Enhancement Flow in Nanoconfined Water

Tsallis and me

Tsallis : Complexity

Our Group

What are the misteries?

Why should we care?

Mistery 1- Diffusion in Nanotubes

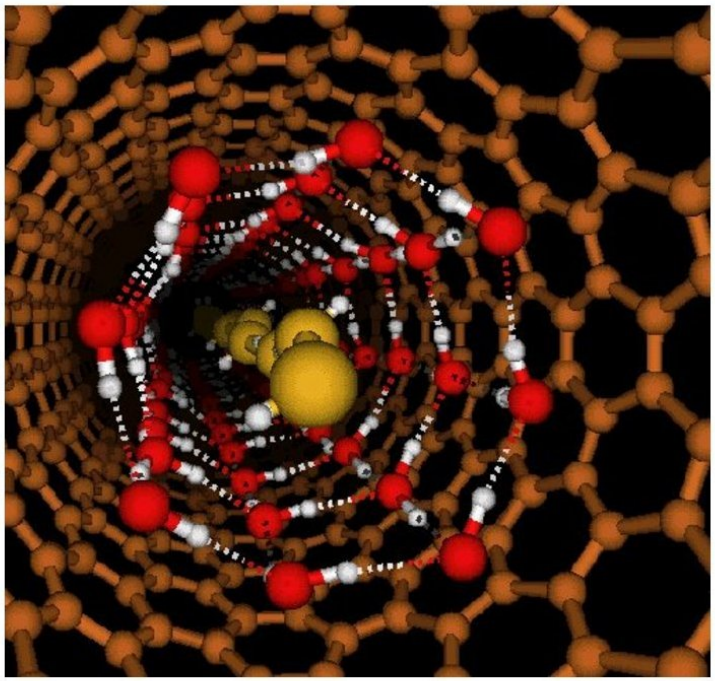
Mistery 2- Flux in Nanotubes

Conclusions

What are the misteries?

- **Diffusion** : INCREASES with the DECREASE of the nanotube diameter

- **Flux** : ENHANCEMENT with the DECREASE of the nanotube diameter



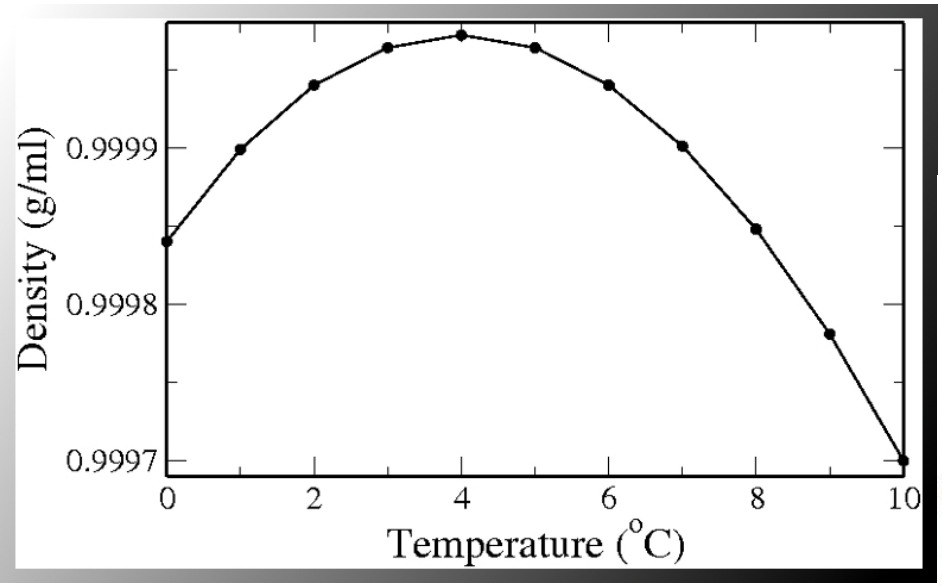
Why should we care?

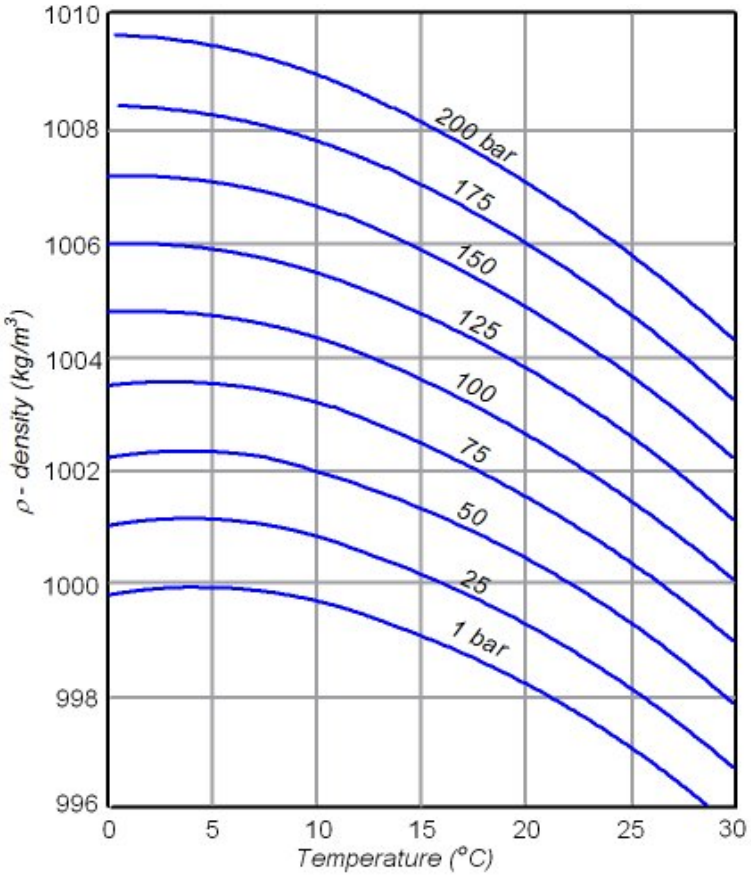
- Interesting new physics at nano scale

- Oil recovery, Second Generation Ethanol, Dissalinazation

Density

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

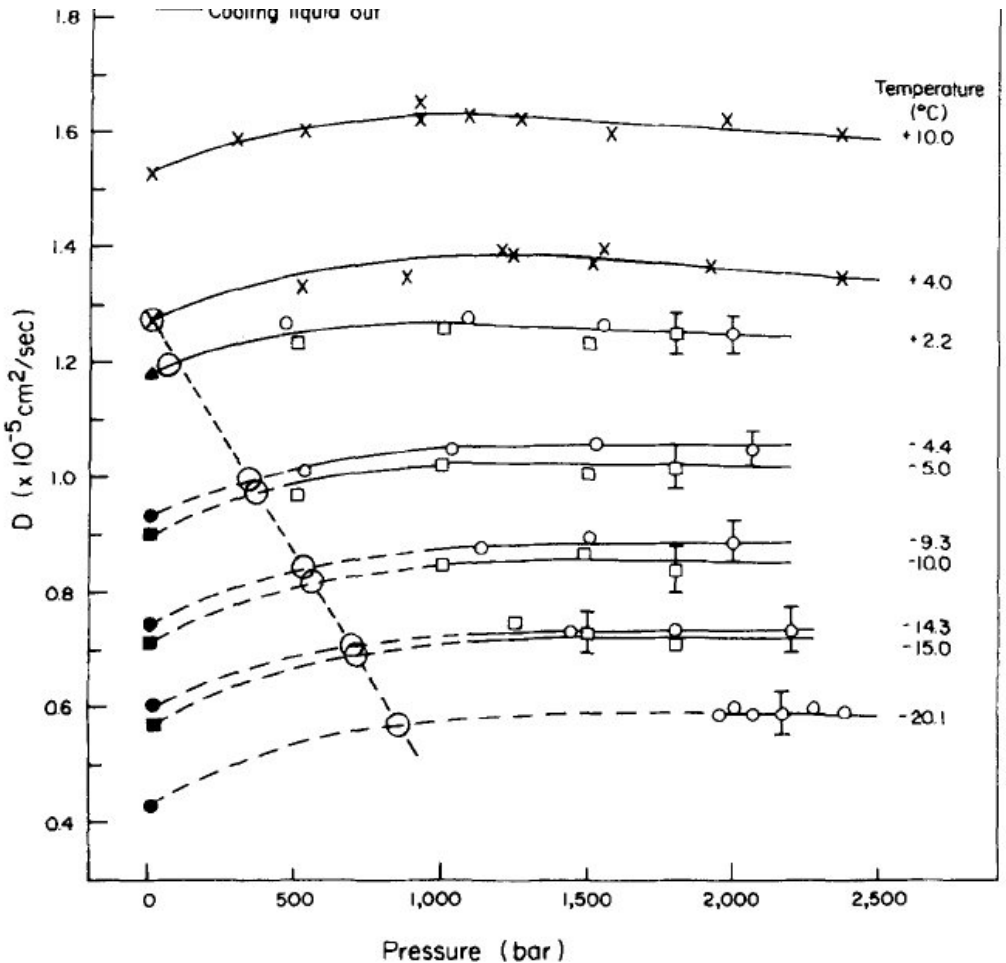




Diffusion

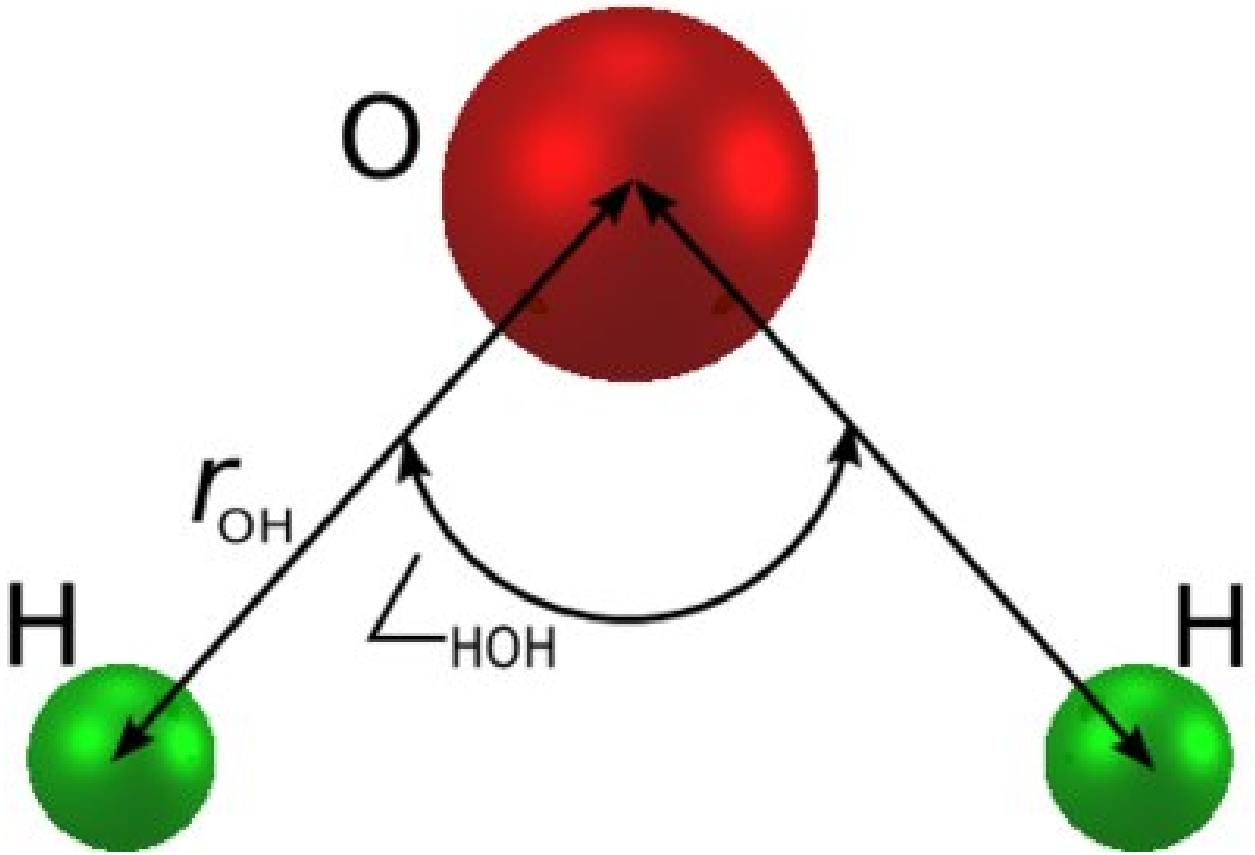
Angell, Finch, Bach 65, 3063 (76)

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



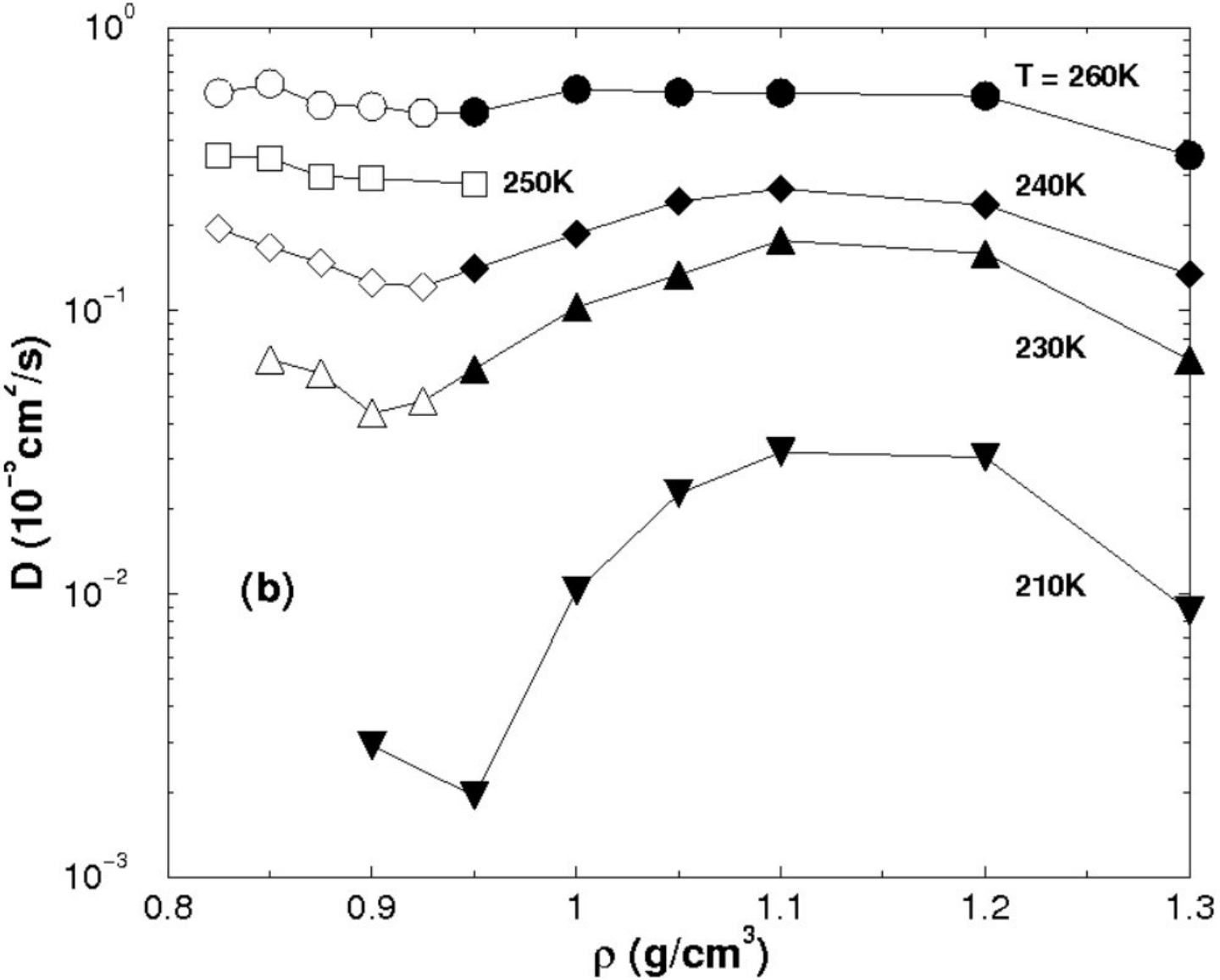
Diffusion - SPC/E

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



Diffusion - SPC/E

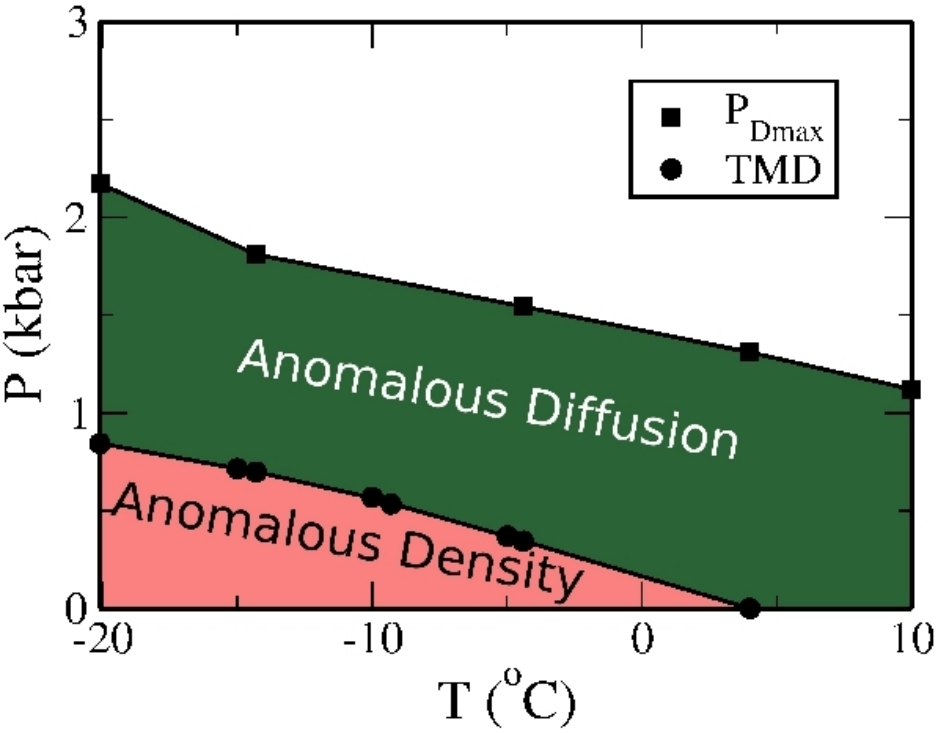
Netz, Starr, Stanley, Barbosa JCP 115, 344 (01)

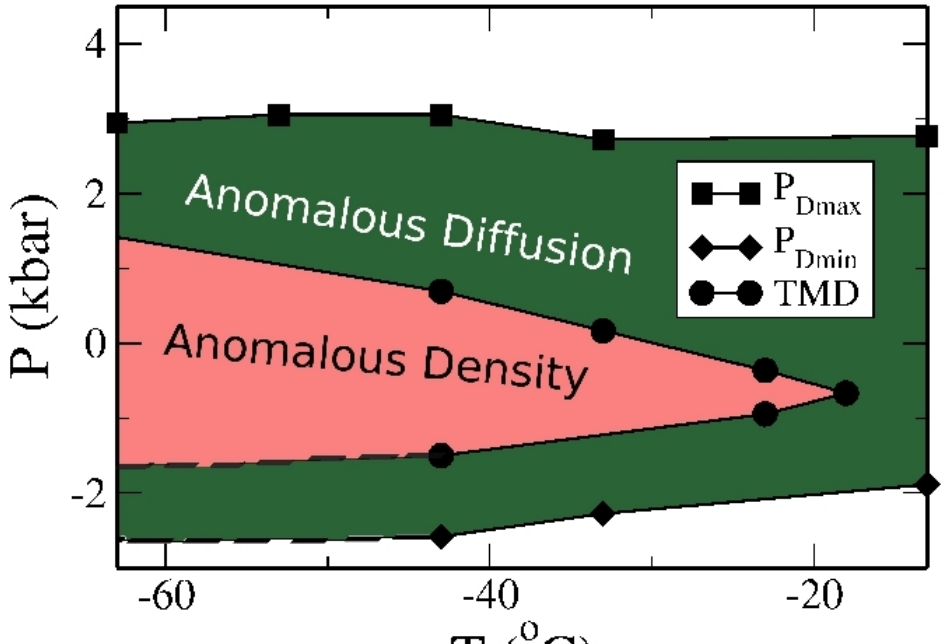


Water SPC/E

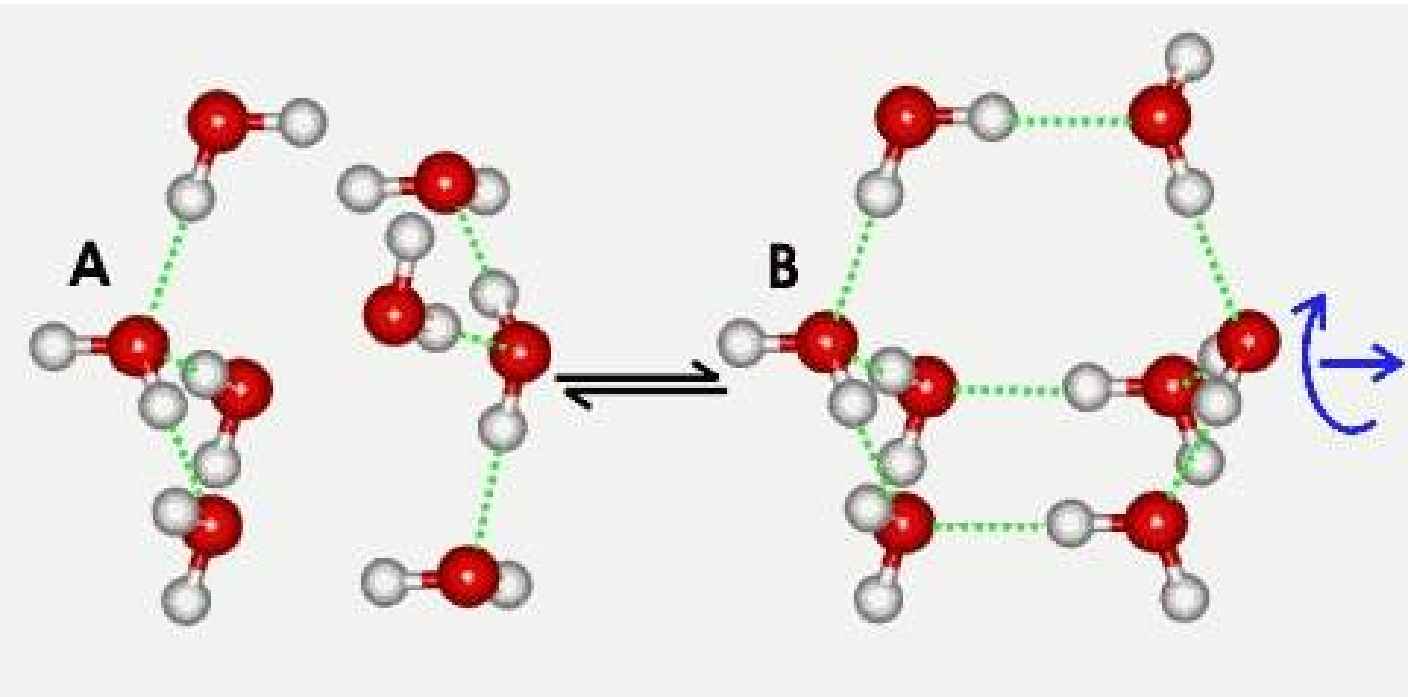
Angell, Finch, Bach 65, 3063 (76)

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



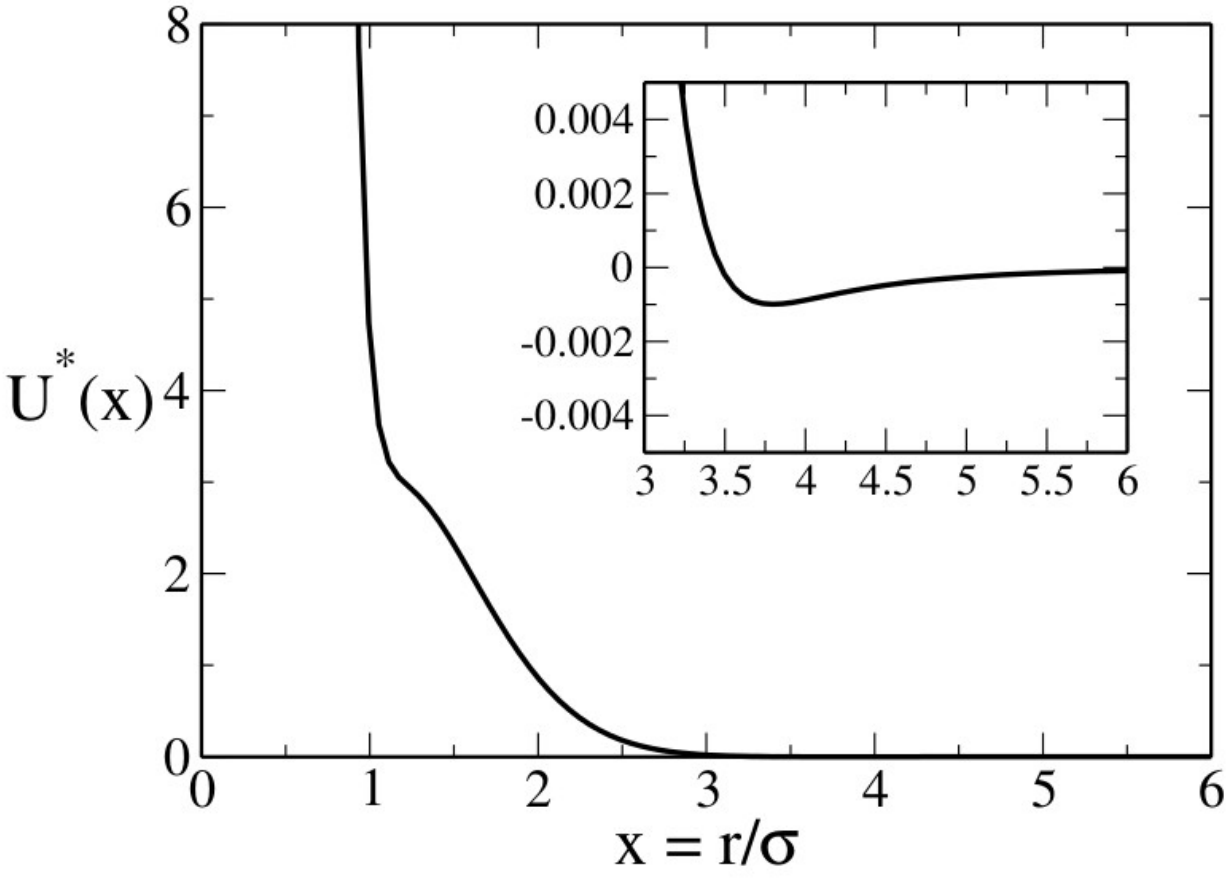


Two Scales



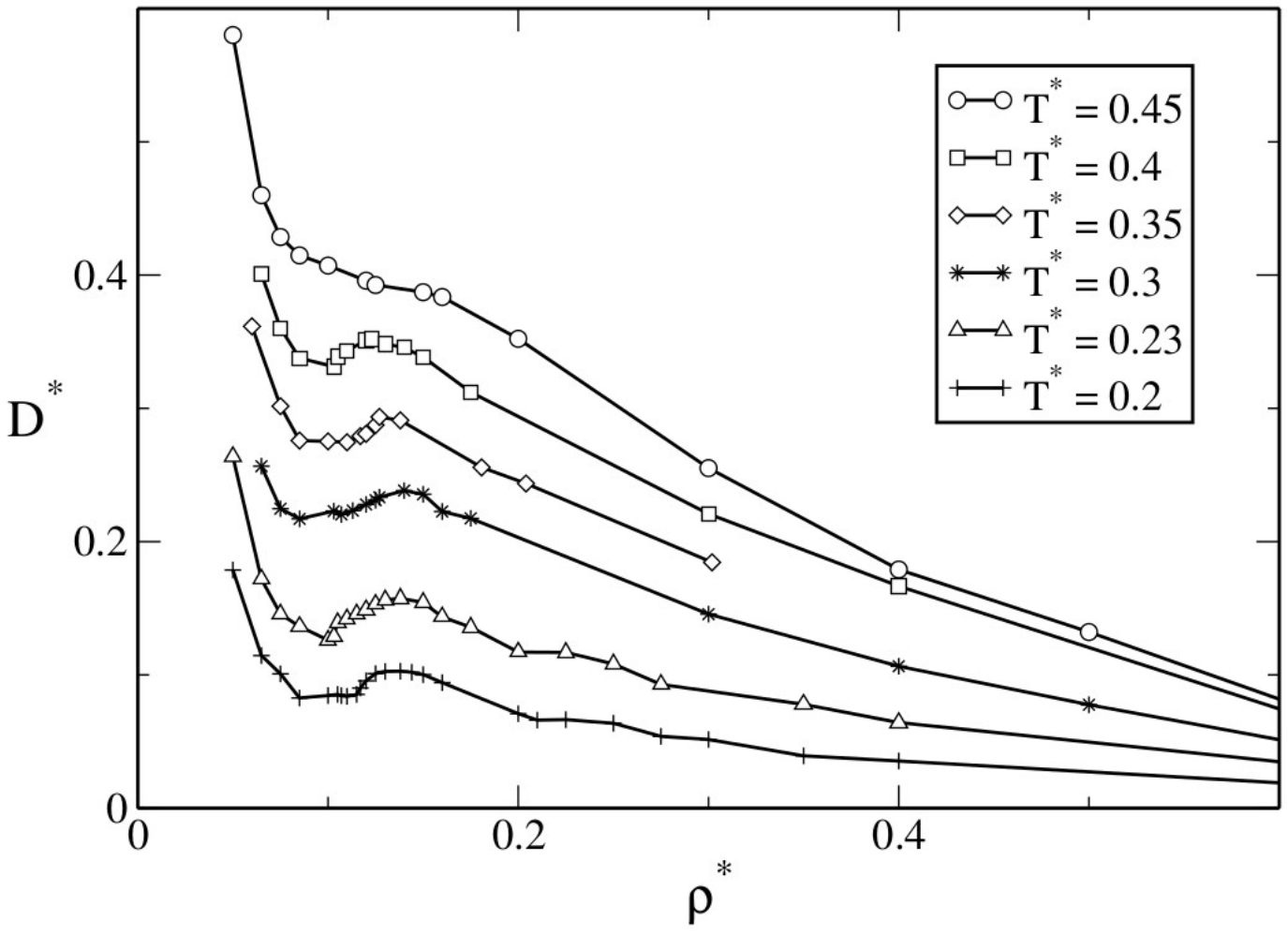
Effective Potential

A. B. de Oliveira, P. Netz and MCB JCP 124, 84505 (2006)



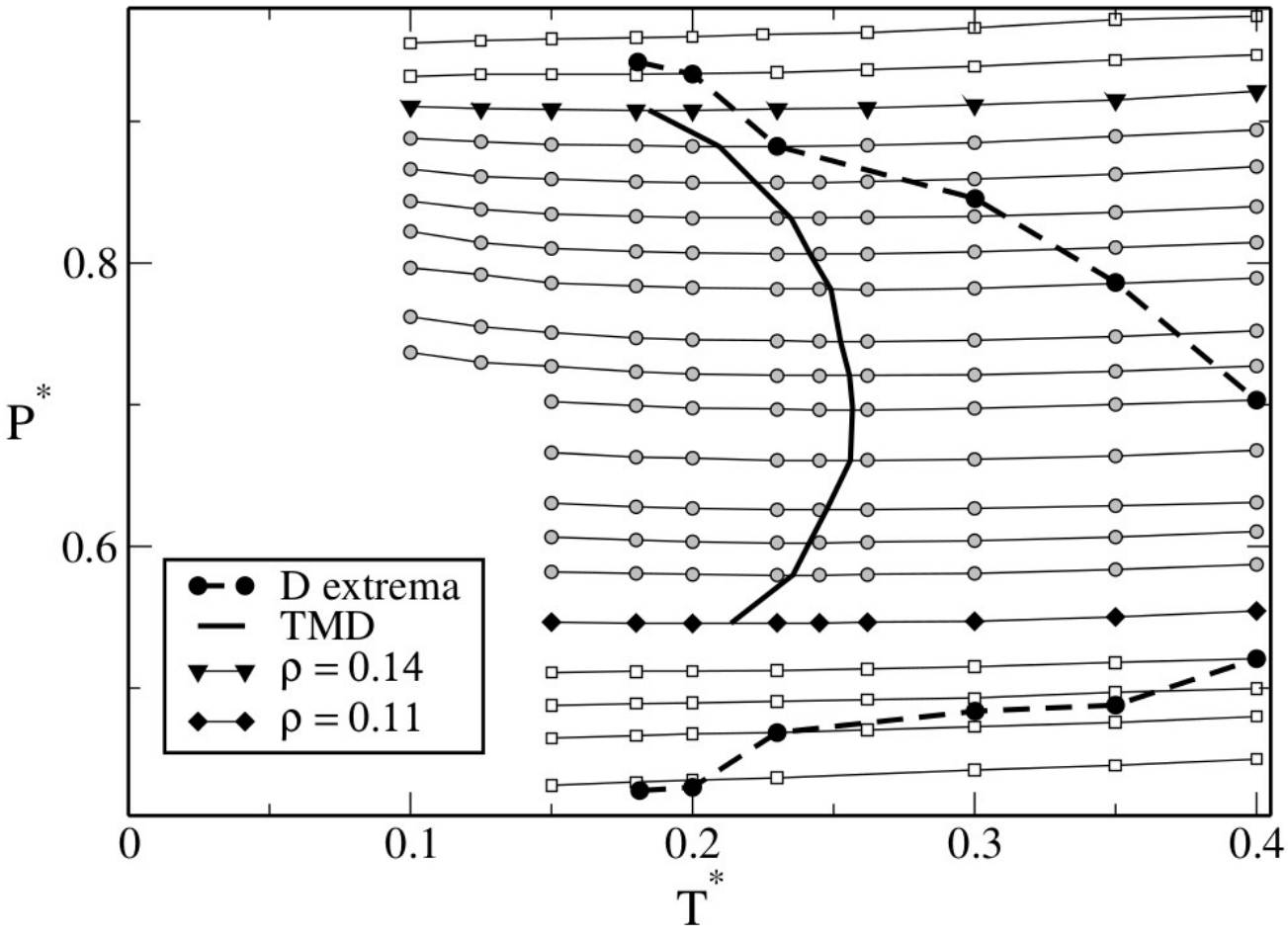
Bulk Diffusion

A. B. de Oliveira, P. Netz and MCB JCP 124, 84505 (2006)



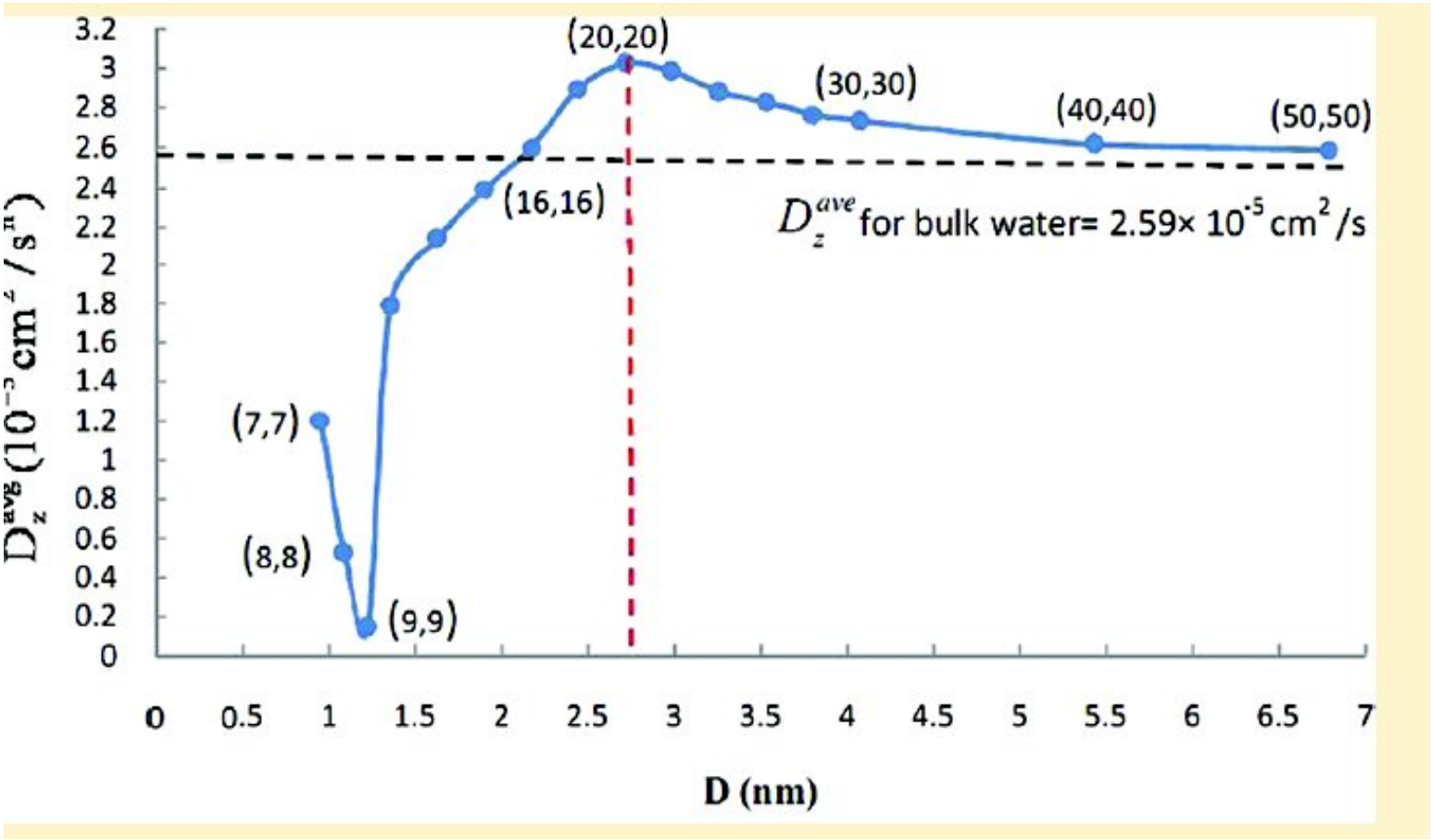
Bulk Phase Diagram

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



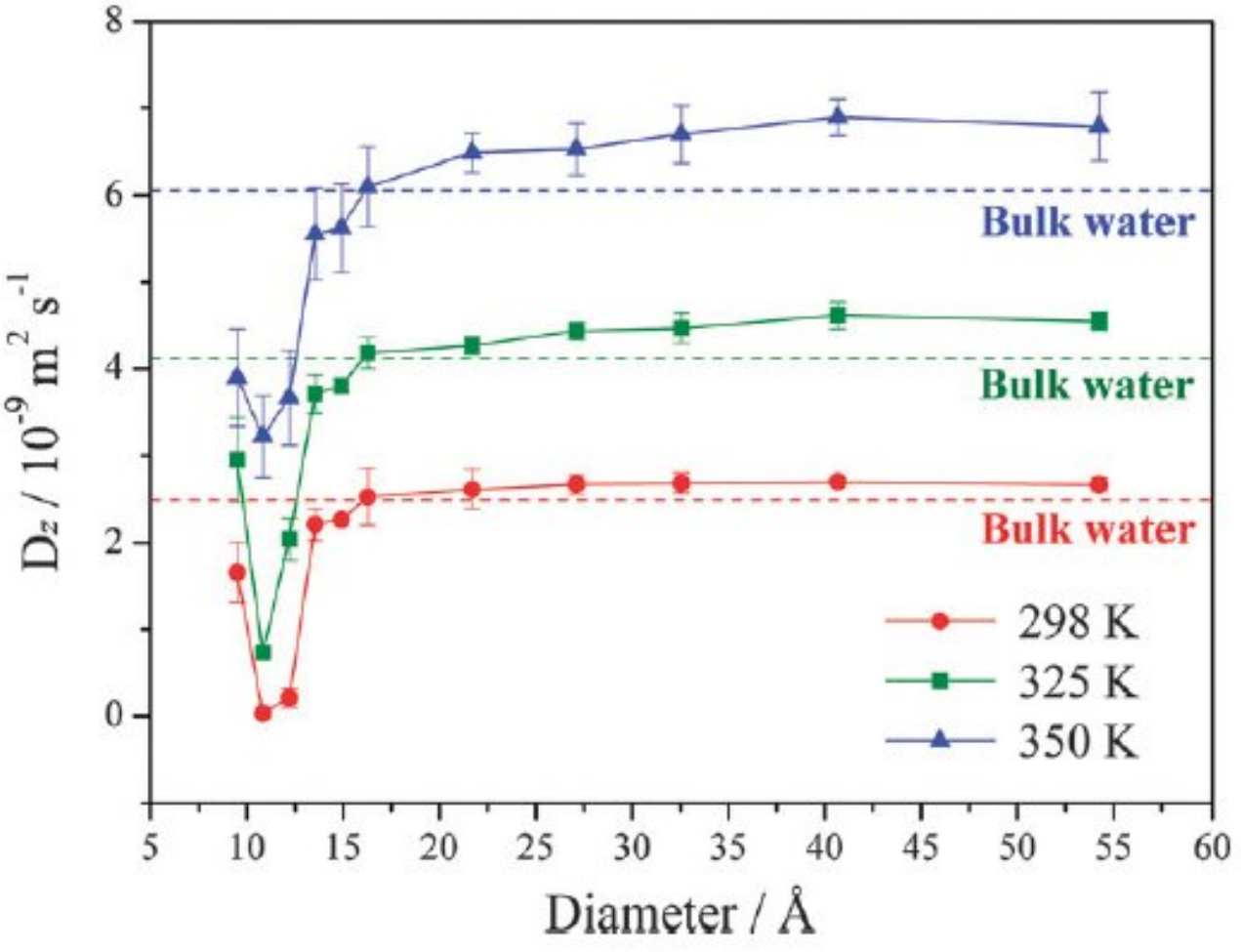
Mistery 1- Diffusion in Nanotubes

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



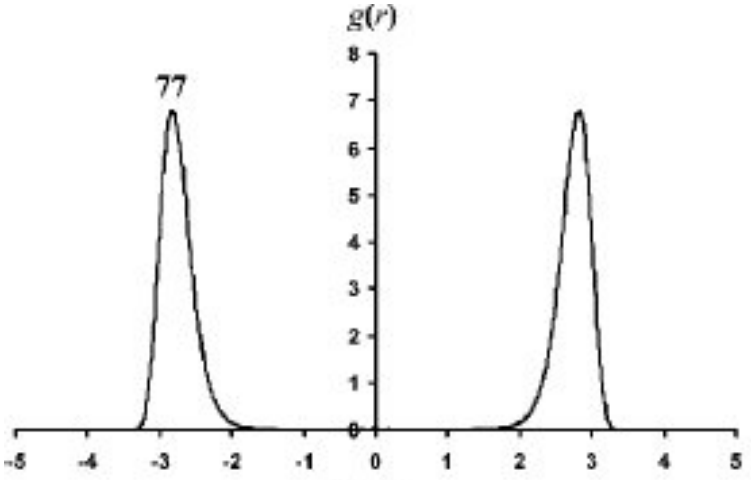
Diffusion in Nanotubes - Temperatures

Y. Zheng, PCCP 14, 964 (2012) - TIP4P-EW

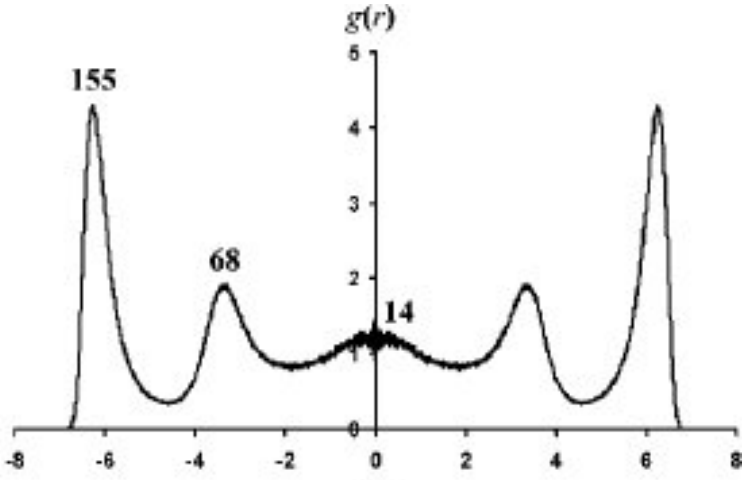


Distribution in Nanotubes - Simulations

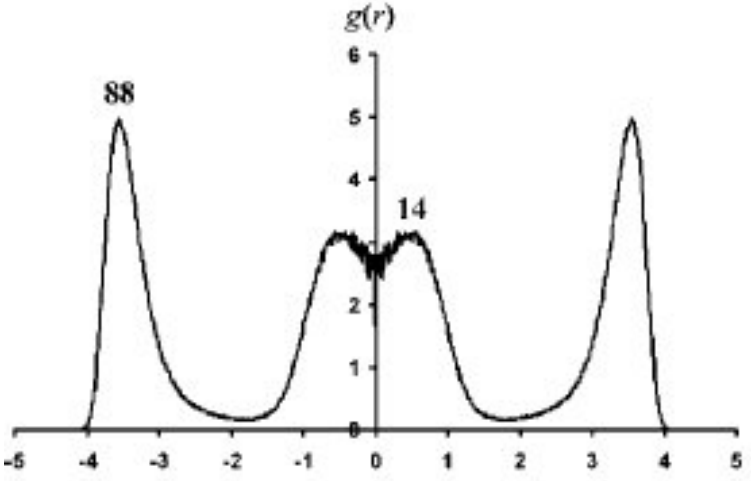
T. Nanok, JCPA 113, 2103 (2009) - SPC/E



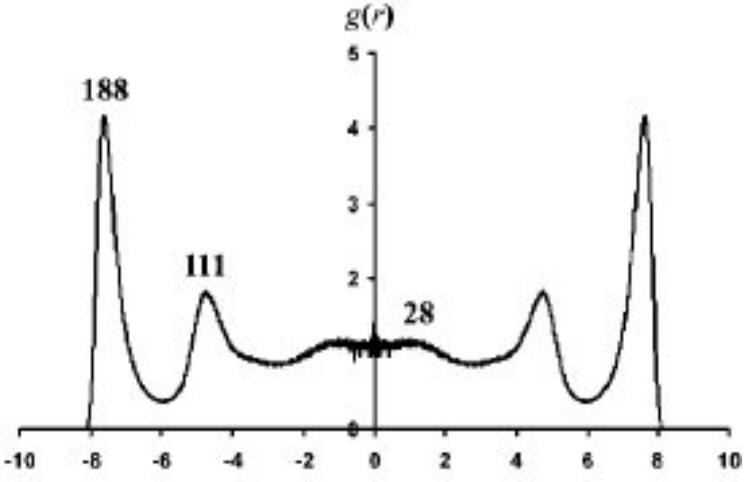
(9,9)-SWBNNT



(14,14)-SWBNNT



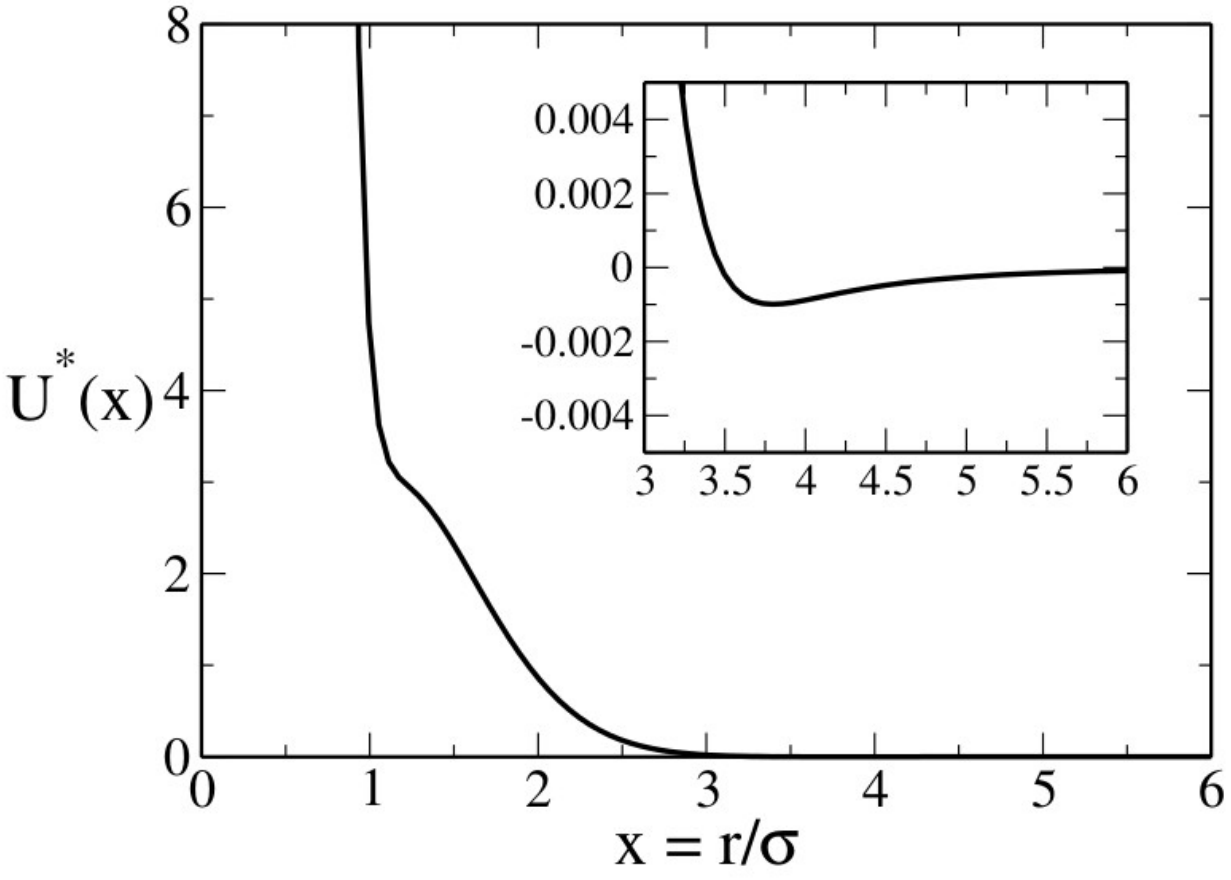
(10,10)-SWBNNT



(16,16)-SWBNNT

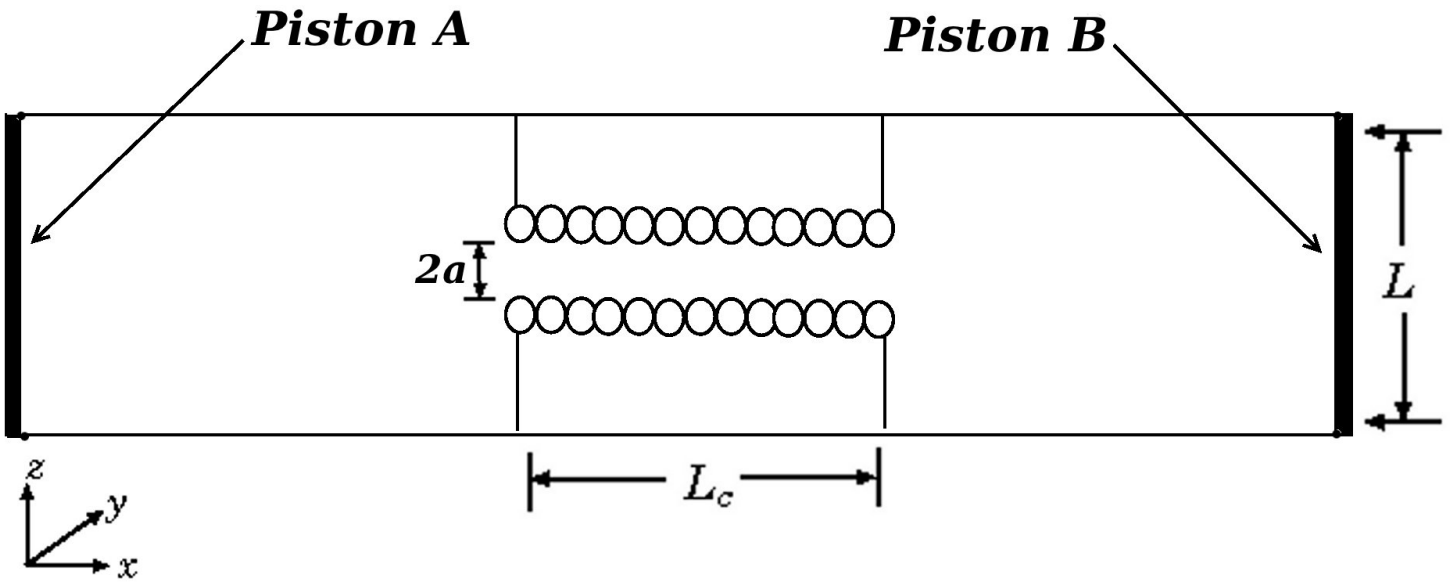
Effective Potential

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



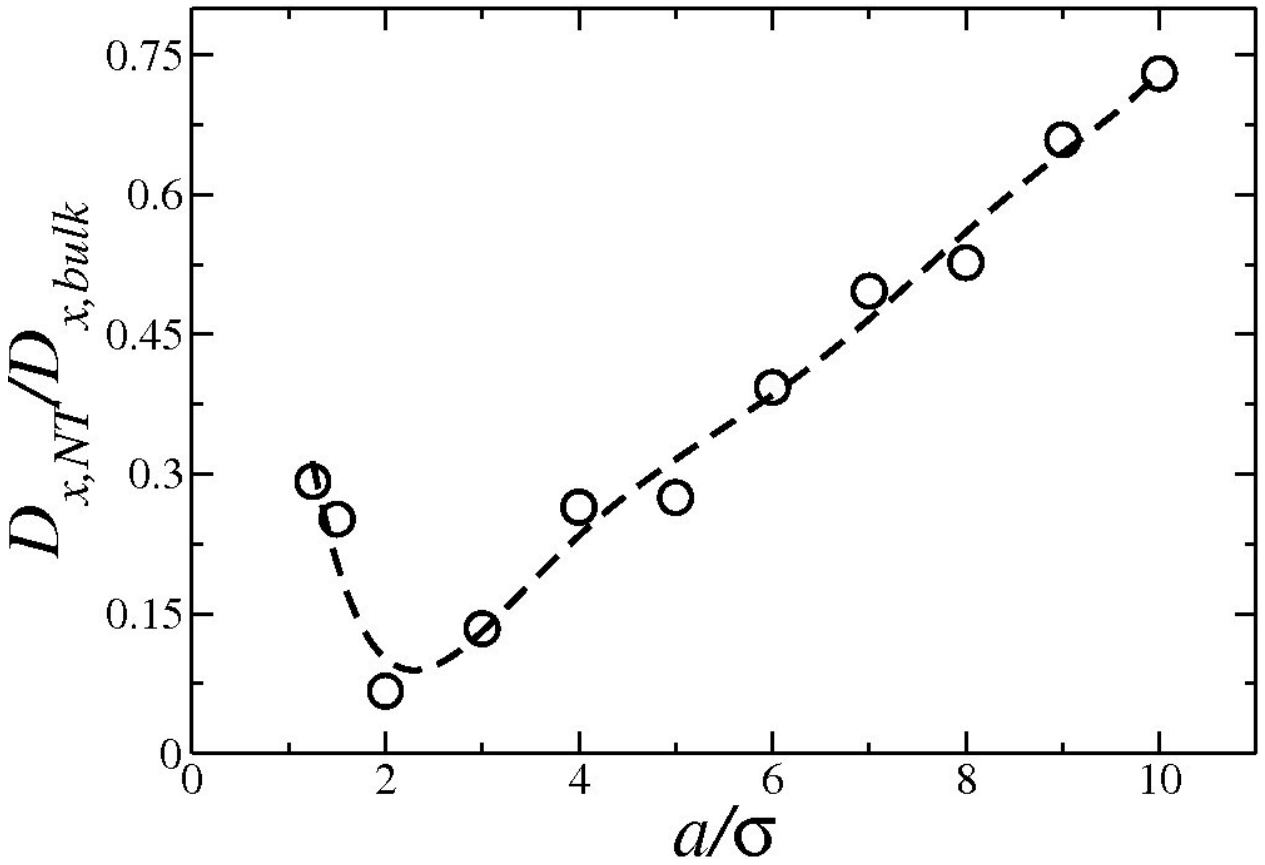
Model for Confining

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



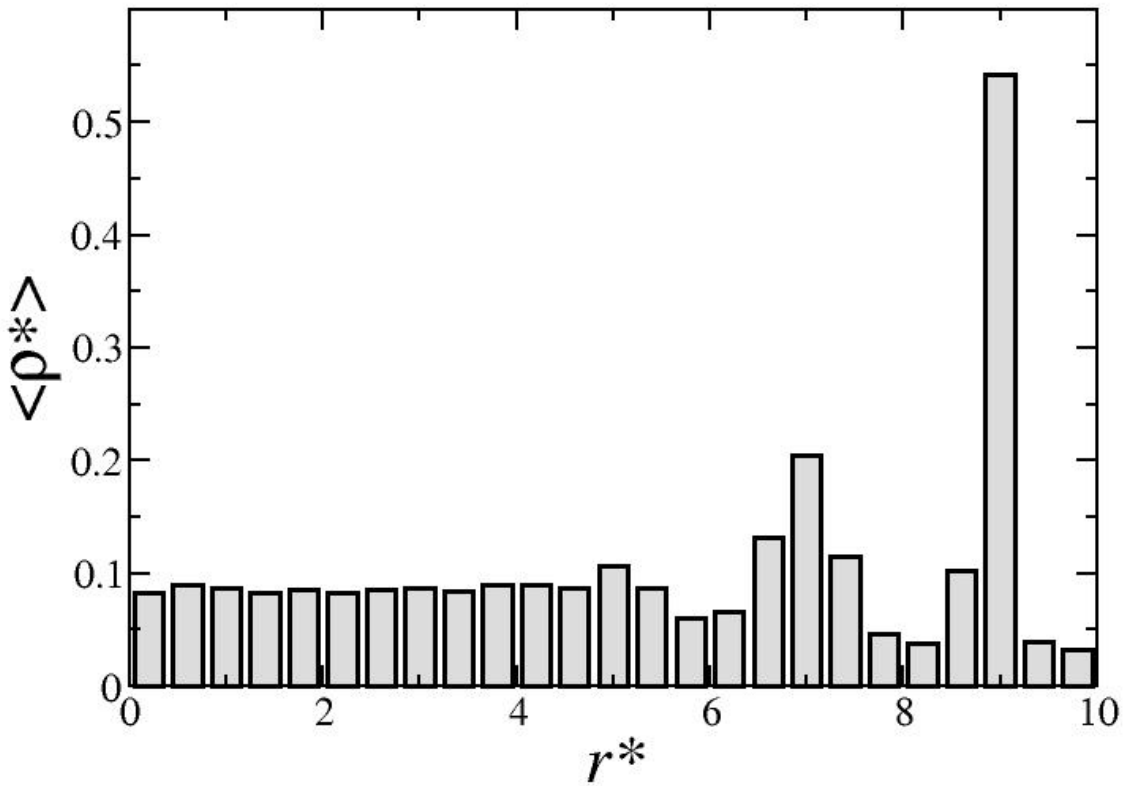
Diffusion

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



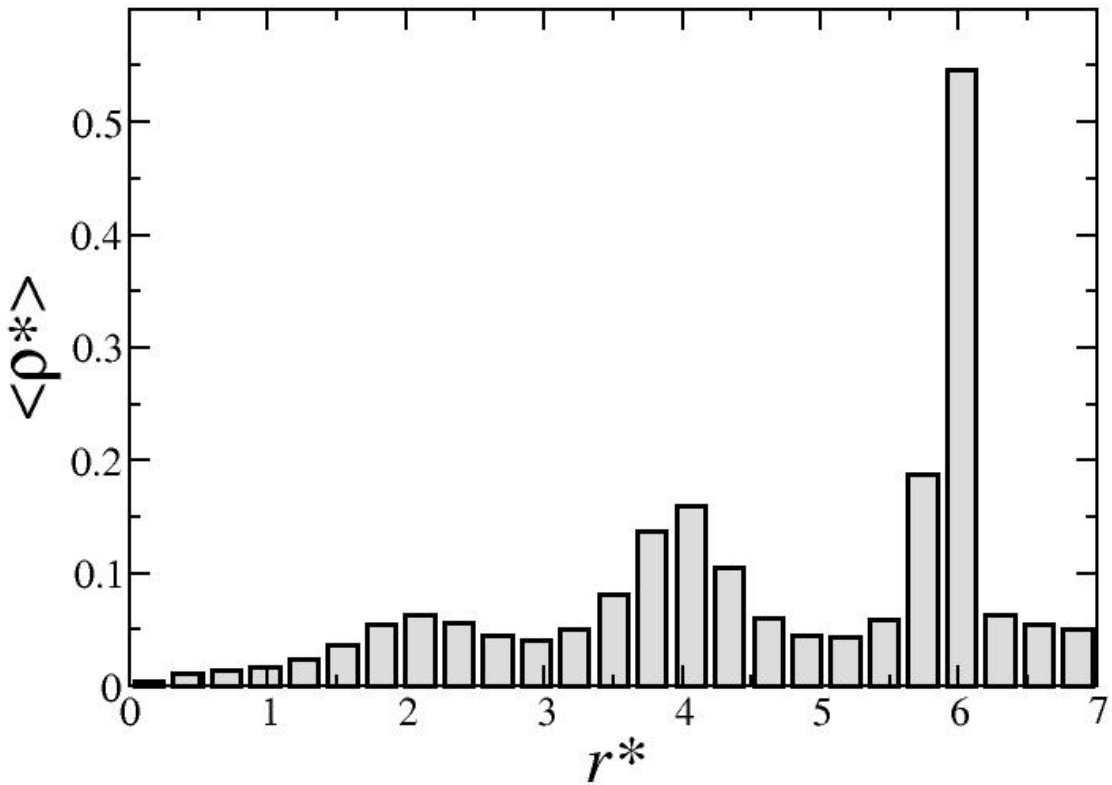
Density vs. r - a=10

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



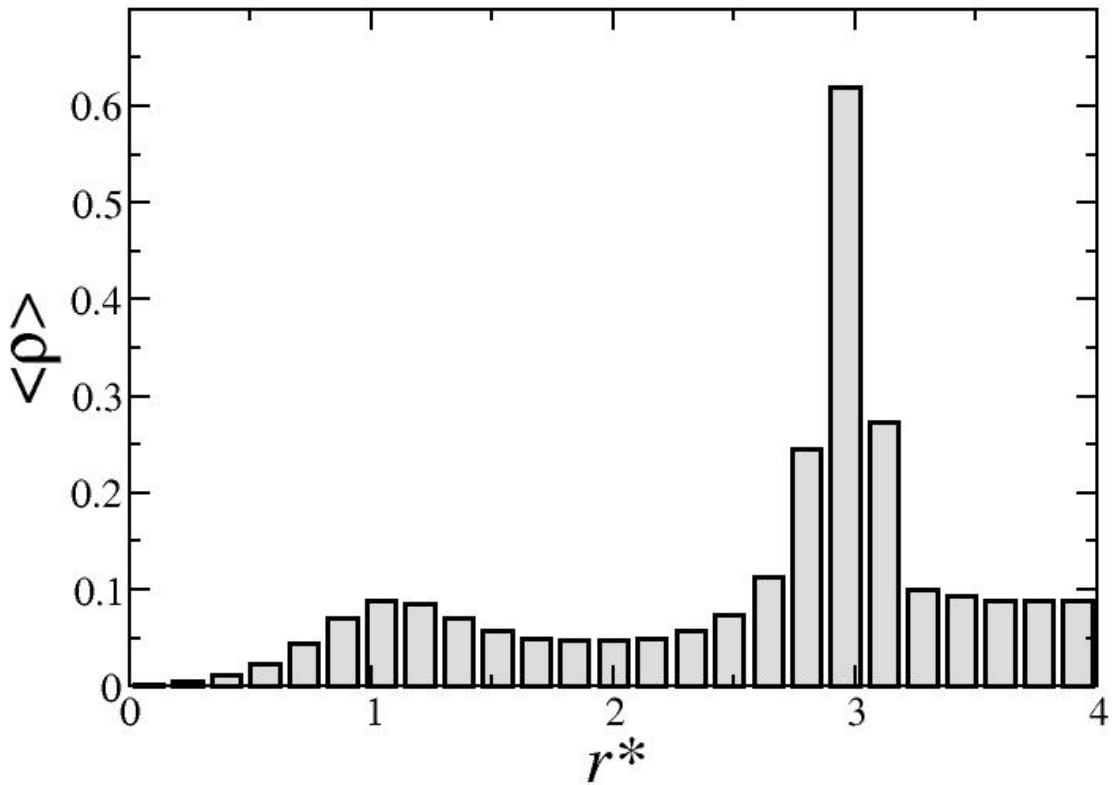
Density vs. r - a=7

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



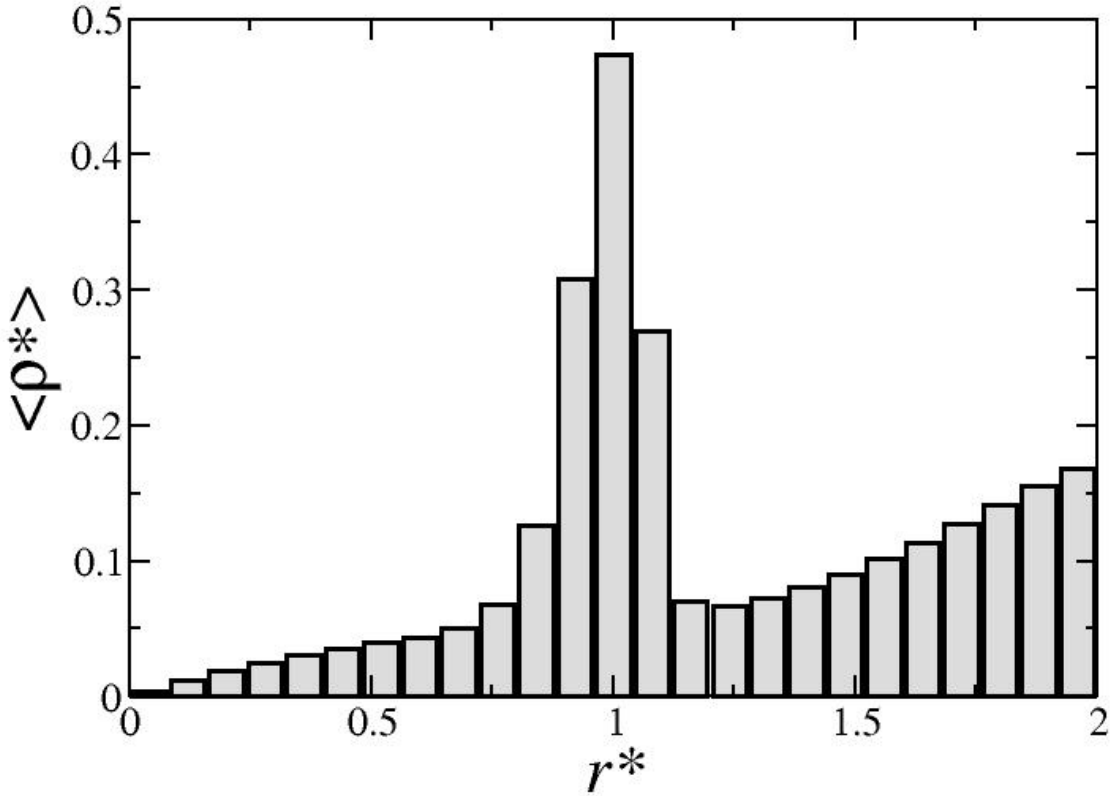
Density vs. r - a=4

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



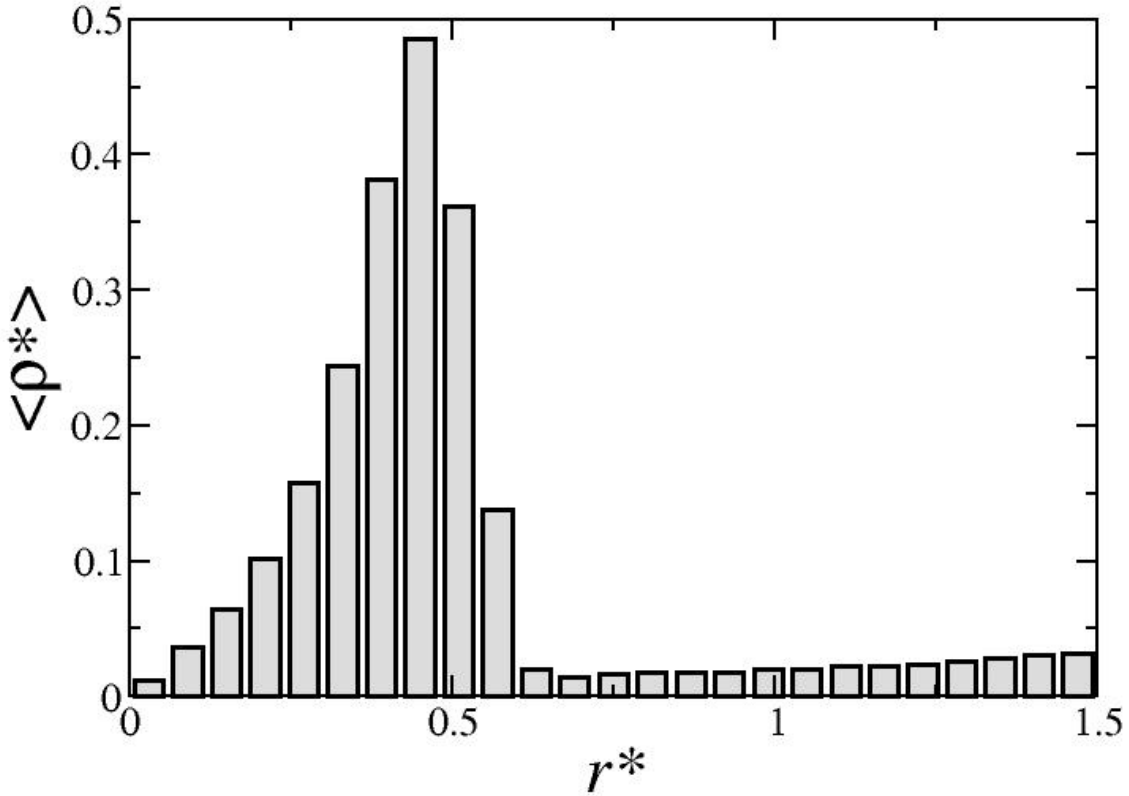
Density vs. r - a=2

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



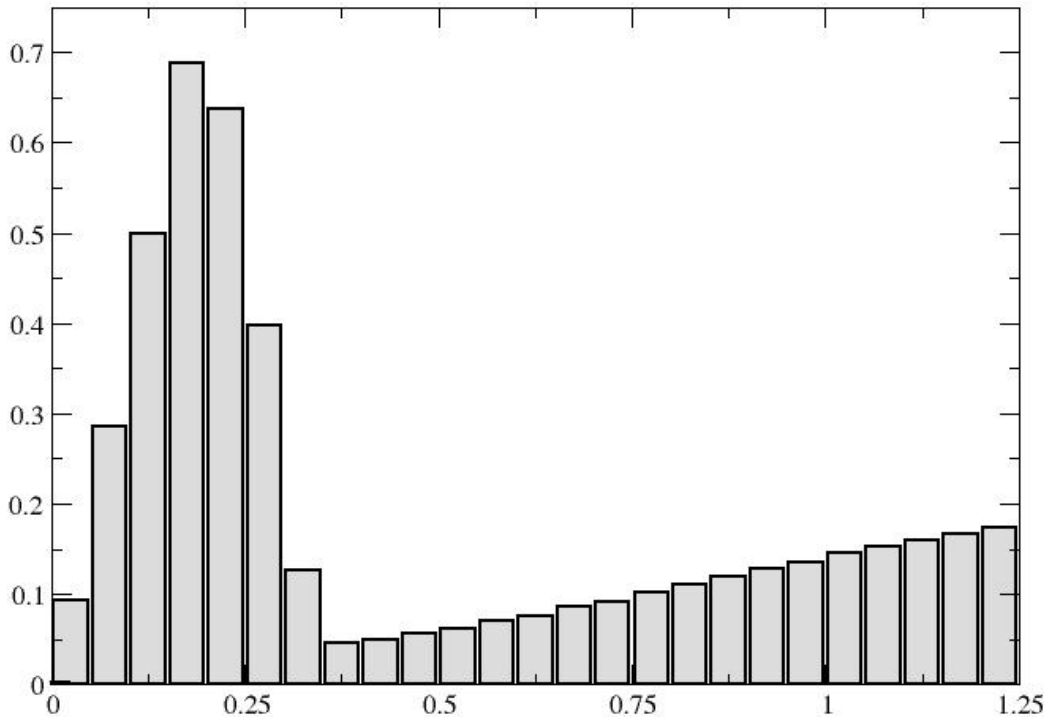
Density vs. r - a=1.5

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



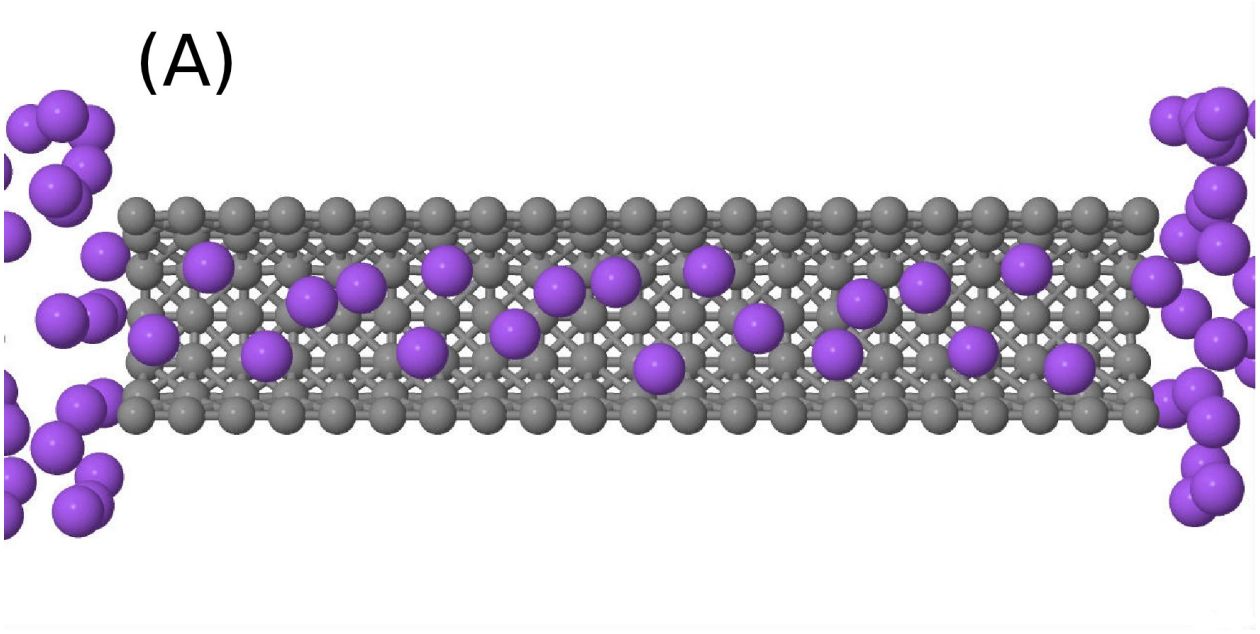
Density vs. r - a=1.25

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



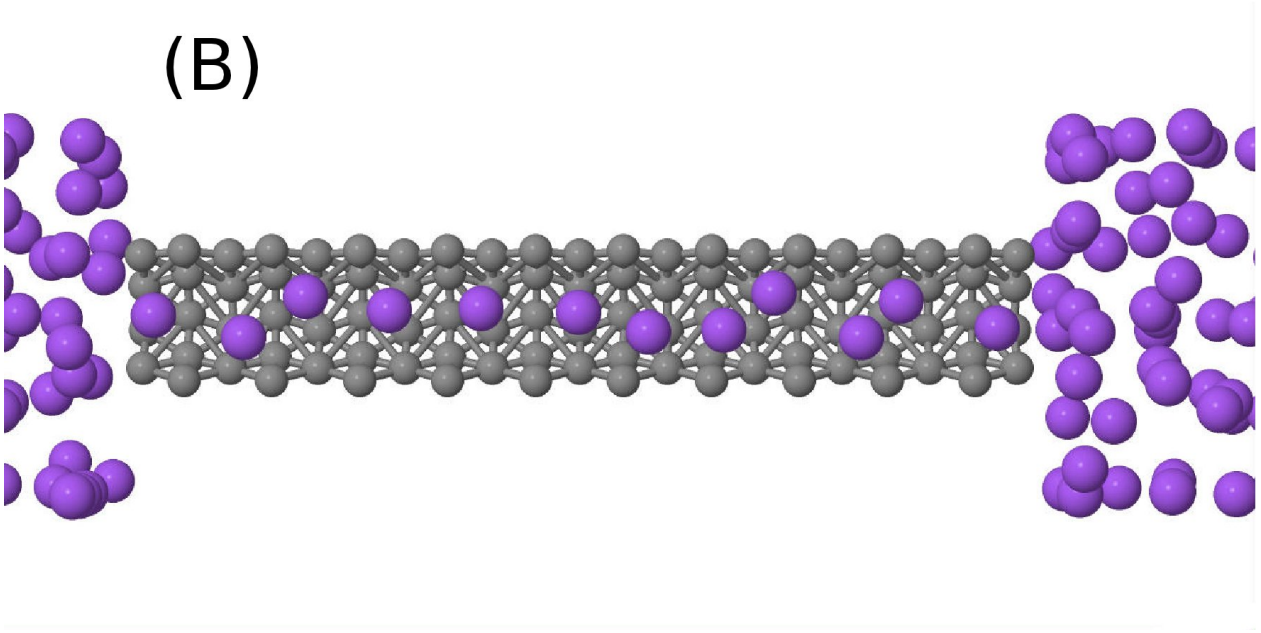
Density vs. r - a=1.25

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



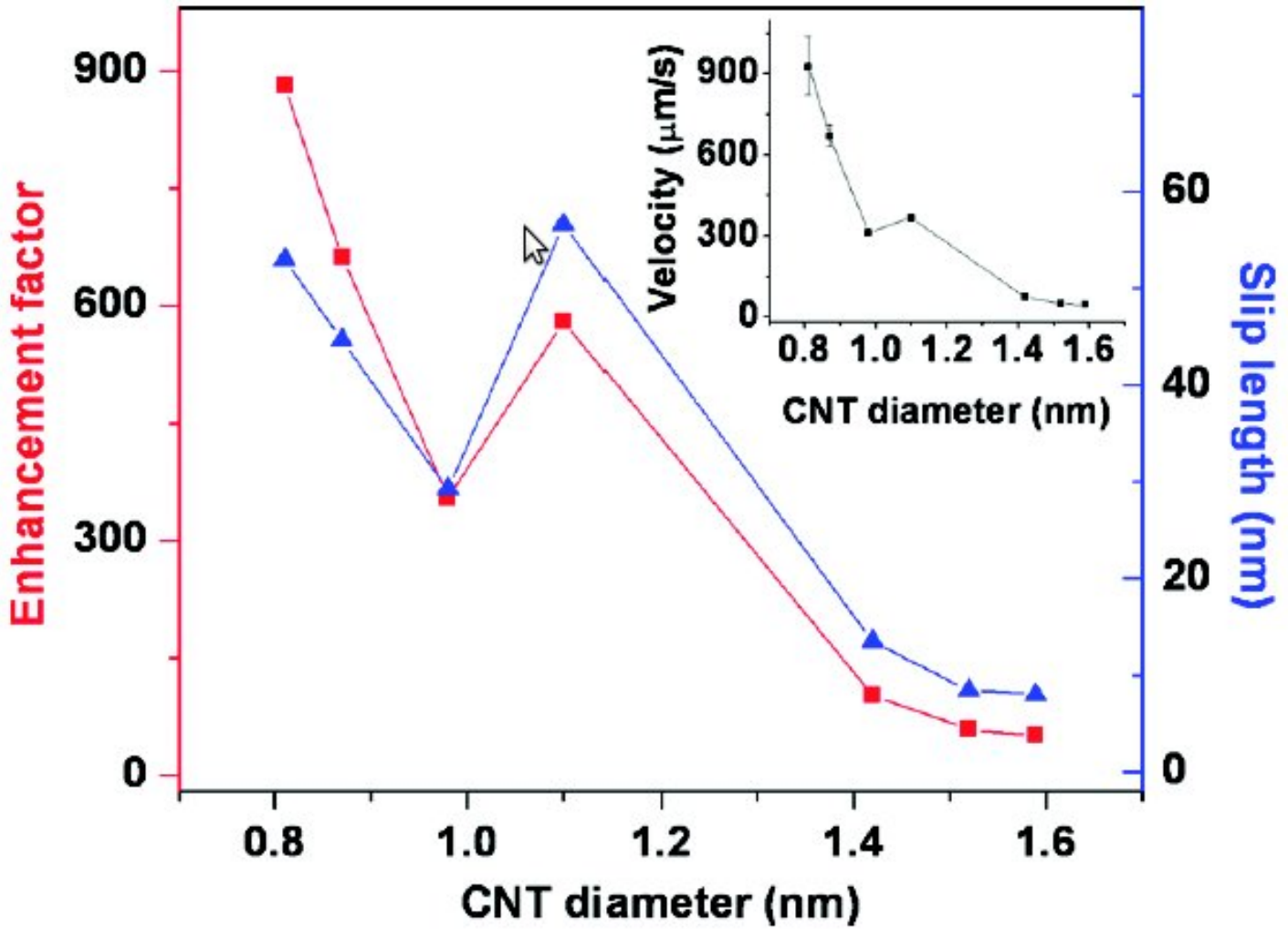
Density vs. r - a=1.25

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



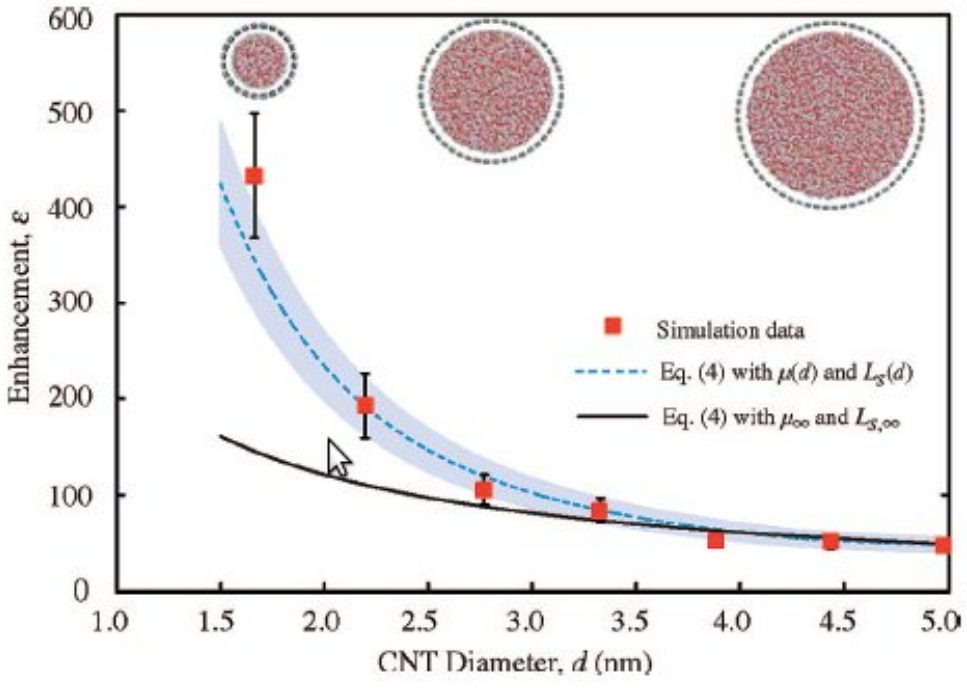
Flux in Nanotubes

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



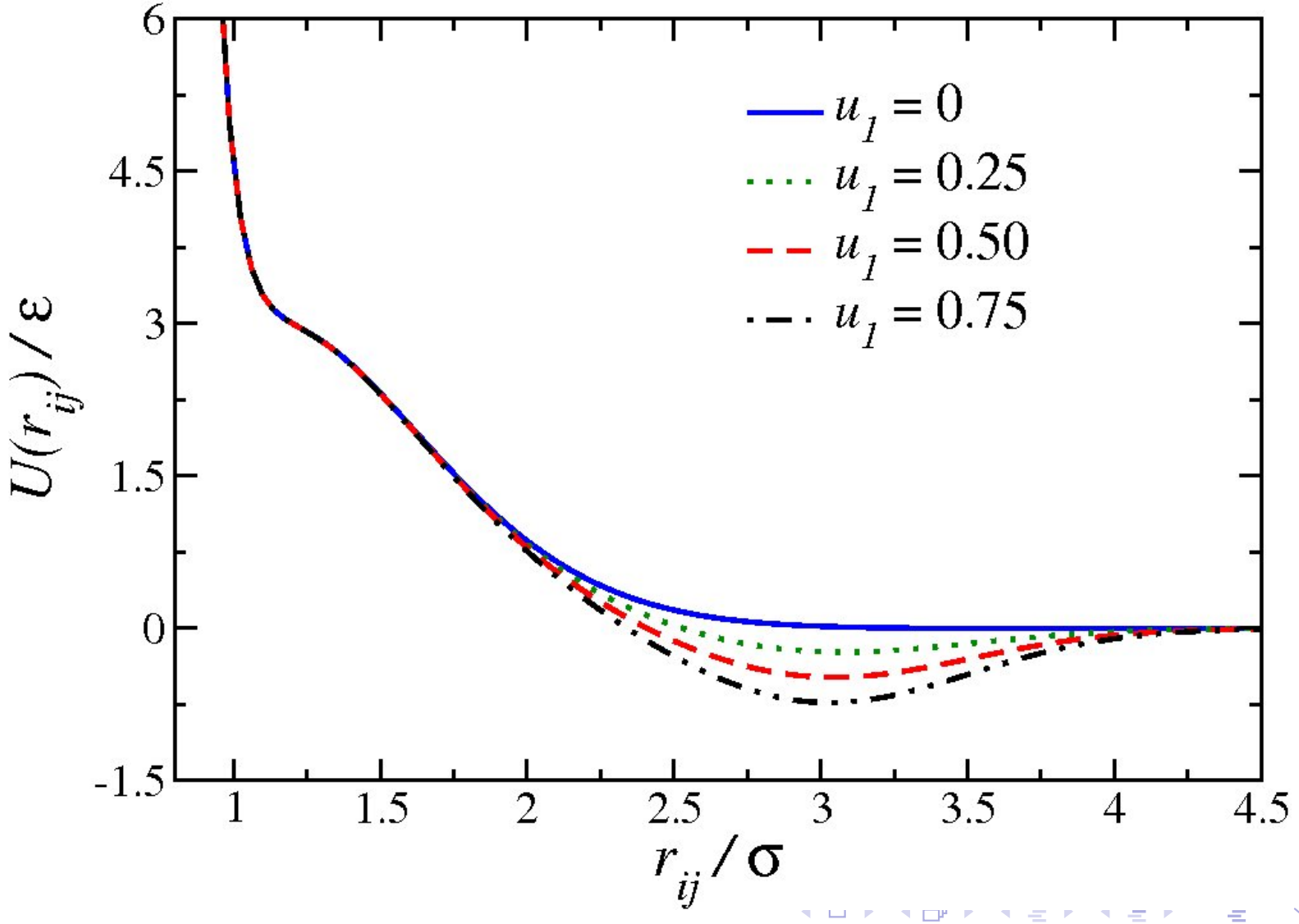
Water Channel - Enhancement Flow

J. A. Thomas and A. J. H. McGaughey, Nanoletters 8, 2788 (2008)



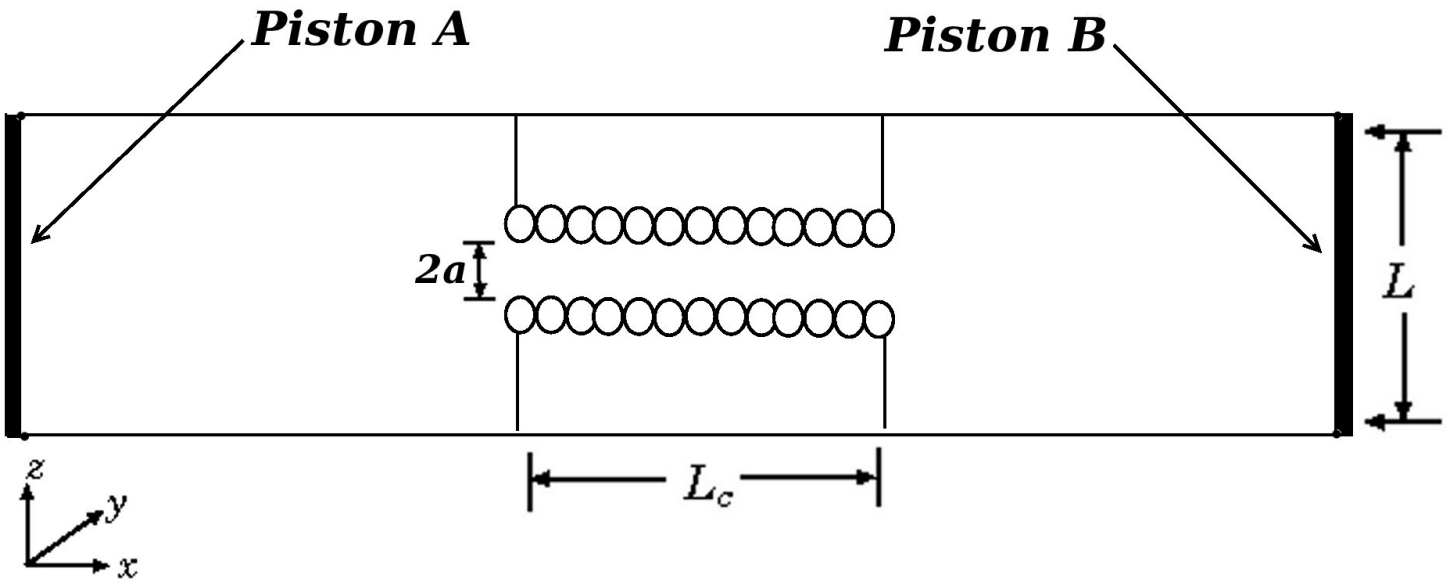
Effective Potential

J. da Silva and MCB, JCP (2010)



Model for Nanotubes

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



Enhancement Flow

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

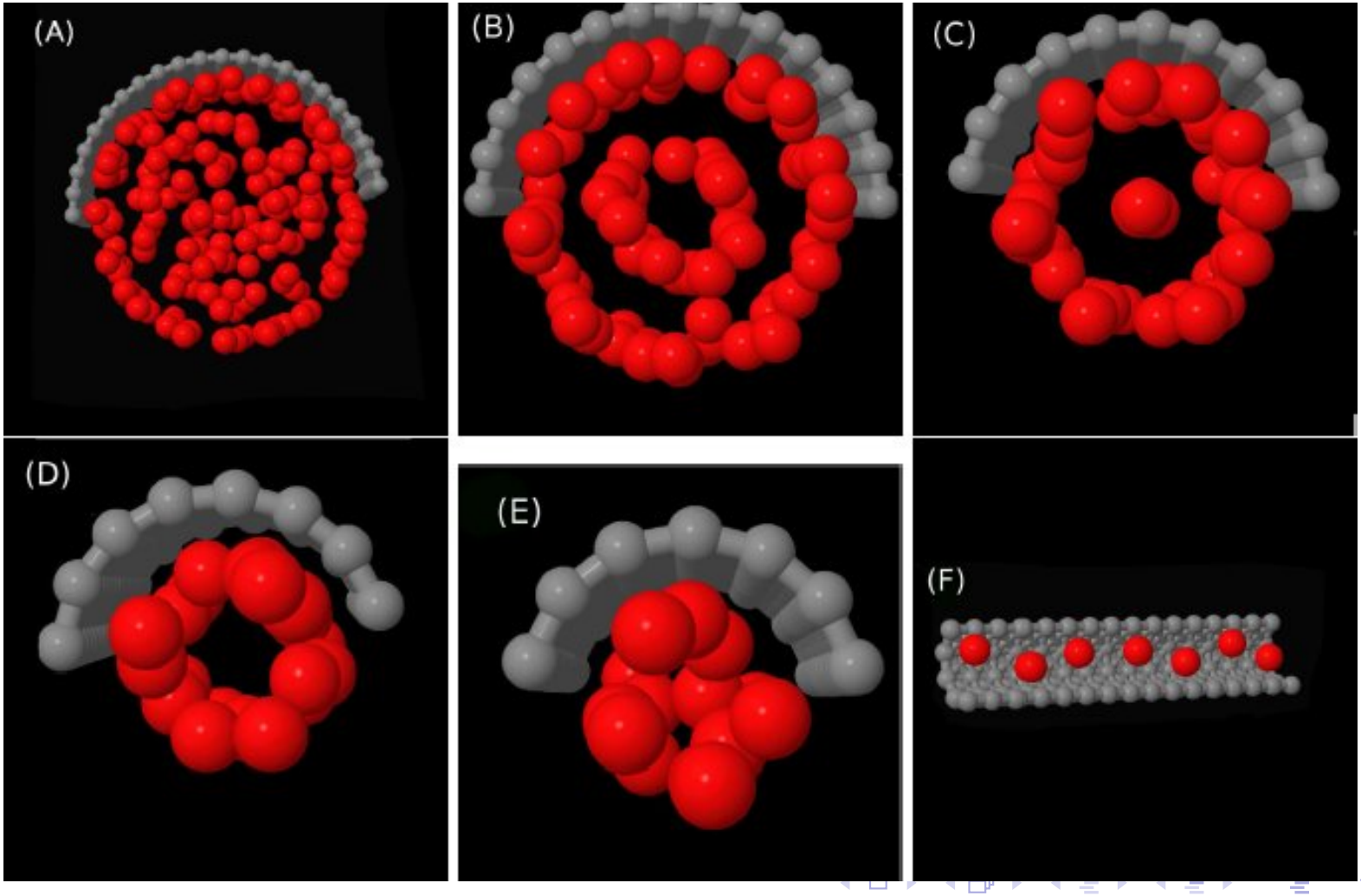
$$\begin{aligned} \langle v_x \rangle &= \gamma_{HP} \frac{\Delta p}{L_{NT}} \\ \gamma_{HP} &= \frac{a^2}{8\eta} \\ \eta &= \frac{k_B T}{3\pi\sigma D_x} \end{aligned}$$

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

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

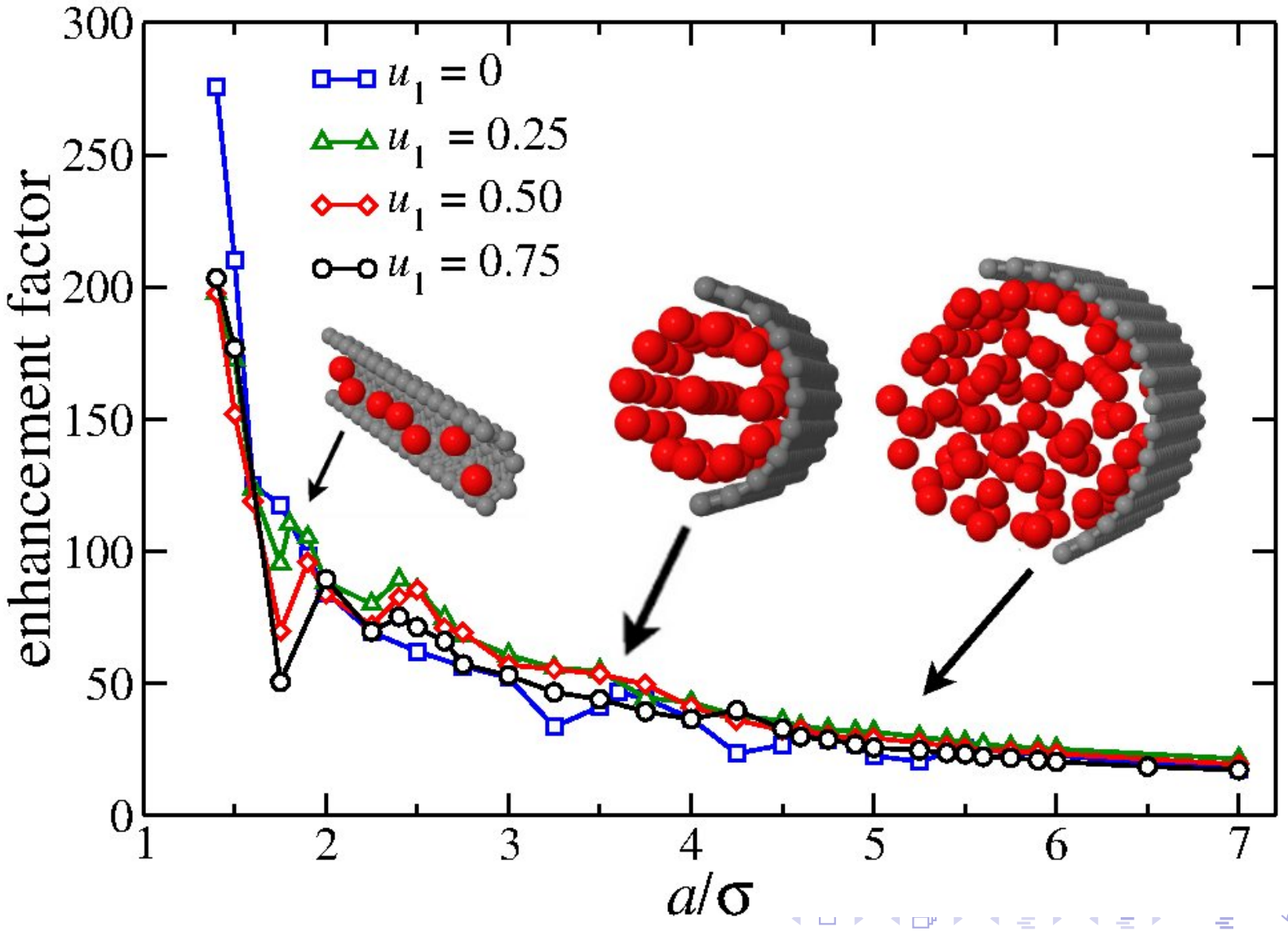
Layers

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



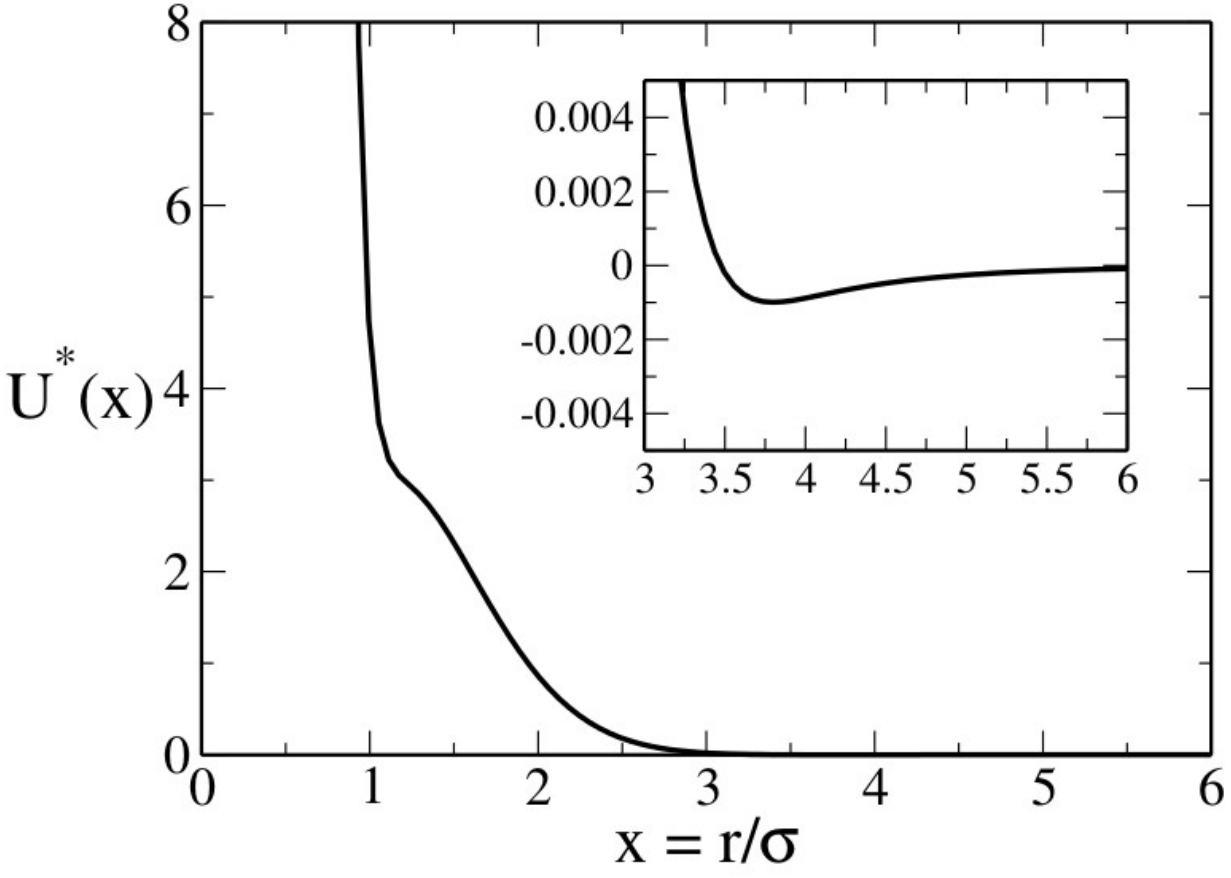
Enhancement Flow

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



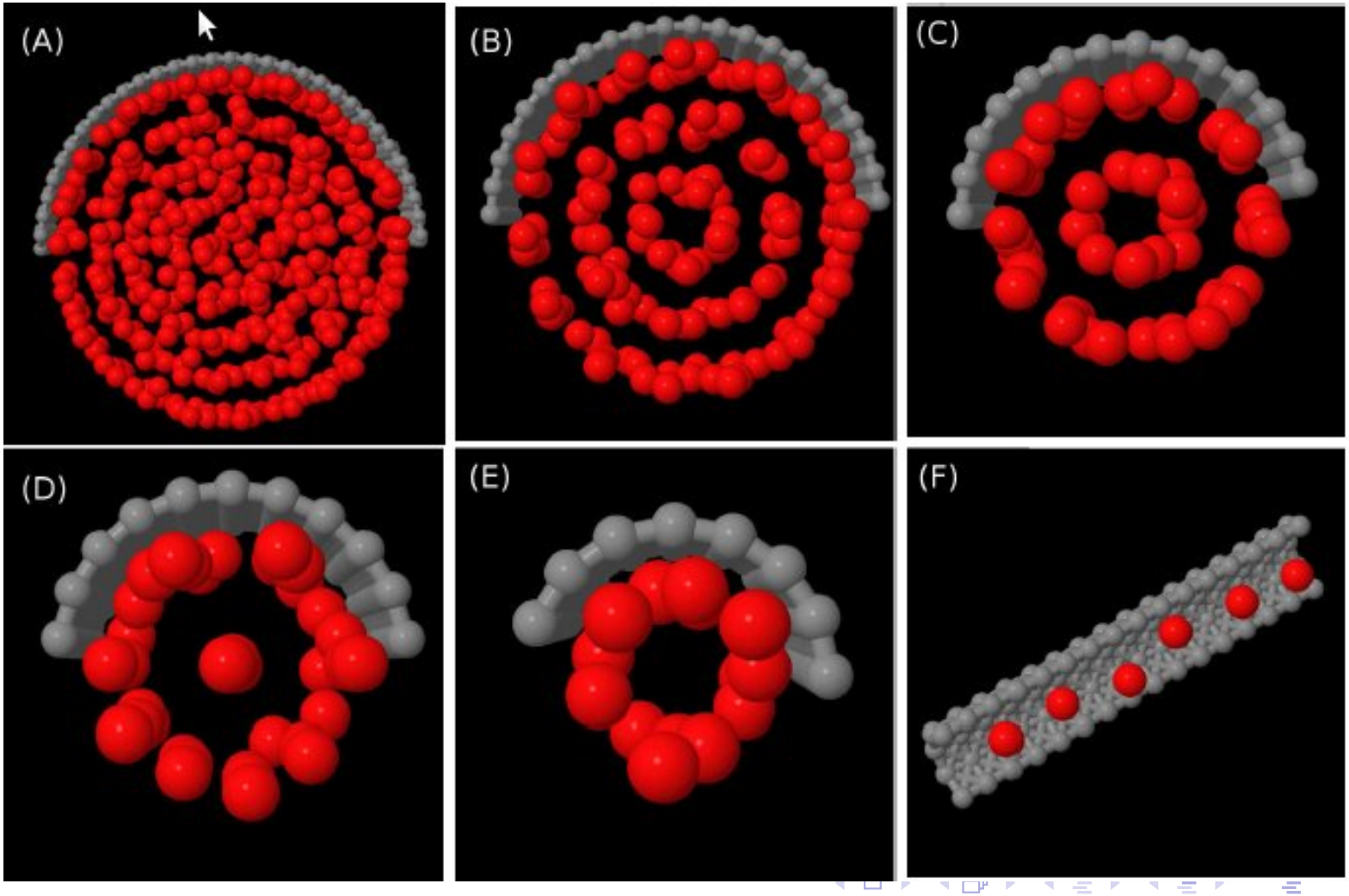
Potential

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



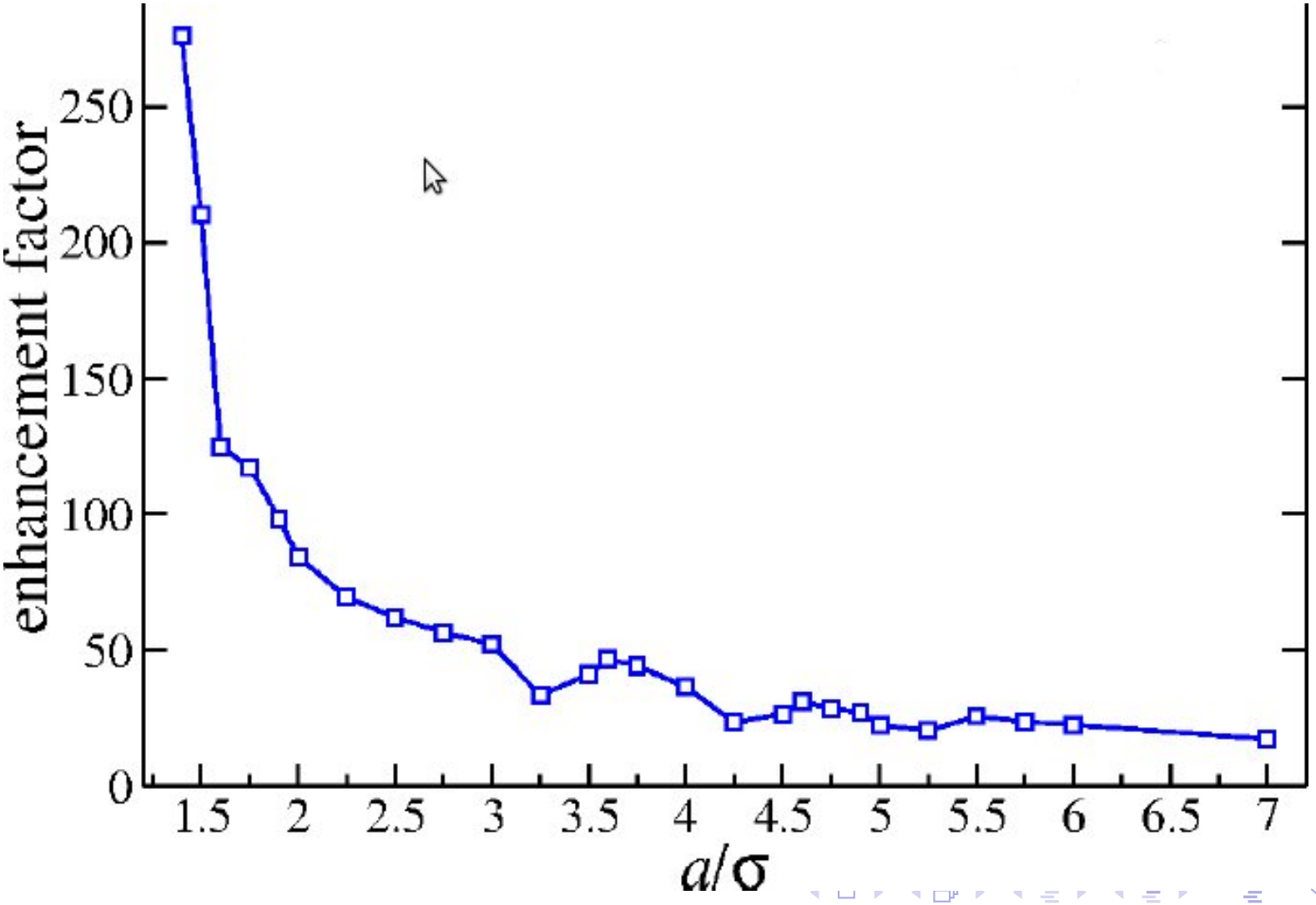
Layers

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



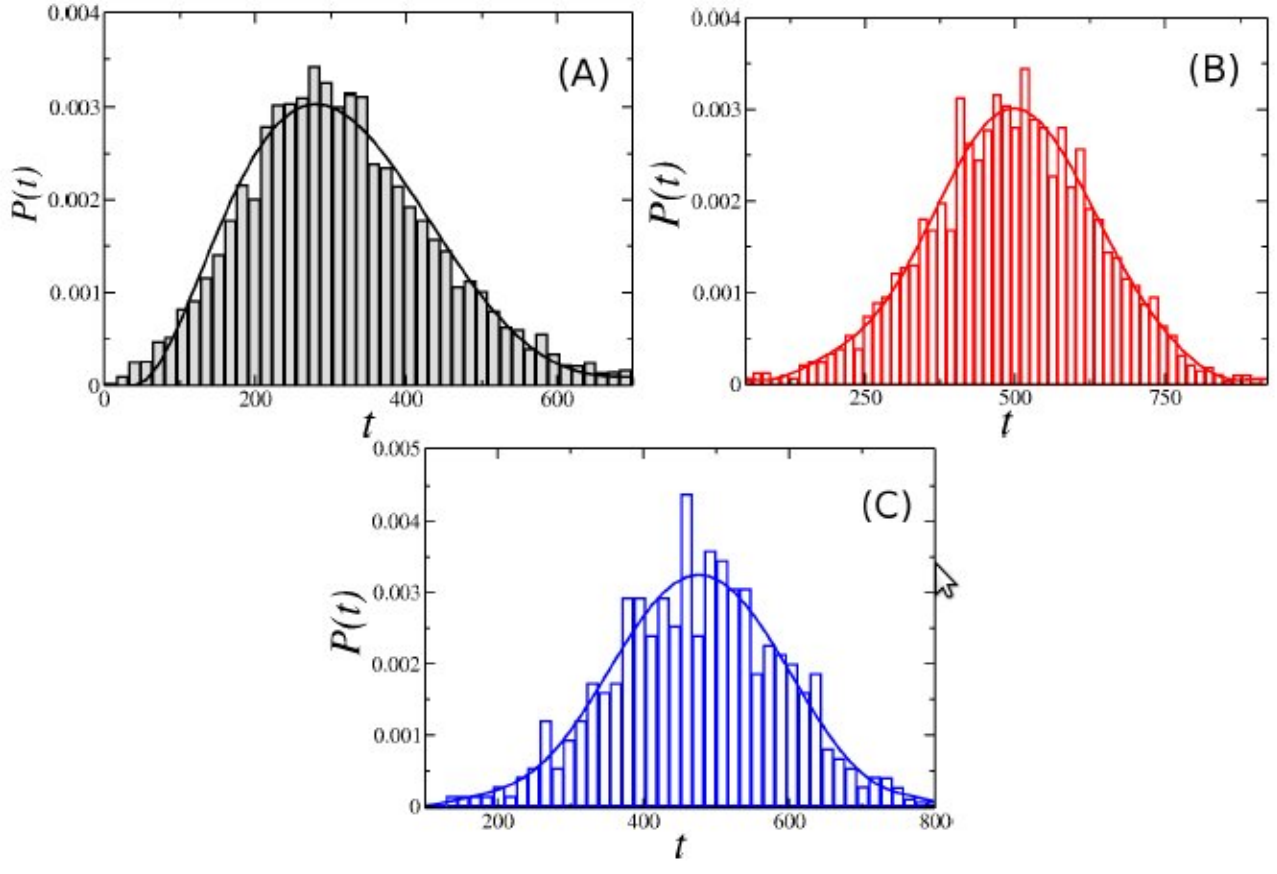
Enhancement Flow

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



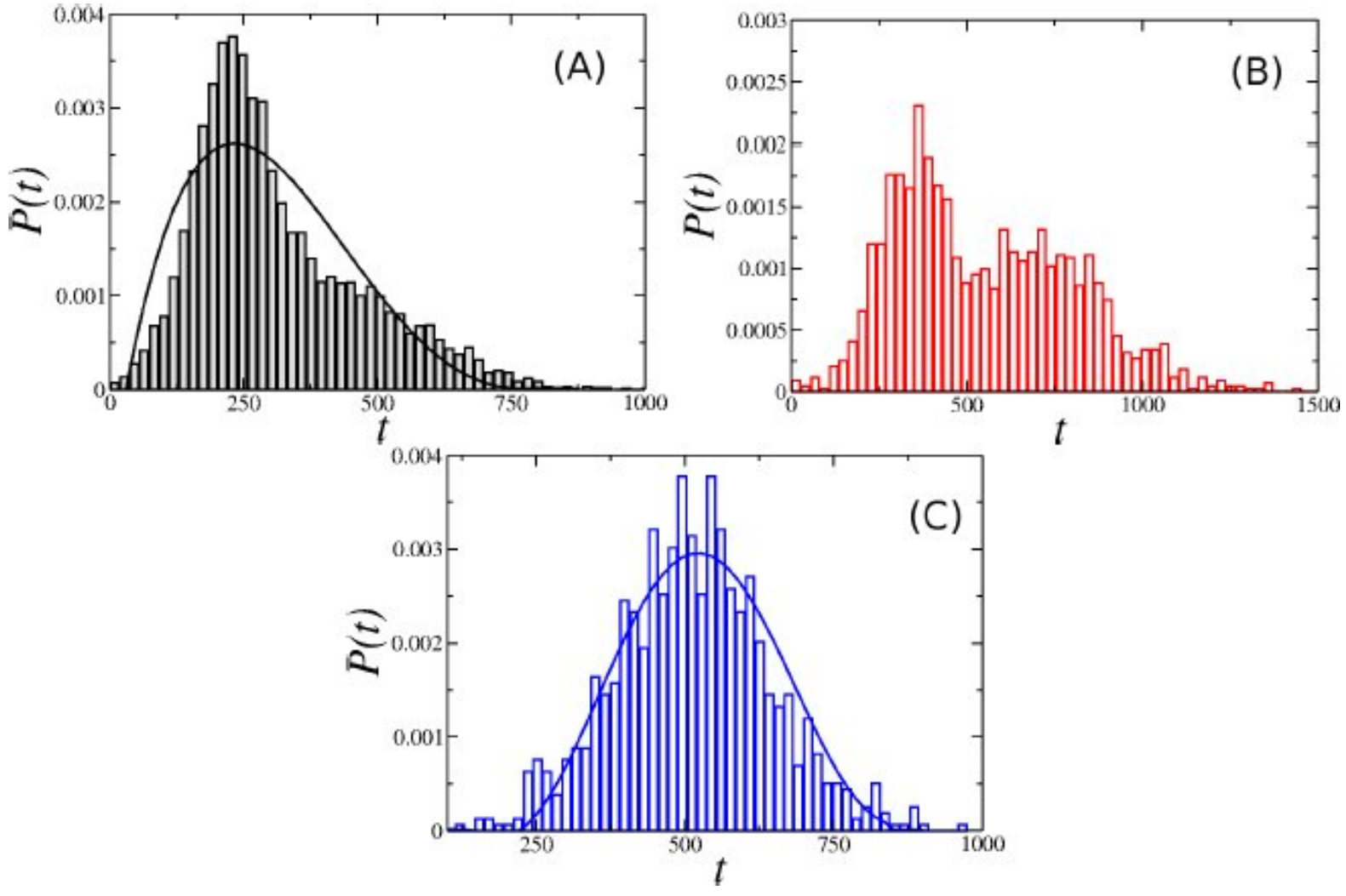
Distribution - Attractive

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



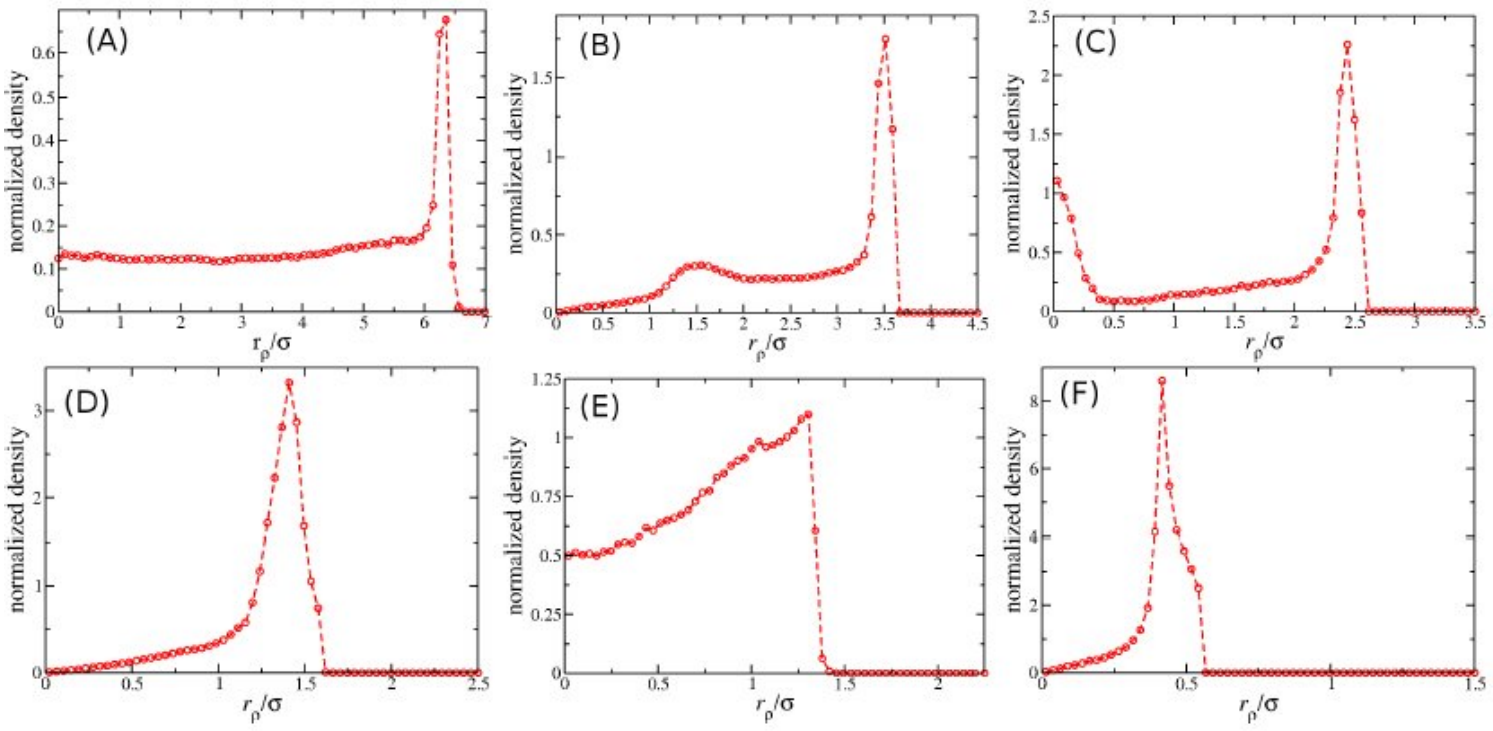
Distribution - Repulsive

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



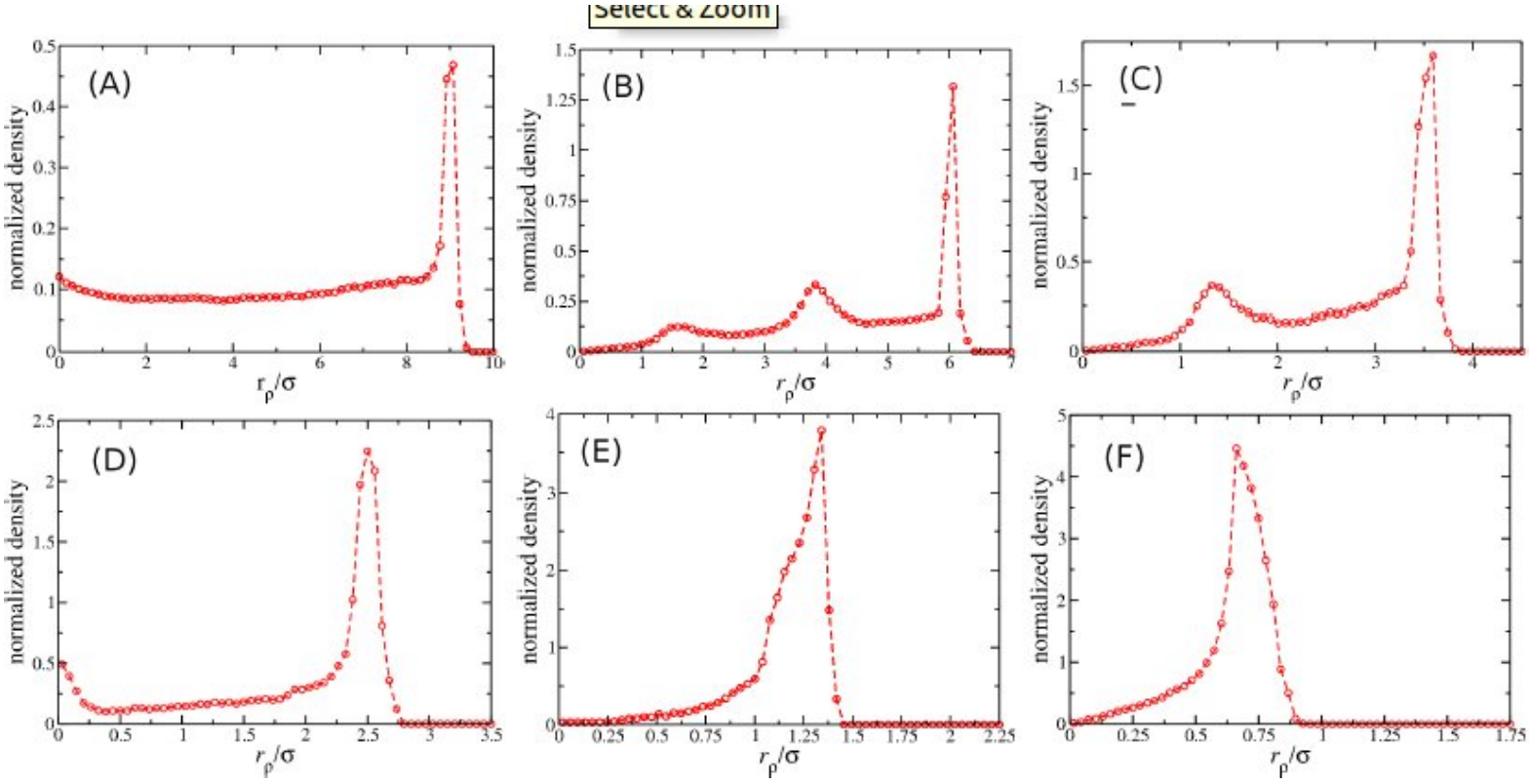
Density - Attractive

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



Density - Repulsive

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



Conclusions

- Diffusion increases
- Enhancement Flow
- Layering