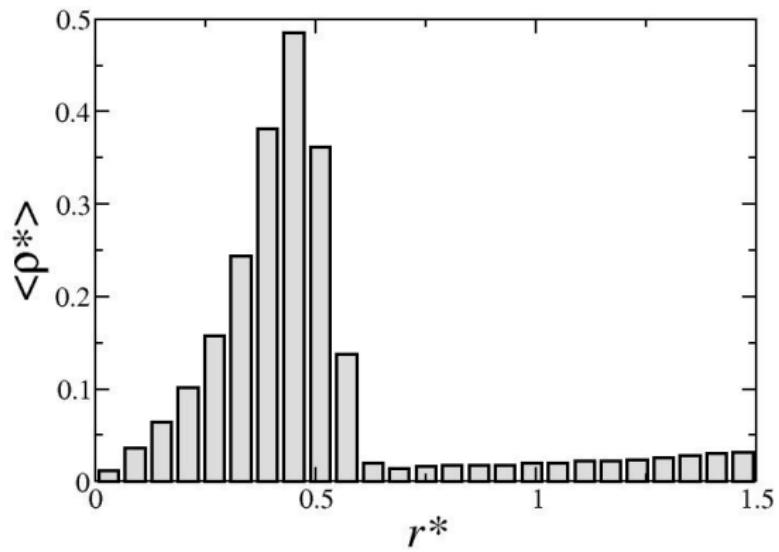
Density vs. r - $a=2$

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



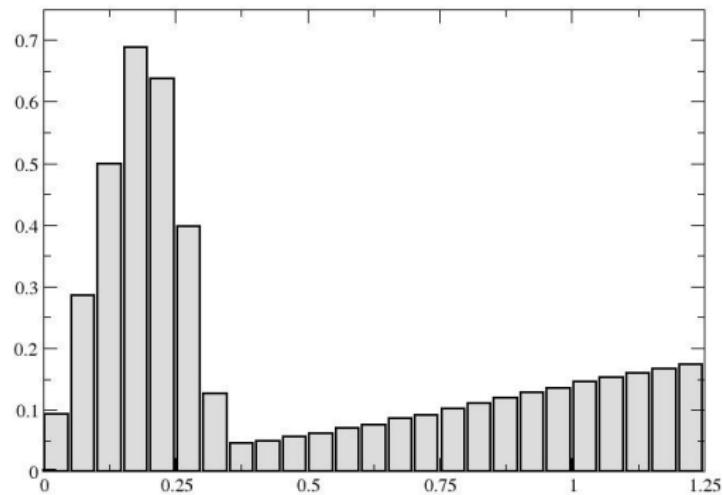
Density vs. r - $a=1.5$

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



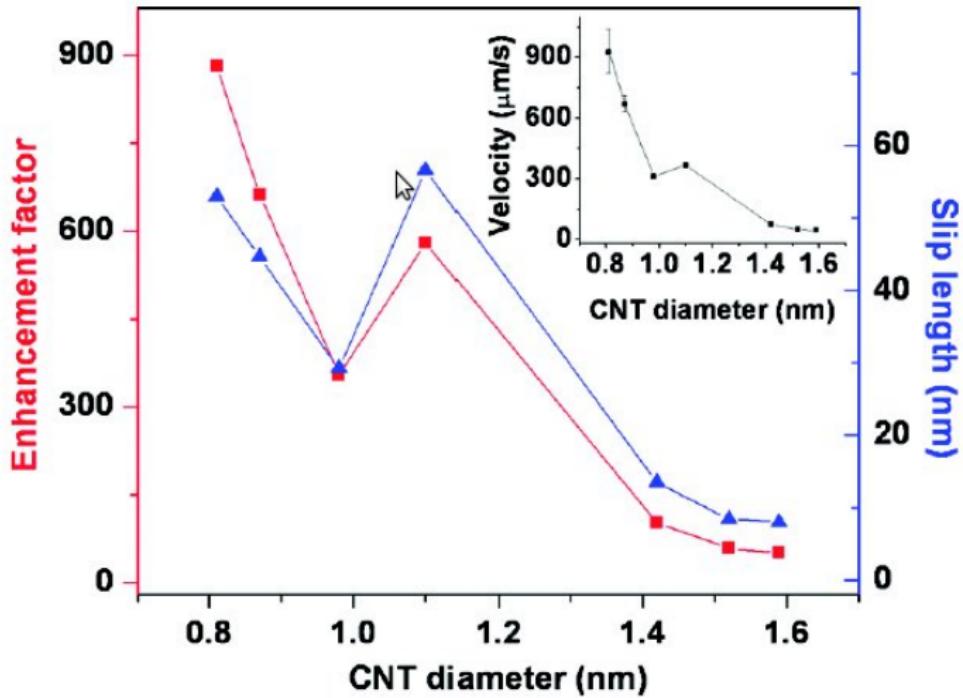
Density vs. r - $a=1.25$

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



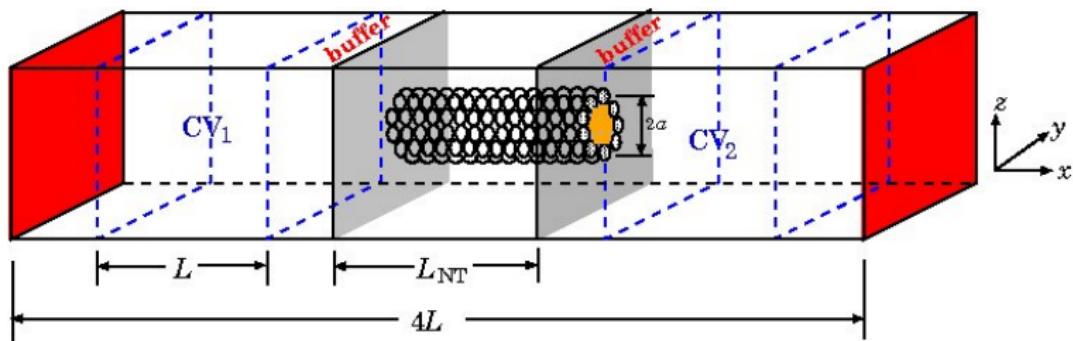
Flux in Nanotubes

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



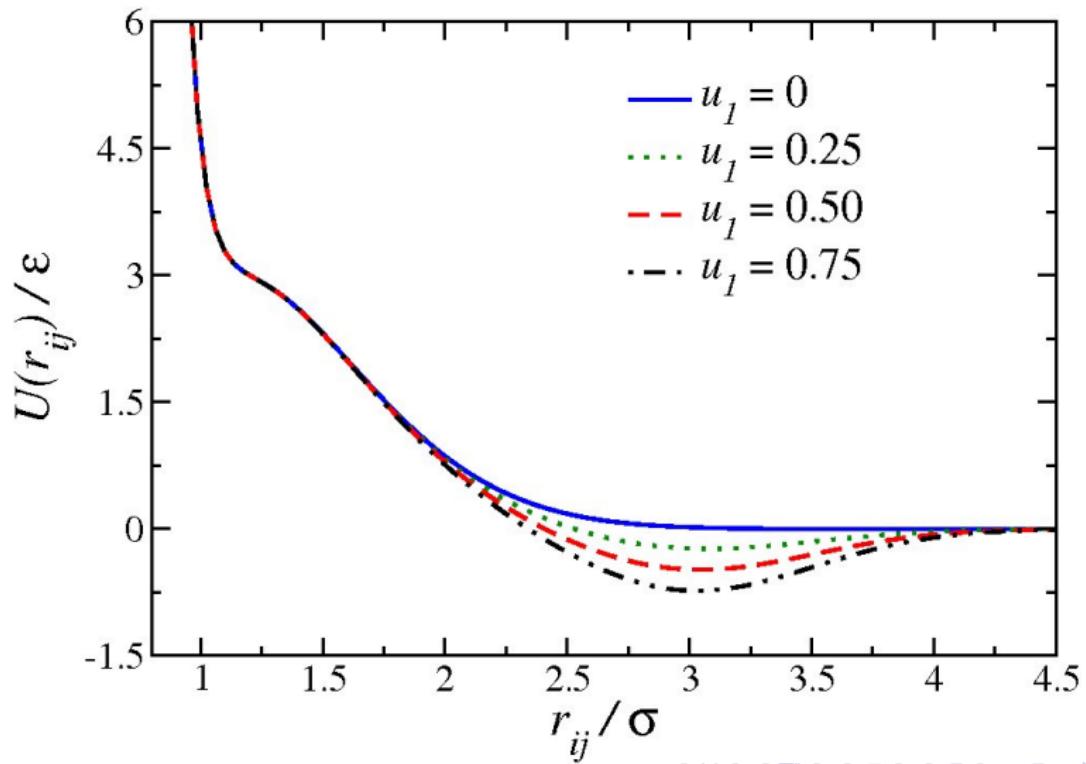
Model for Nanotubes

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



Fluid-Fluid Effective Potential

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



Enhancement Flow

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

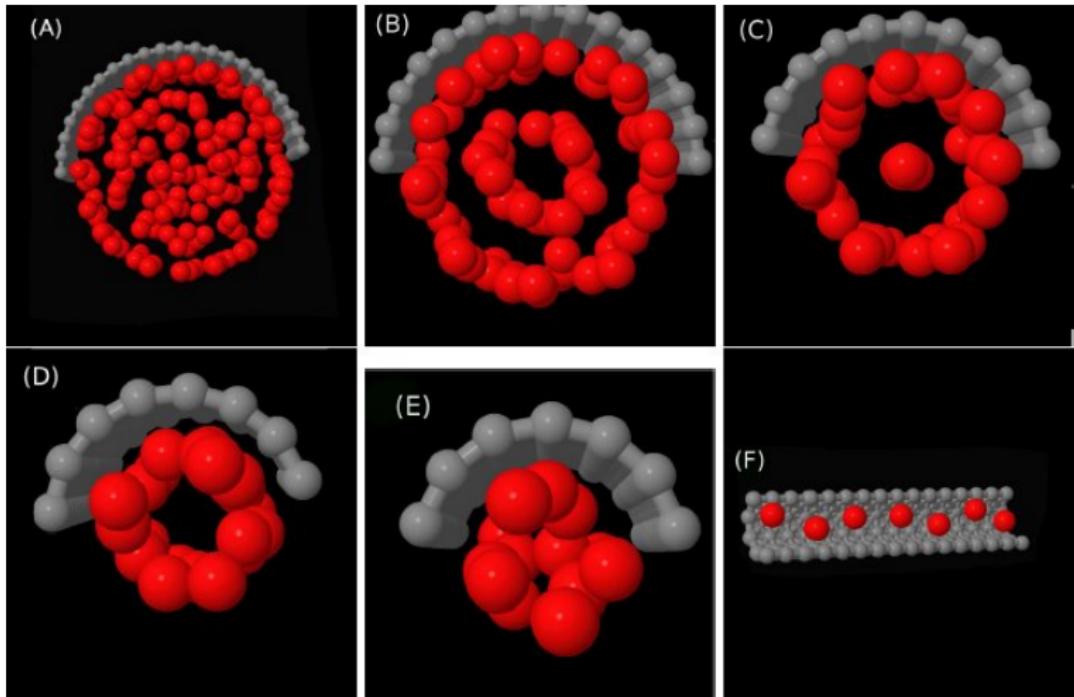
$$\begin{aligned}\langle v_x \rangle &= \gamma_{HP} \frac{\Delta p}{L_{NT}} \\ \gamma_{HP} &= \frac{a^2}{8\eta} \\ \eta &= \frac{k_B T}{3\pi\sigma D_x}\end{aligned}$$

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

$$\epsilon = \frac{\gamma_{MD}}{\gamma_{HP}} \quad (1)$$

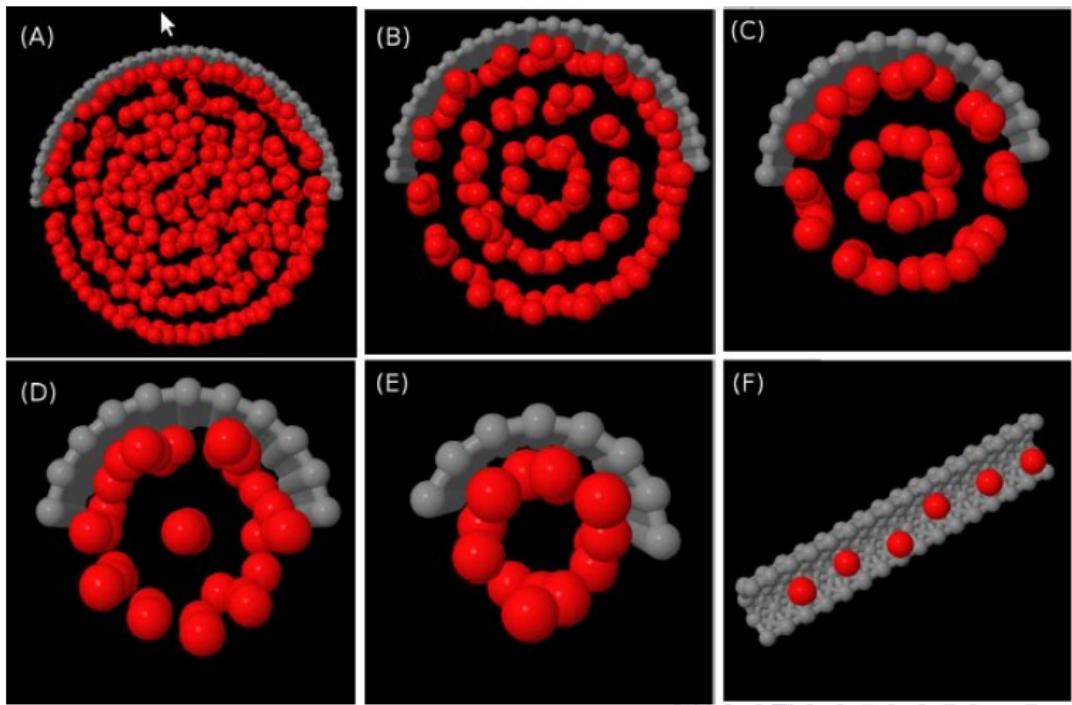
Layers - Attractive

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



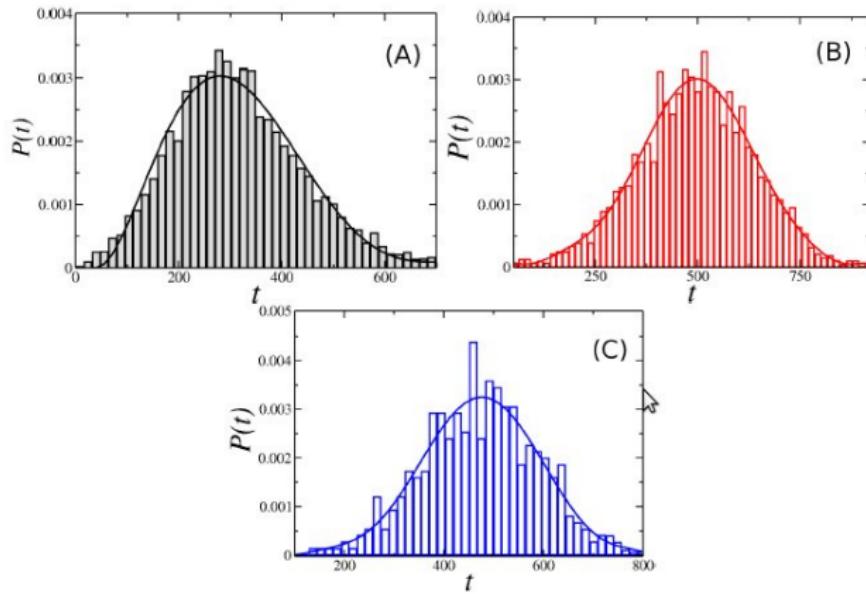
Layers - Repulsive

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



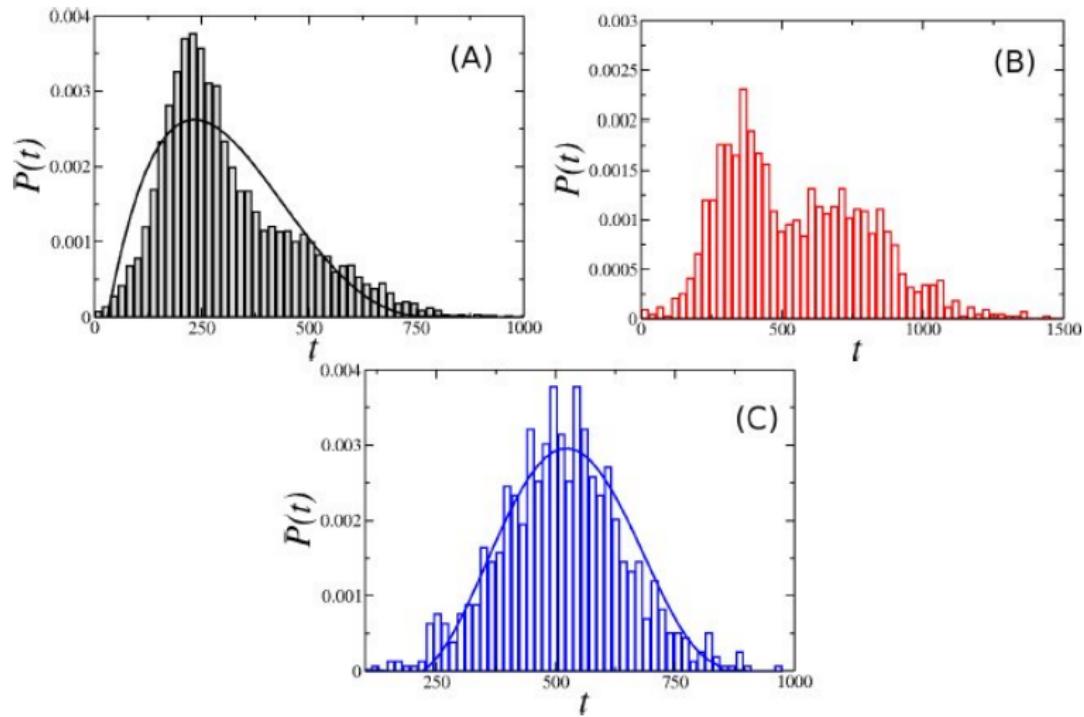
Distribution - Attractive

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



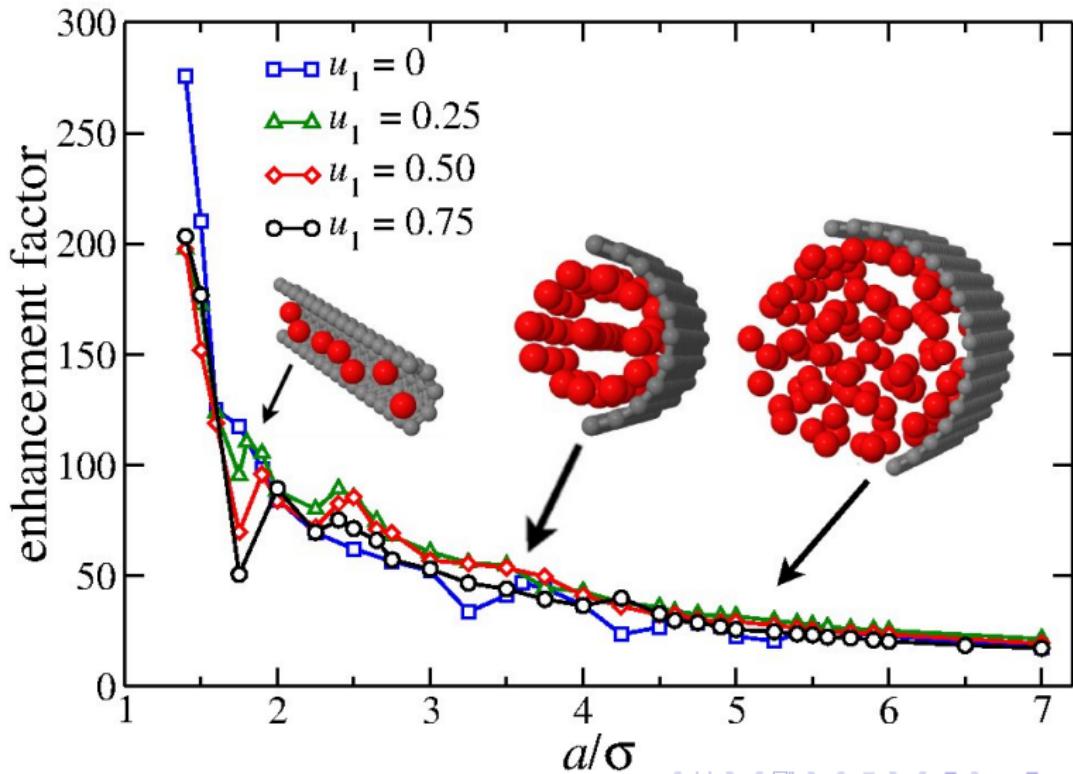
Distribution - Repulsive

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



Enhancement Flow

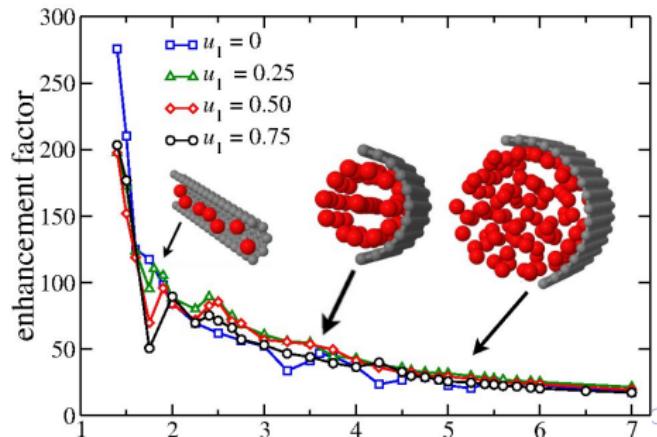
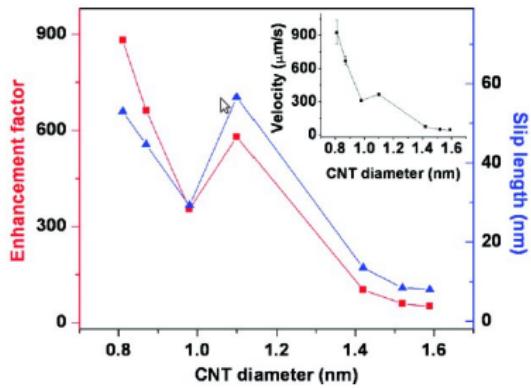
J. R. Bordin, A. Diehl and MCB, JPCB 117, 7047(2013)



Enhancement Flow

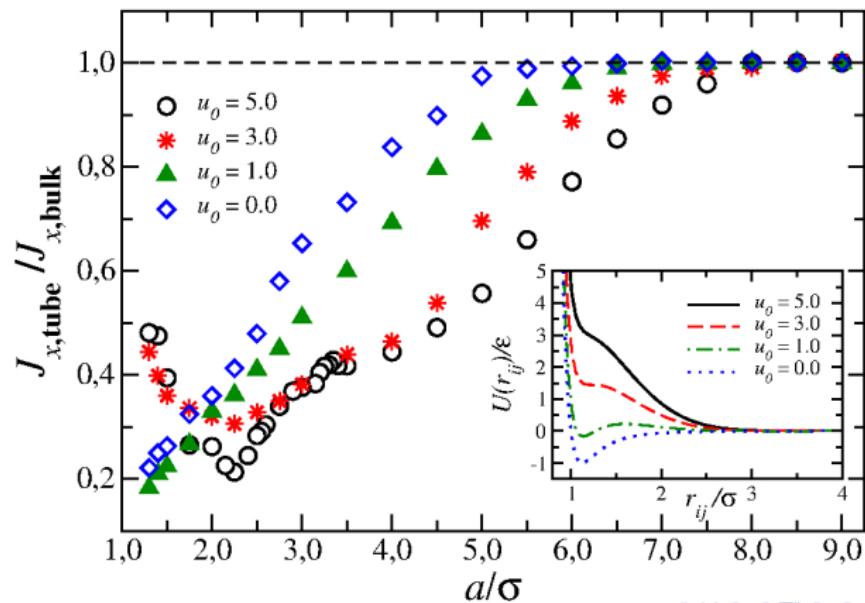
X. Qin et al, Nanoletters 11, 2173 (2011)

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



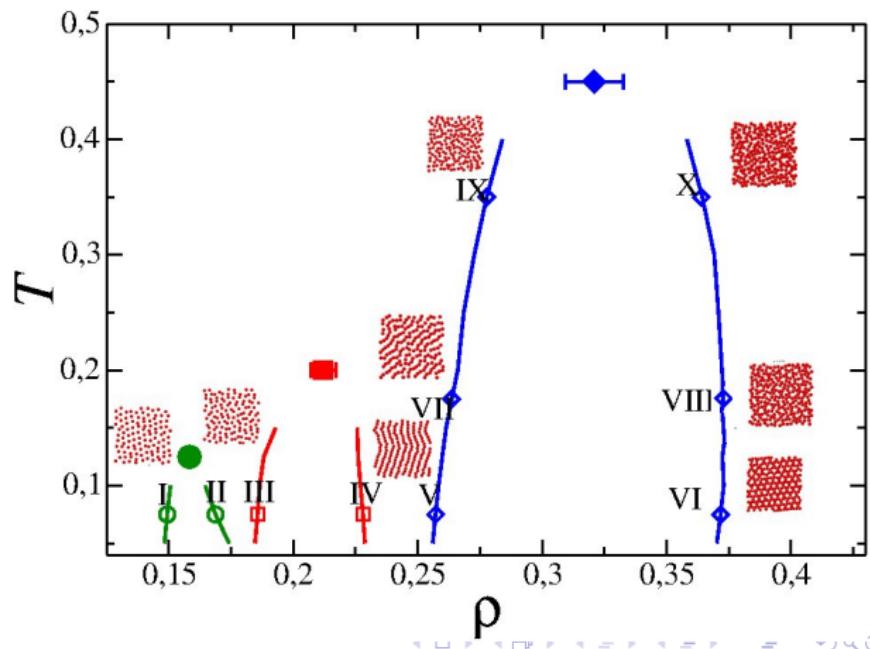
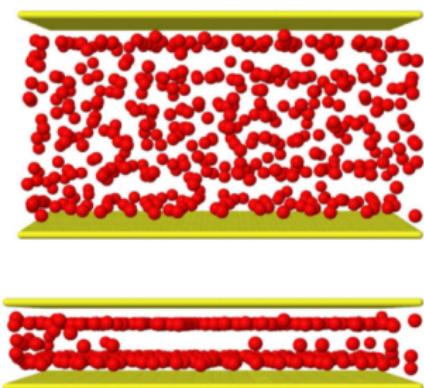
Flux increases is only for two length scales?

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



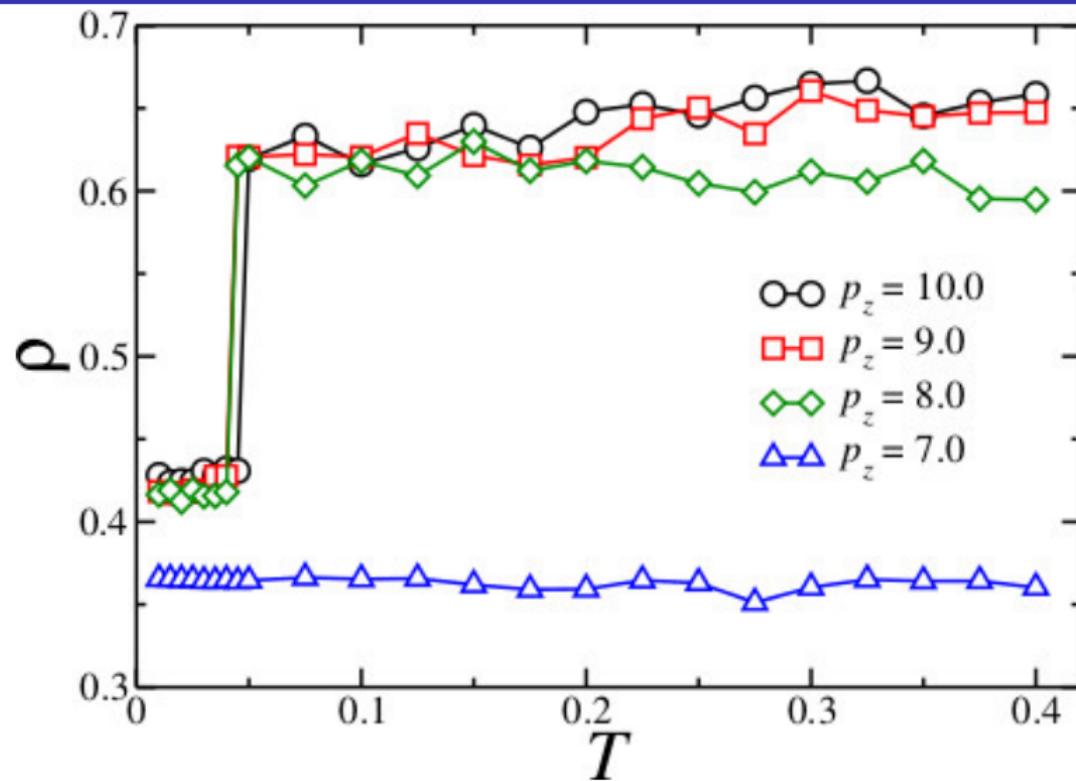
Phases in a fixed Plane

Bordin, Krott and MCB, JPC C 118 9497 (2014)



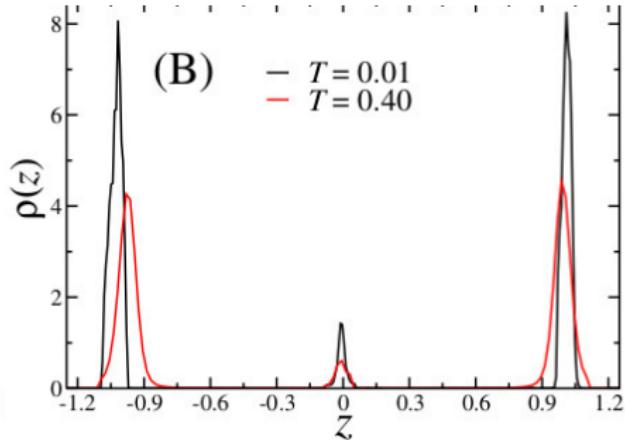
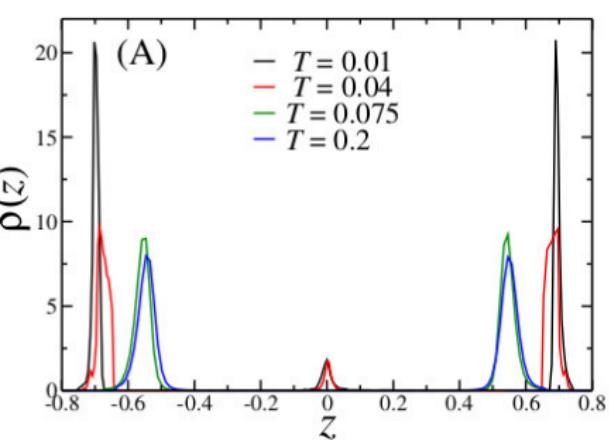
Plane

Bordin, Krott and MCB, JCP. 141 144502 (2014)



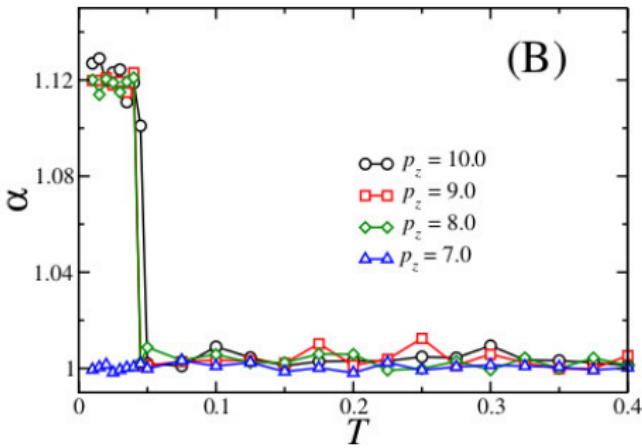
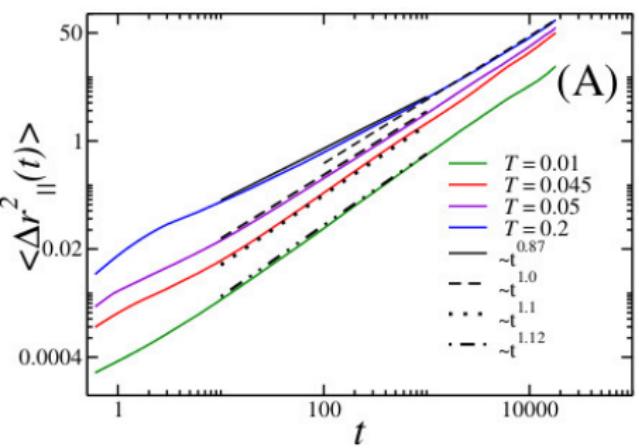
Plane

Bordin, Krott and MCB, JCP. 141 144502 (2014)



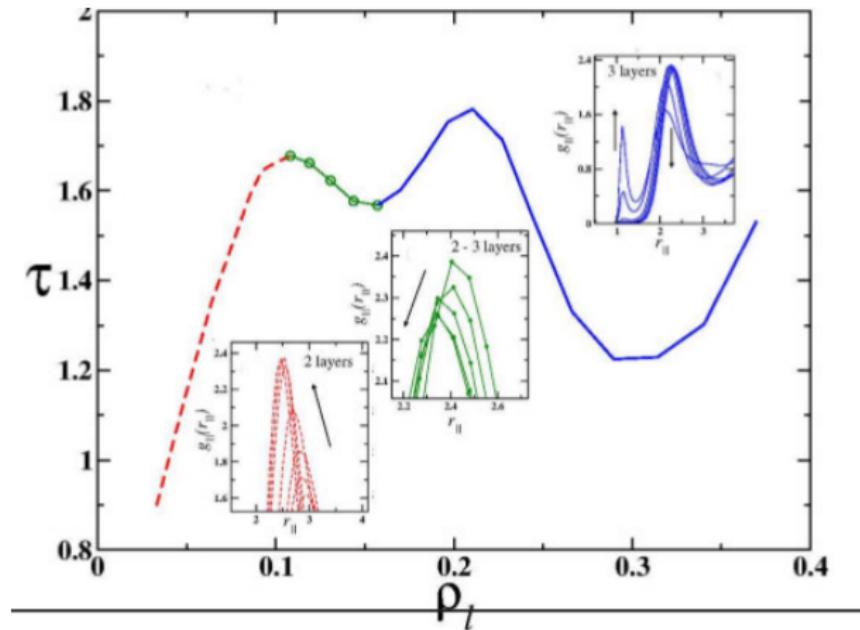
Plane

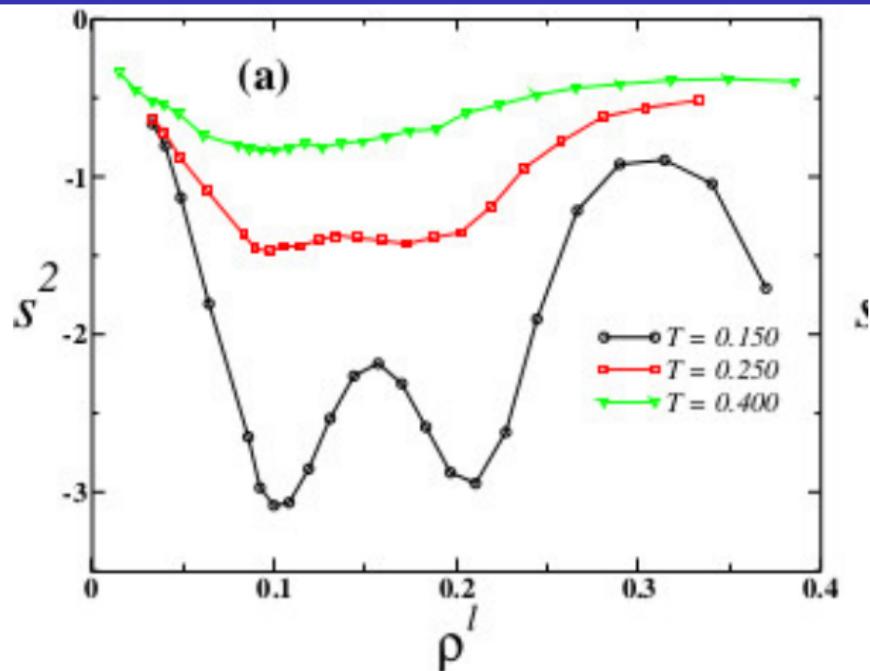
Bordin, Krott and MCB, JCP. 141 144502 (2014)



Plane - Translational Order Parameter

Krott, Bordin and MCB JPC B 119, 291 (2015).





Namibia Beatle

Stenocara dentata Herbst, 1799 by Hans Hillewaert

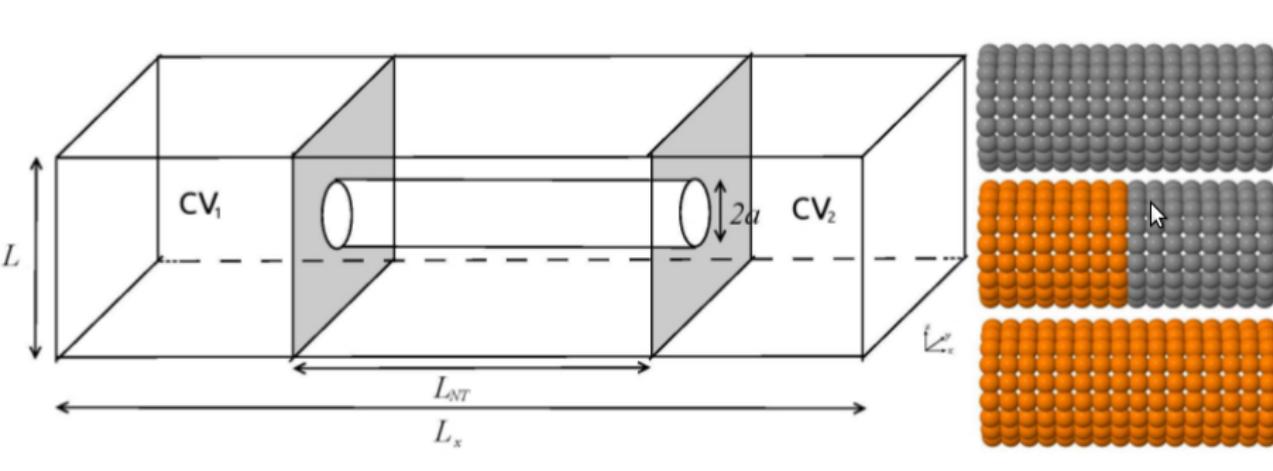
http://commons.wikimedia.org/wiki/File:Stenocara_dentata.jpg

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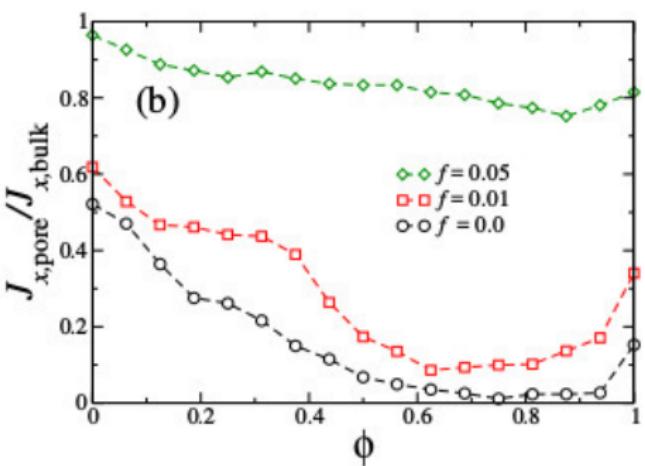
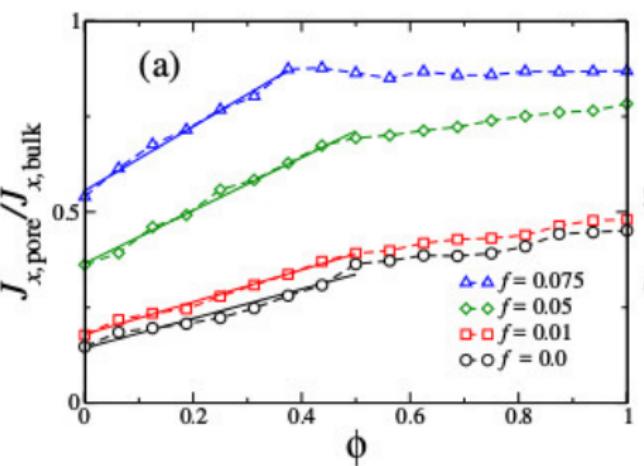
Nanotube

Bordin and MCB



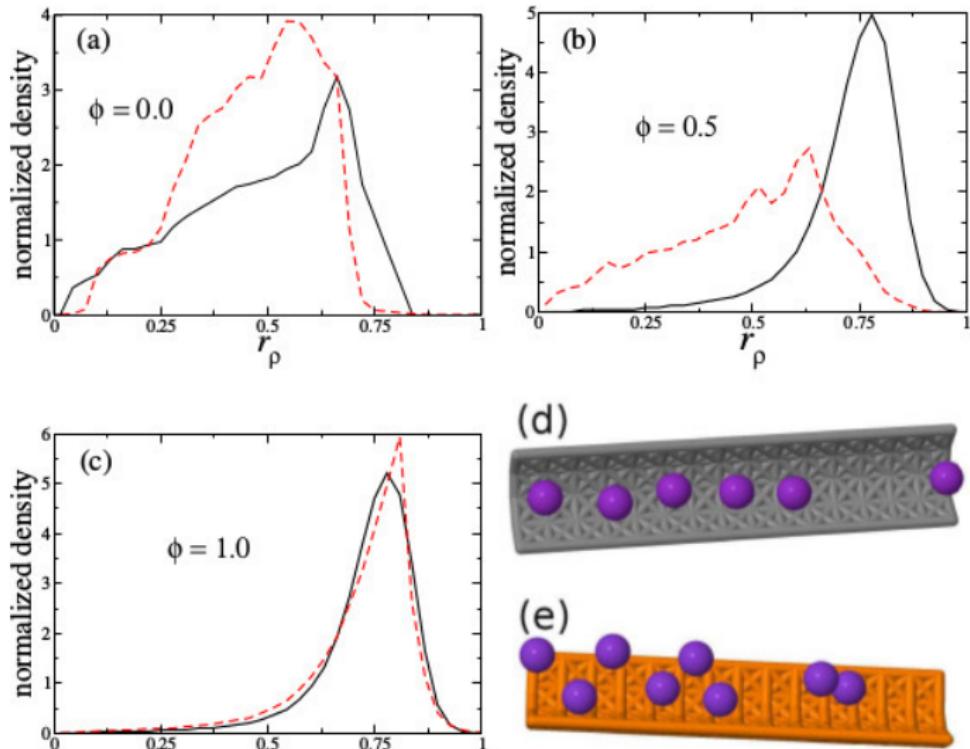
Nanotube Density versus ϕ

Bordin and MCB



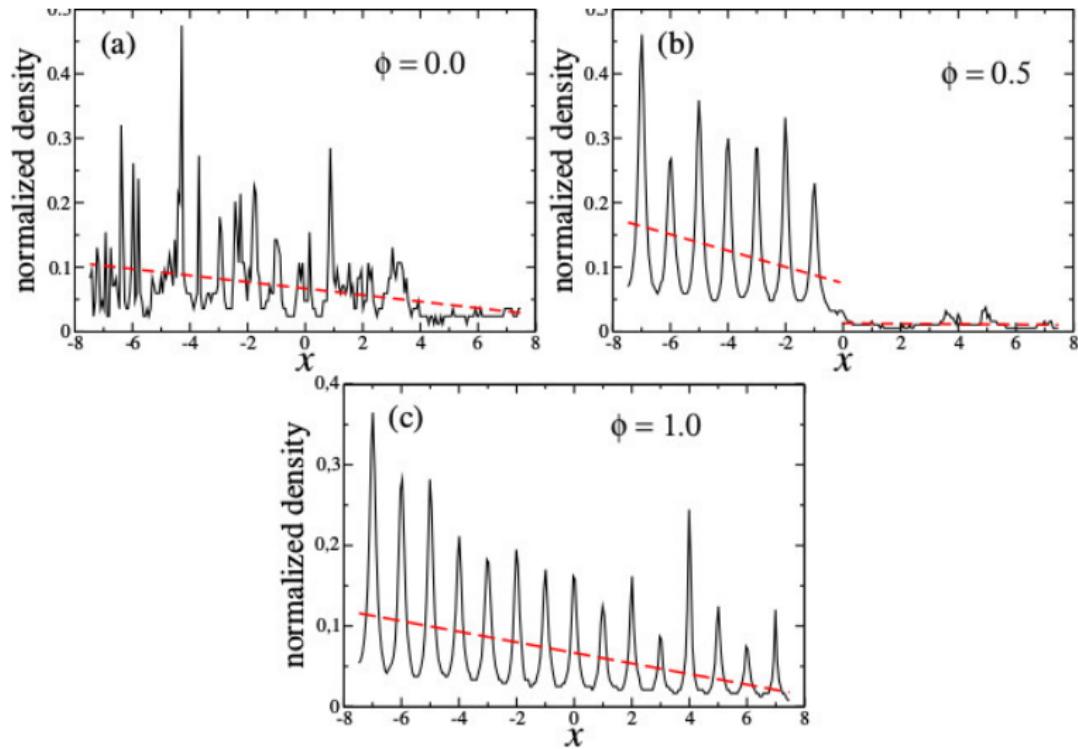
Nanotube Density versus r

Bordin and MCB



Nanotube Density versus x

Bordin and MCB



Conclusions

- ▶ Diffusion increases
- ▶ Enhancement Flow
- ▶ Transformation depends on hydrophobic or hydrophilic