Molecular Probes Used to Elucidate the Thermodynamics of Nanoparticle Diffusion

Steven Fiedler

Department of Biology and Chemistry

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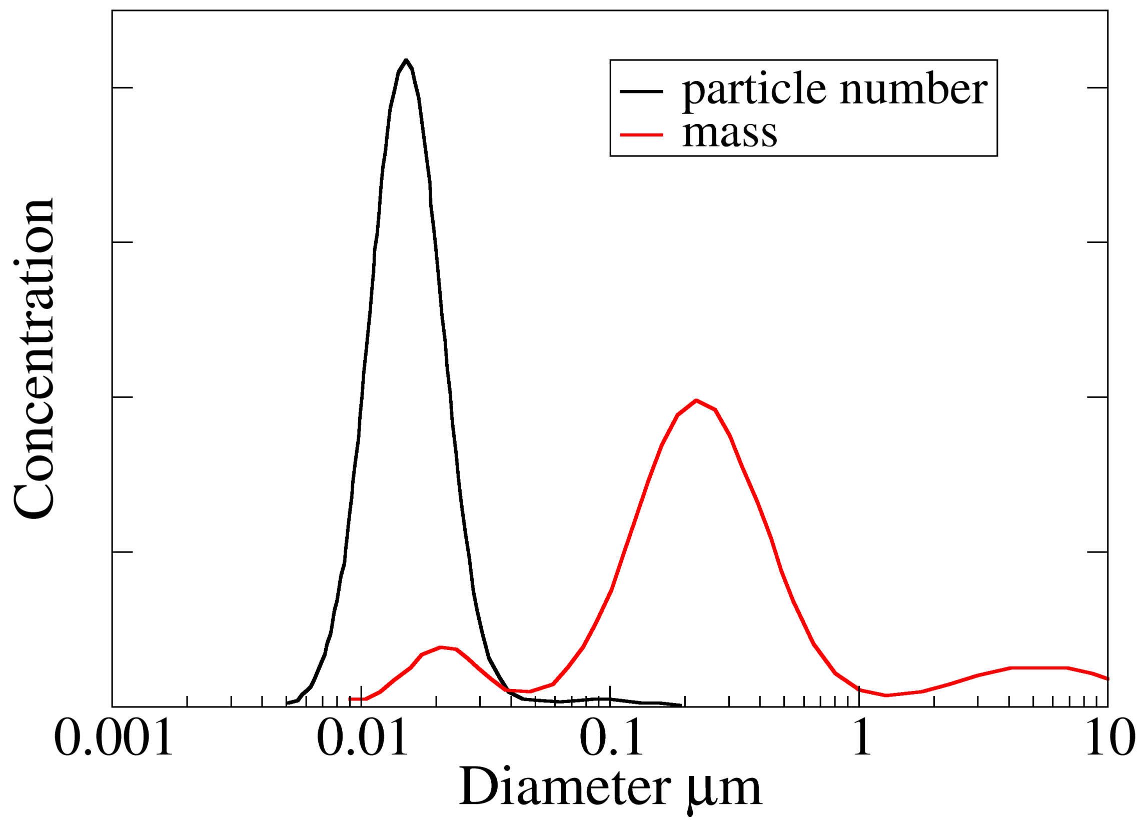
Nanoparticle Permeation

Understanding interactions of carbonaceous material with a lipid bilayer using MD simulation

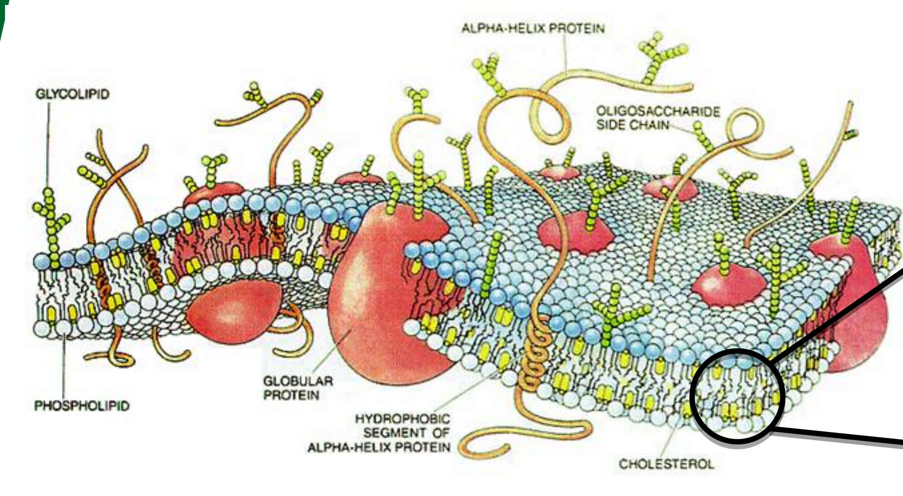
Airborne Particulate Matter

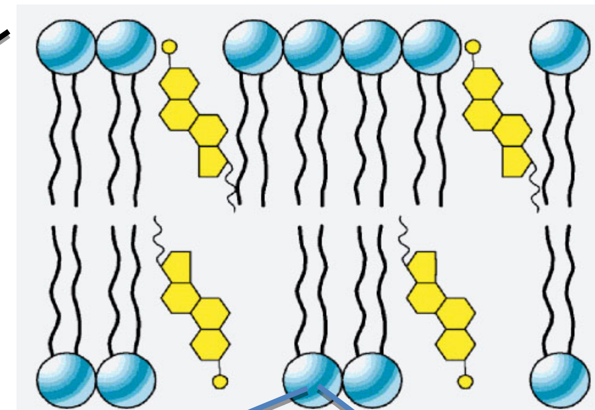
Typical diesel engine exhaust

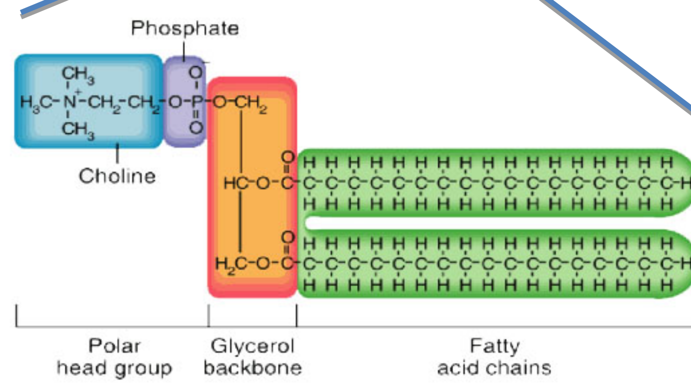


Kittelson, J. Aerol Sci. 29, 575 (1998)

Membrane





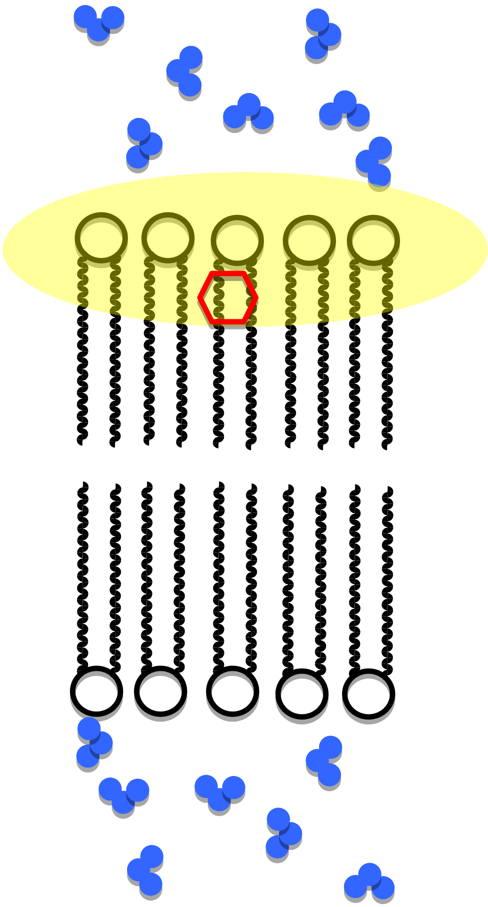


Phosopholipids

Head: Hydrophyllic, polar, PO_4 group(s)

Tail: Hydrophobic, non-polar HC chain

Permeation Thermodynamics

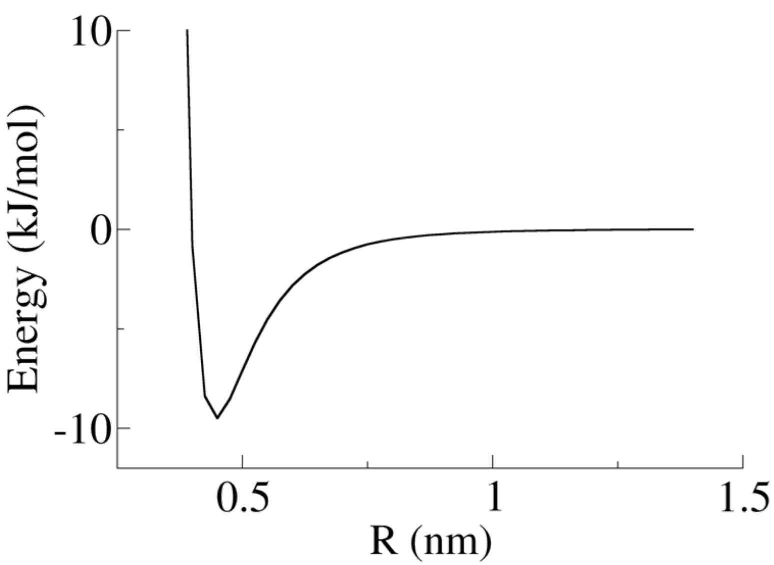


- ΔG driven by entropy
- Head group region
  - High density
  - Enthapic favorable
- Tail group region
  - free volume
  - Entropically favored

Free Energy

Constraint Force

$$\Delta G \approx \sum_{\lambda=0}^{1} \left\langle \frac{\partial E}{\partial \lambda} \right\rangle_{\lambda} \Delta\lambda$$



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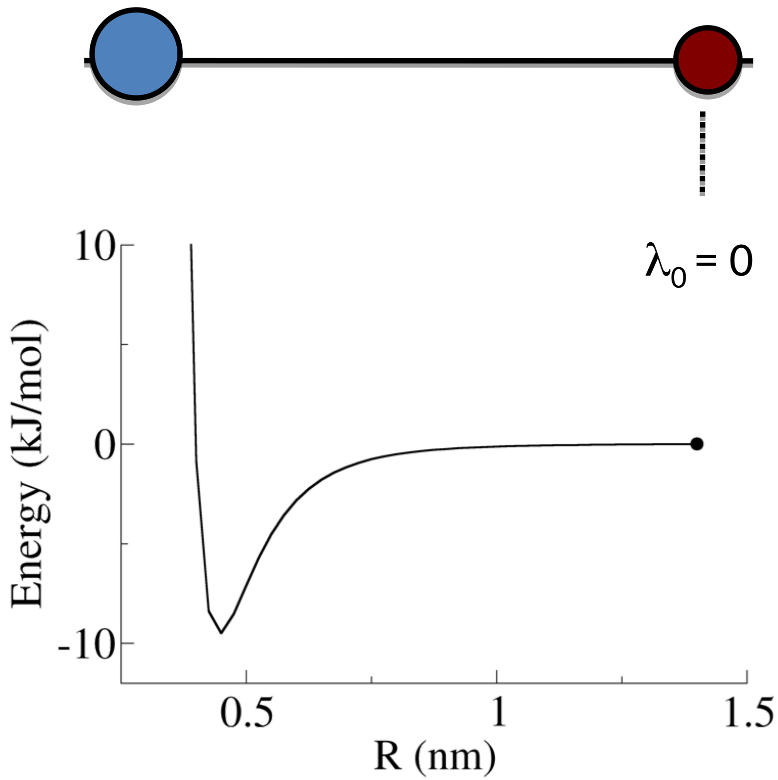

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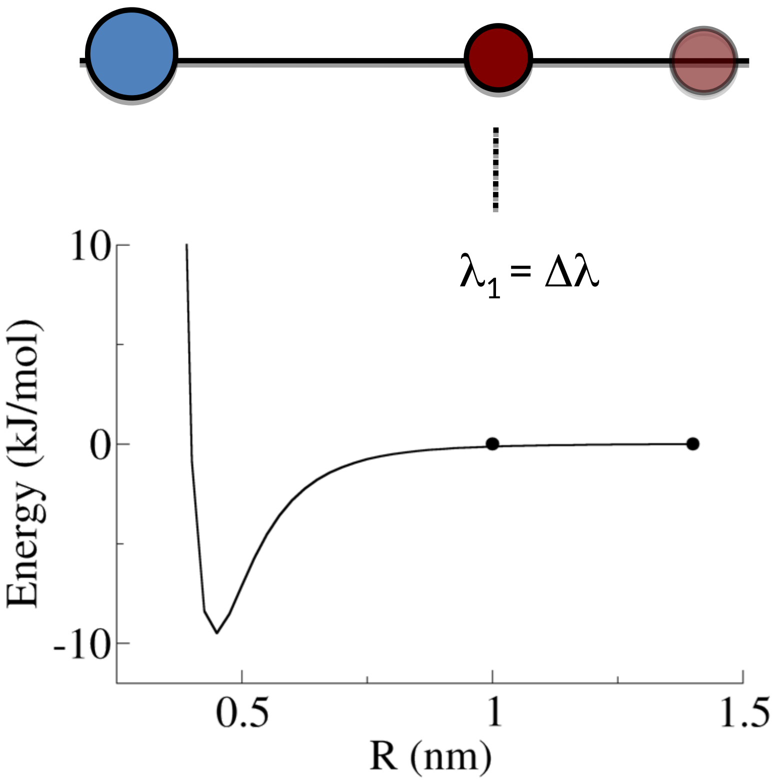

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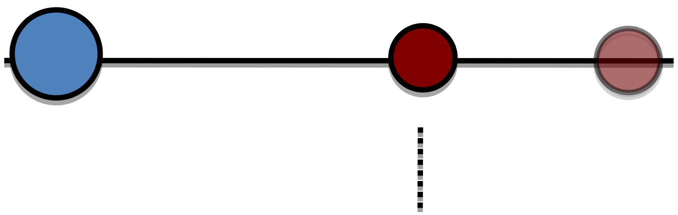
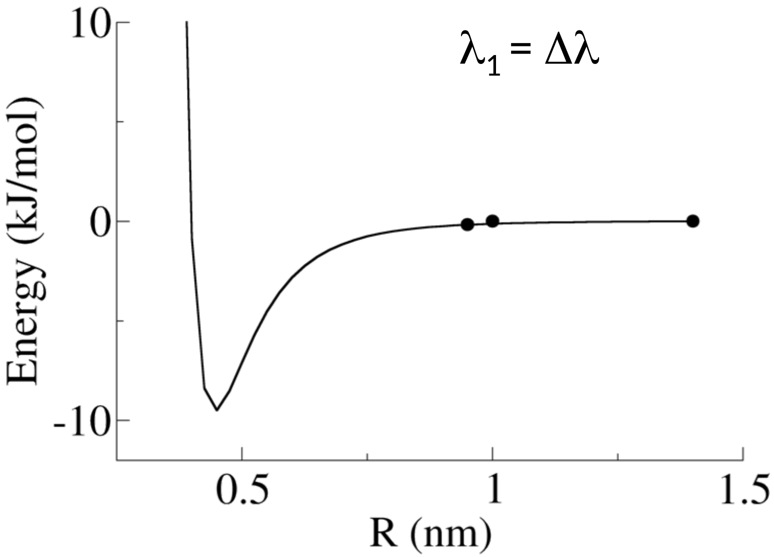


$\lambda_1 = \Delta\lambda$



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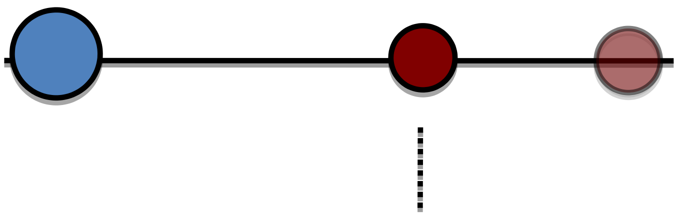

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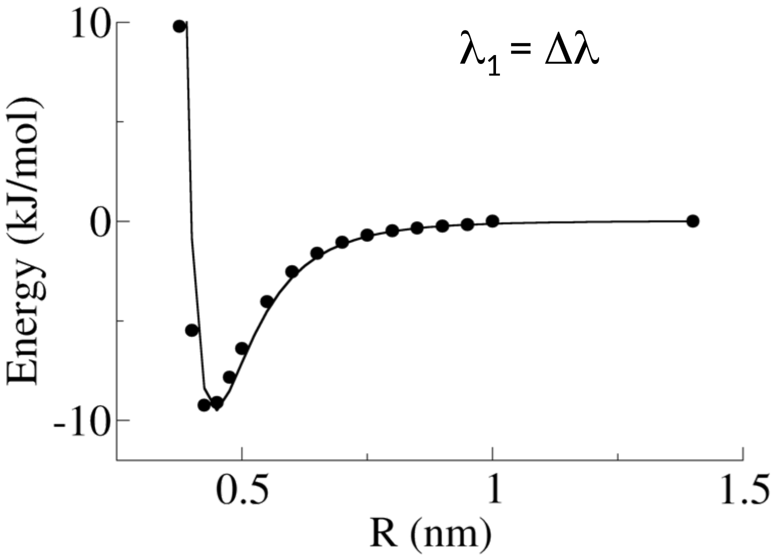

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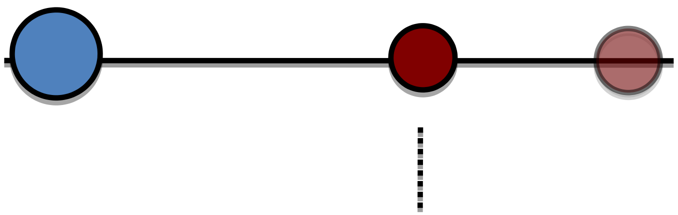

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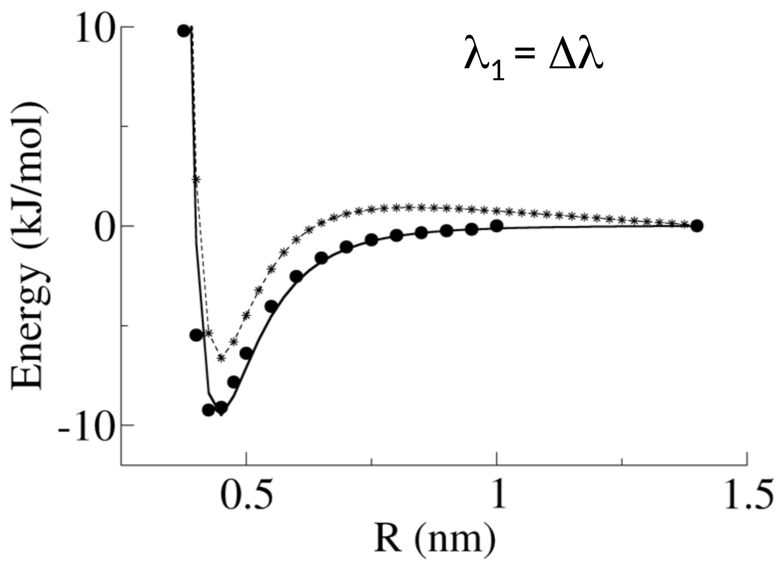

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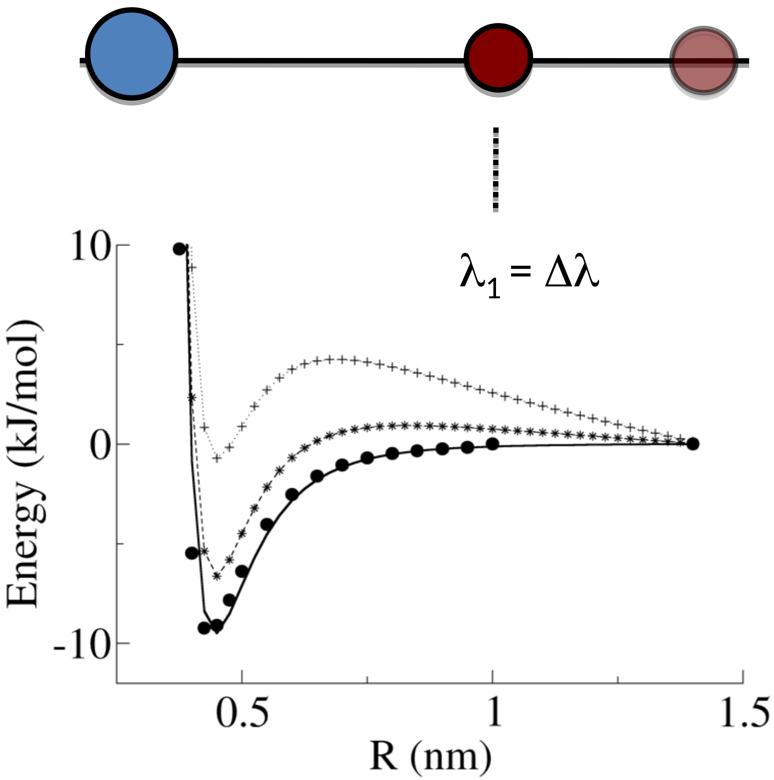
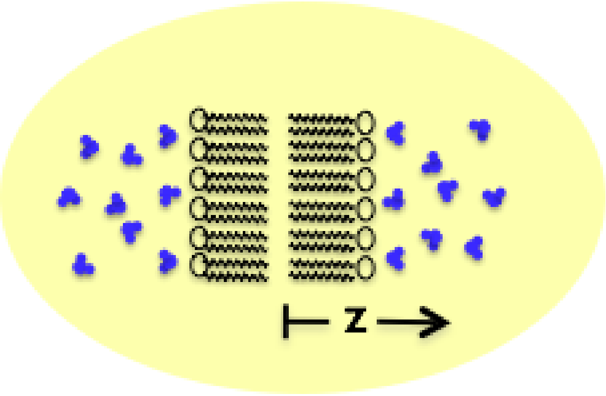
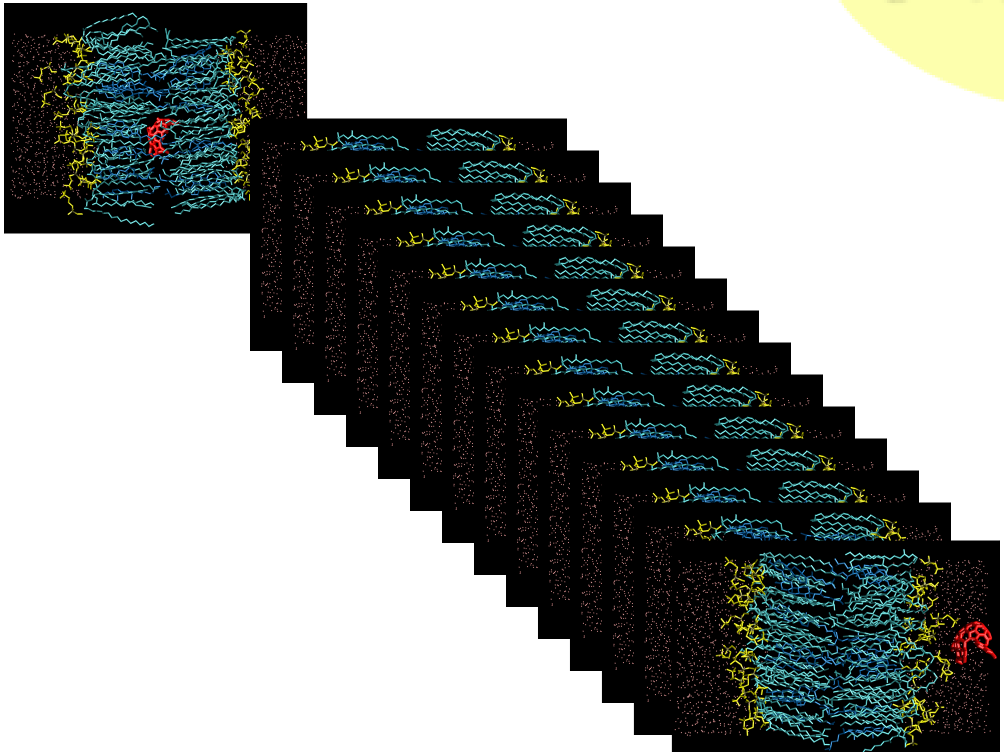


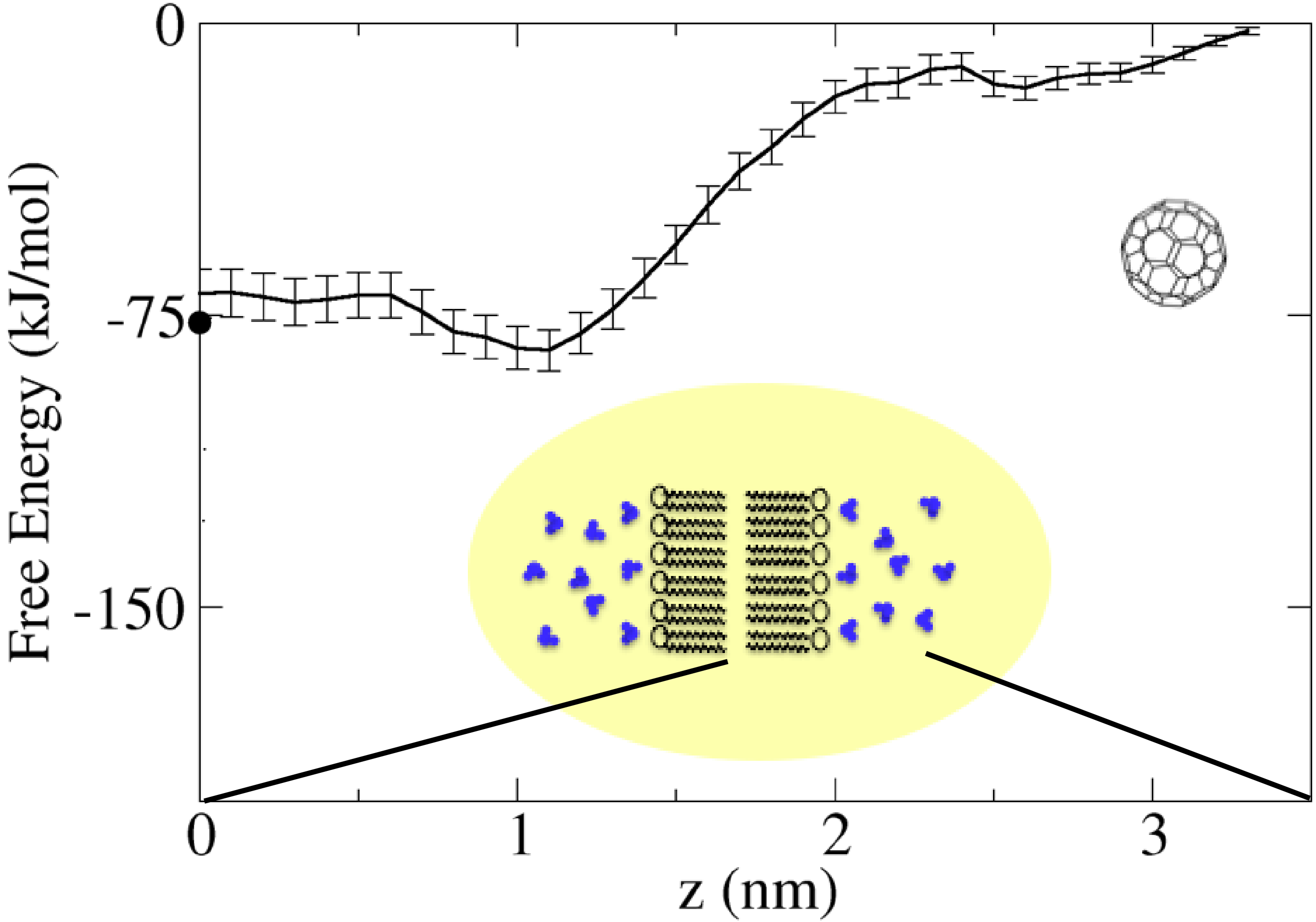
Required Simulations

Permeability function of: $\Delta G(z)$, $D(z)$





Potential of Mean Force



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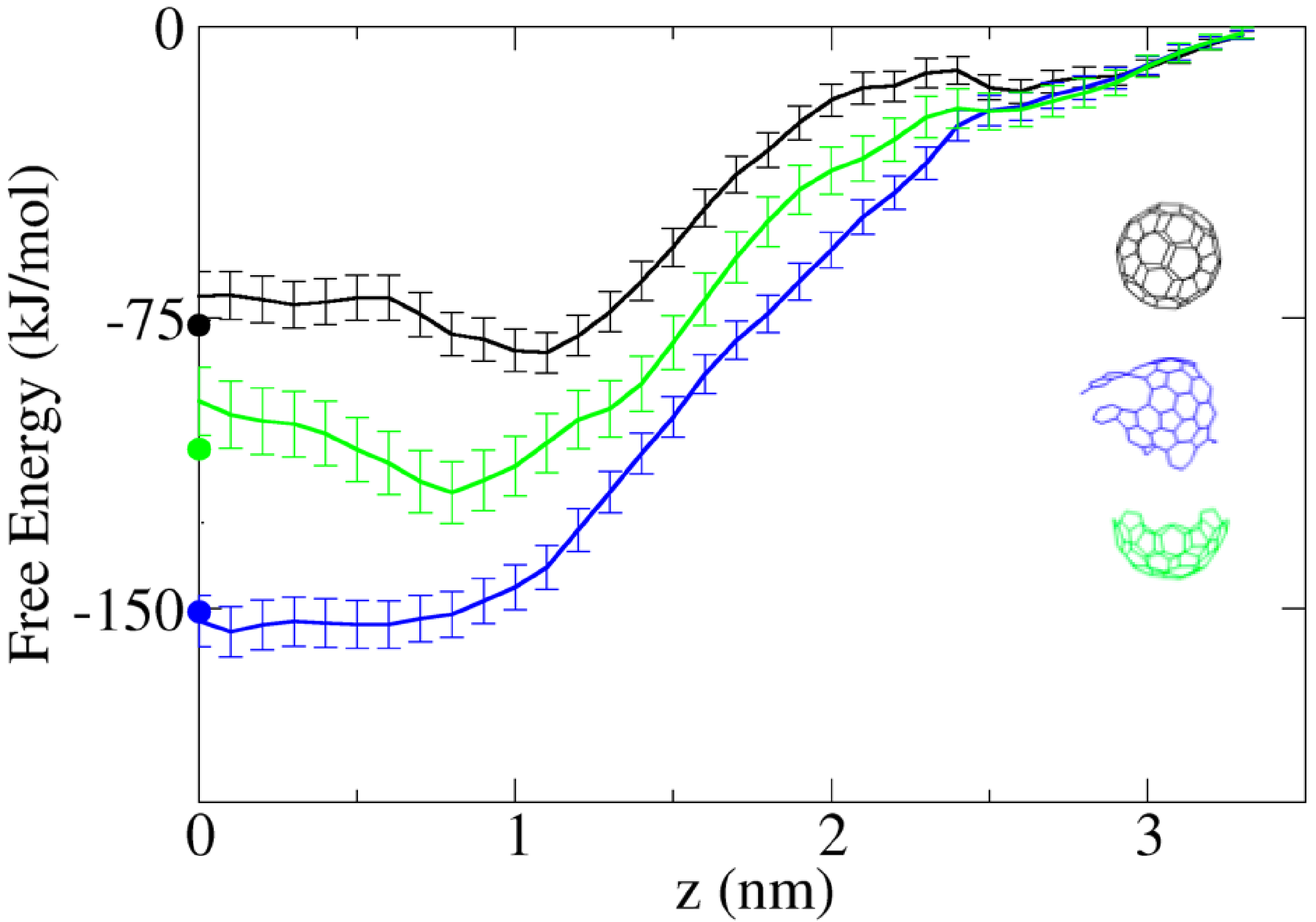


Advancements

Familiarity with the Linux environment

- Text editing (vi)

Molecular visualization (VMD)

Molecular modeling (GROMACS)

- Ensembles
- **Elimination of bad-contacts (shell scripting)**

Simulation techniques

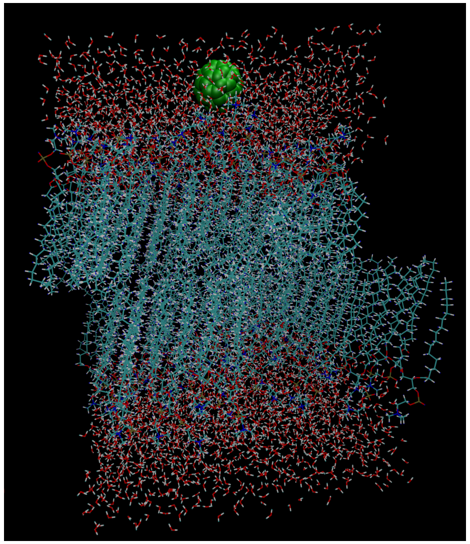
- Equations of motion
- Periodic boundaries

Data Analysis (Xmgrace, OriginPro)

- Integration and differentiation
- Fitting

Literature Search (ARC Card)

Presentation



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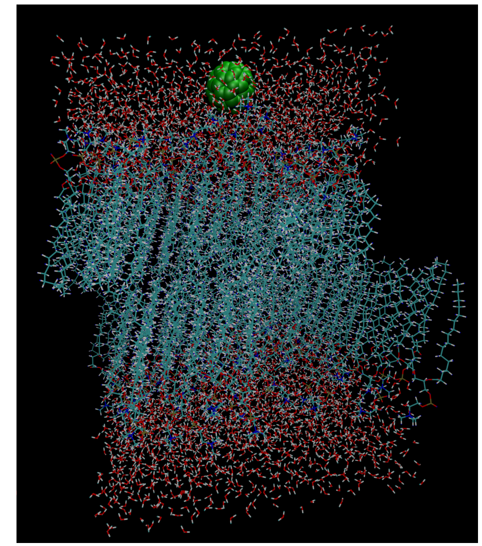
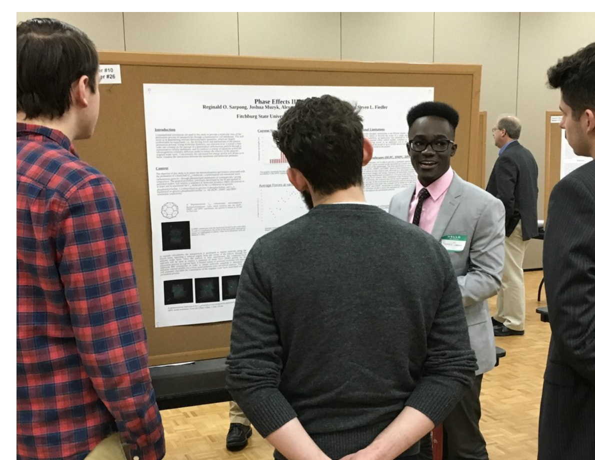
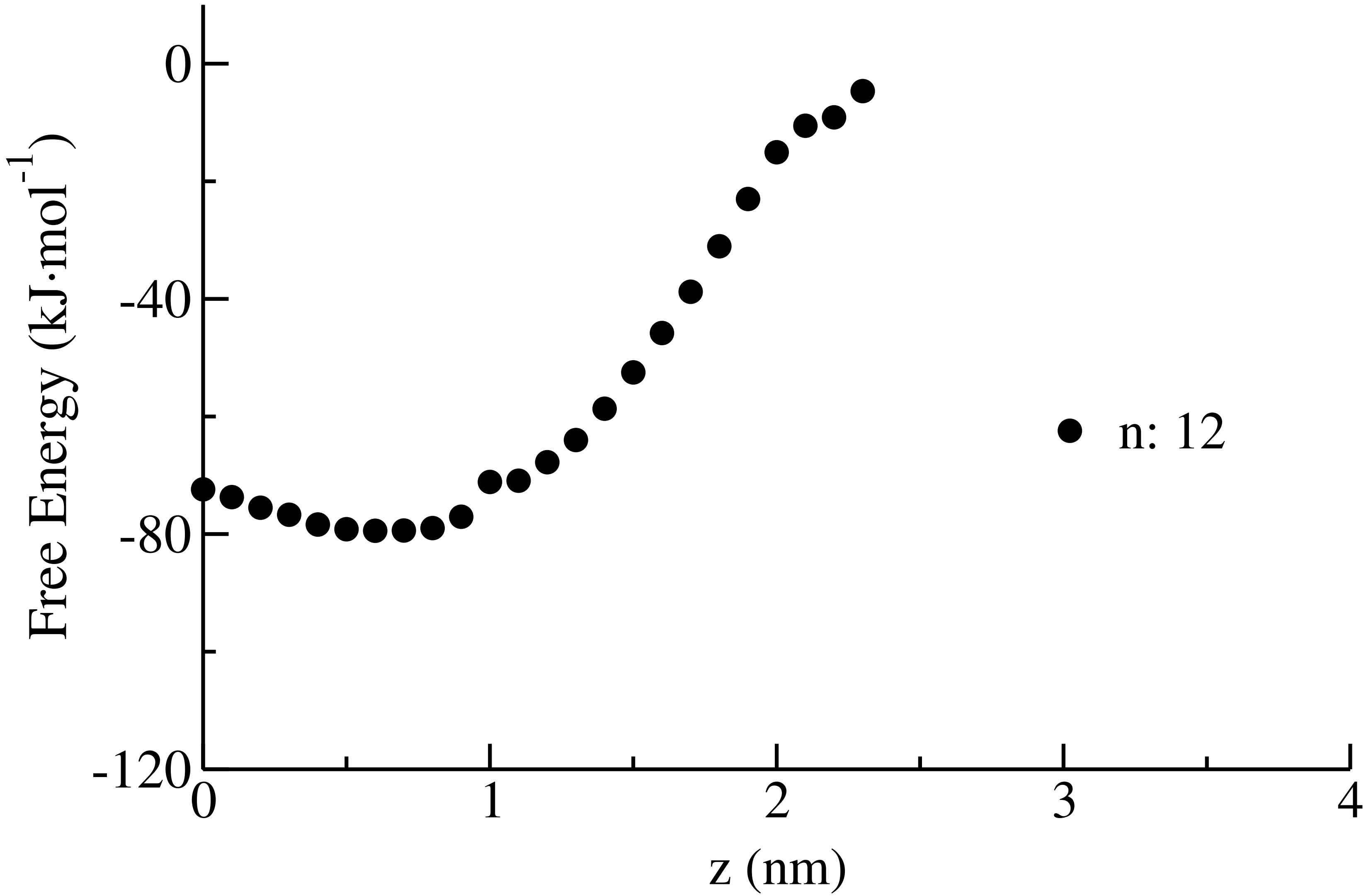




Potential of Mean Force (C_{60})



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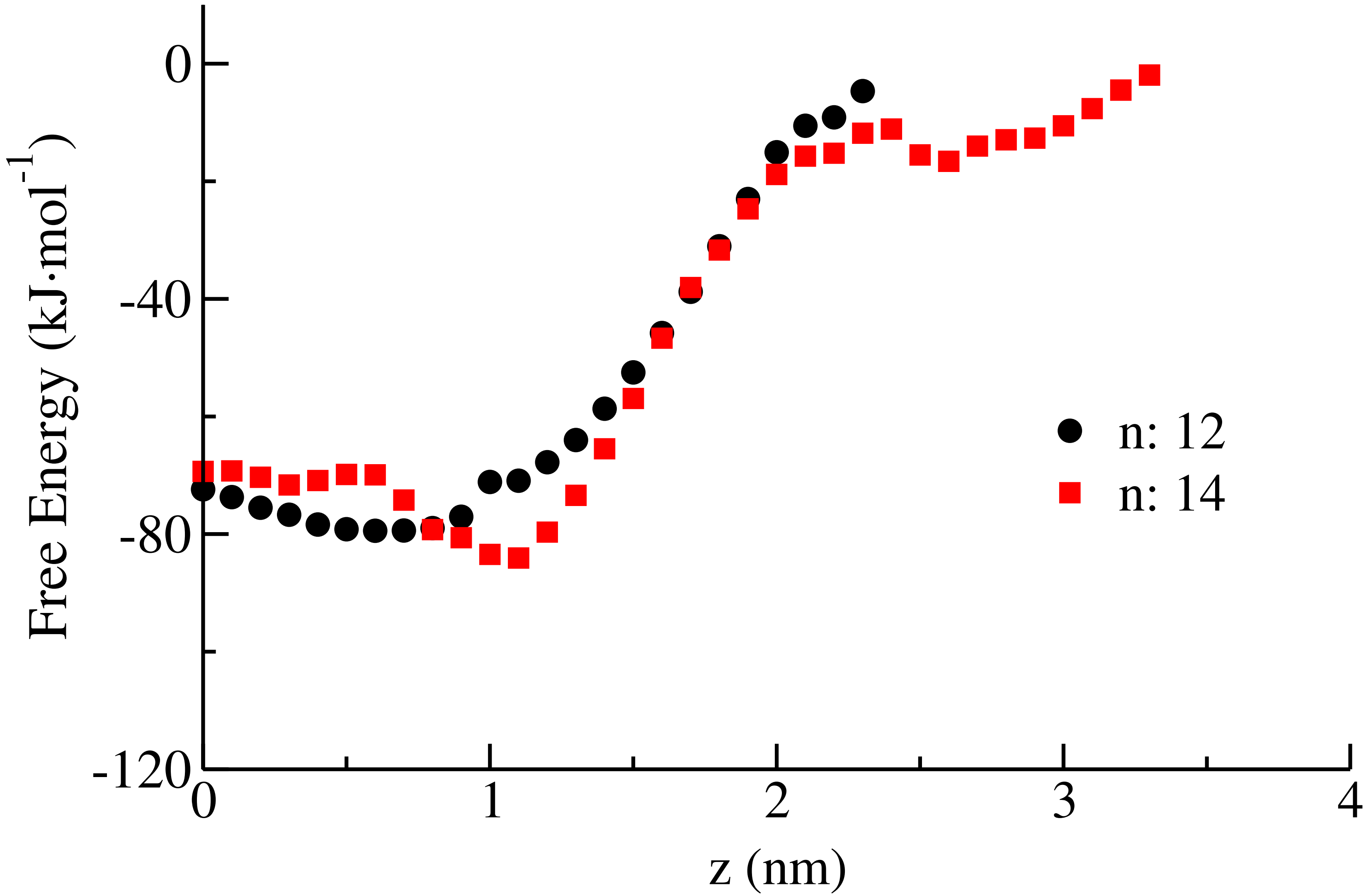

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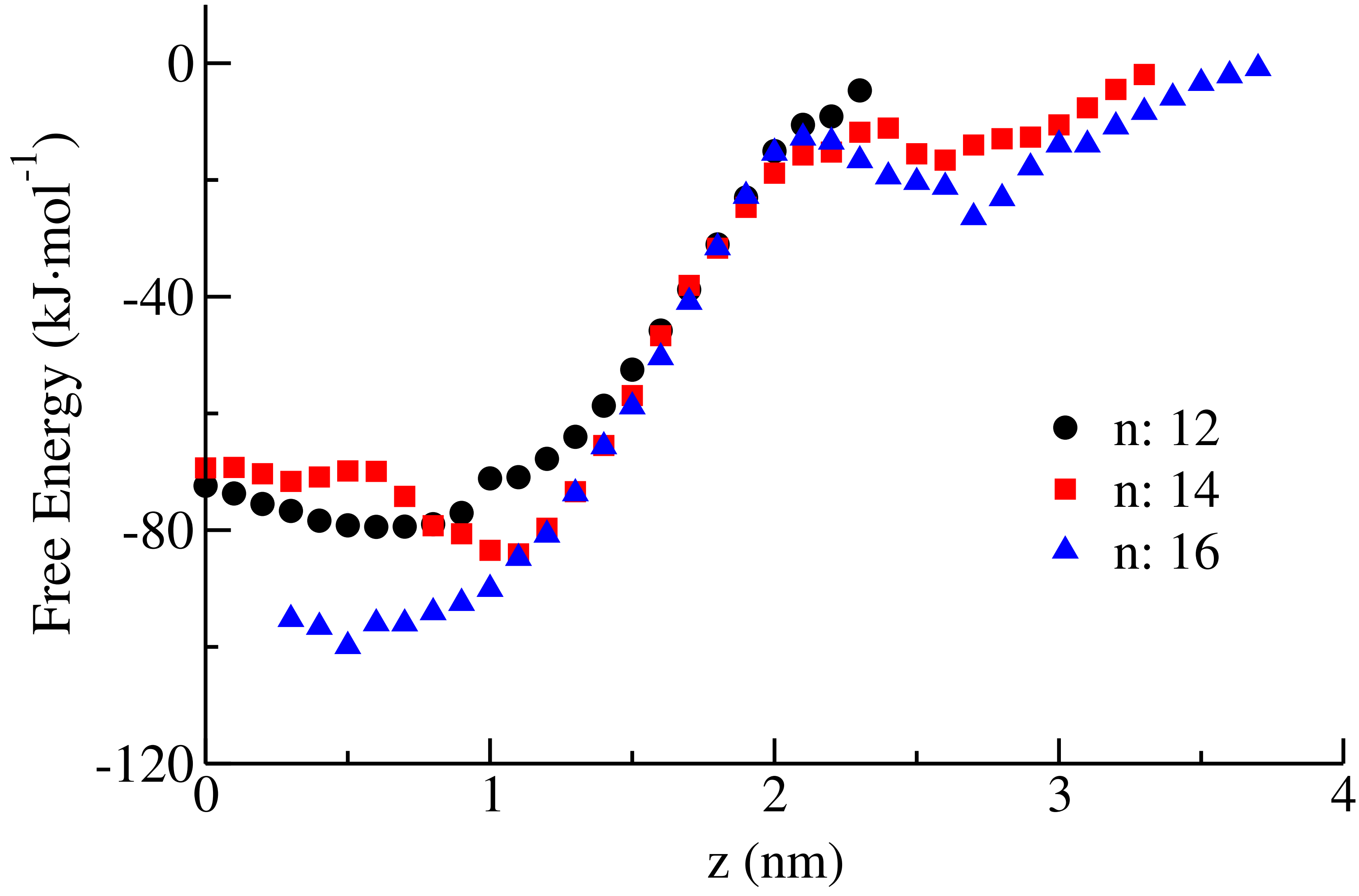
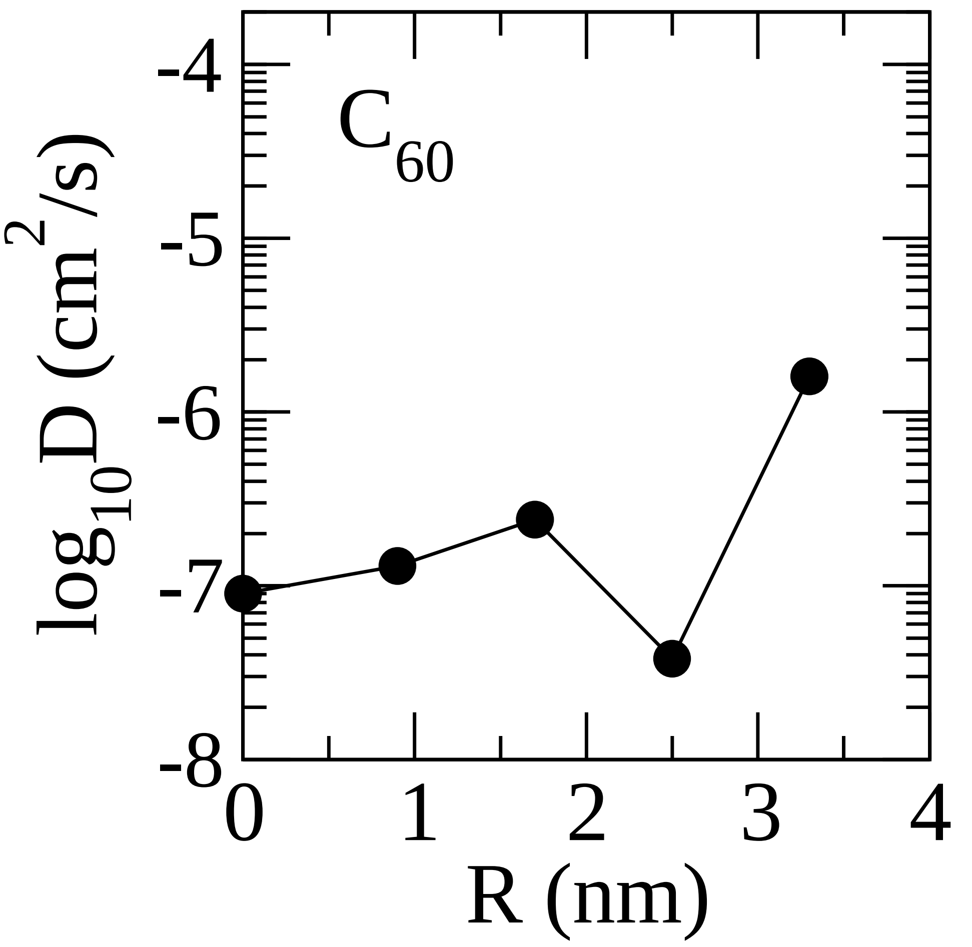
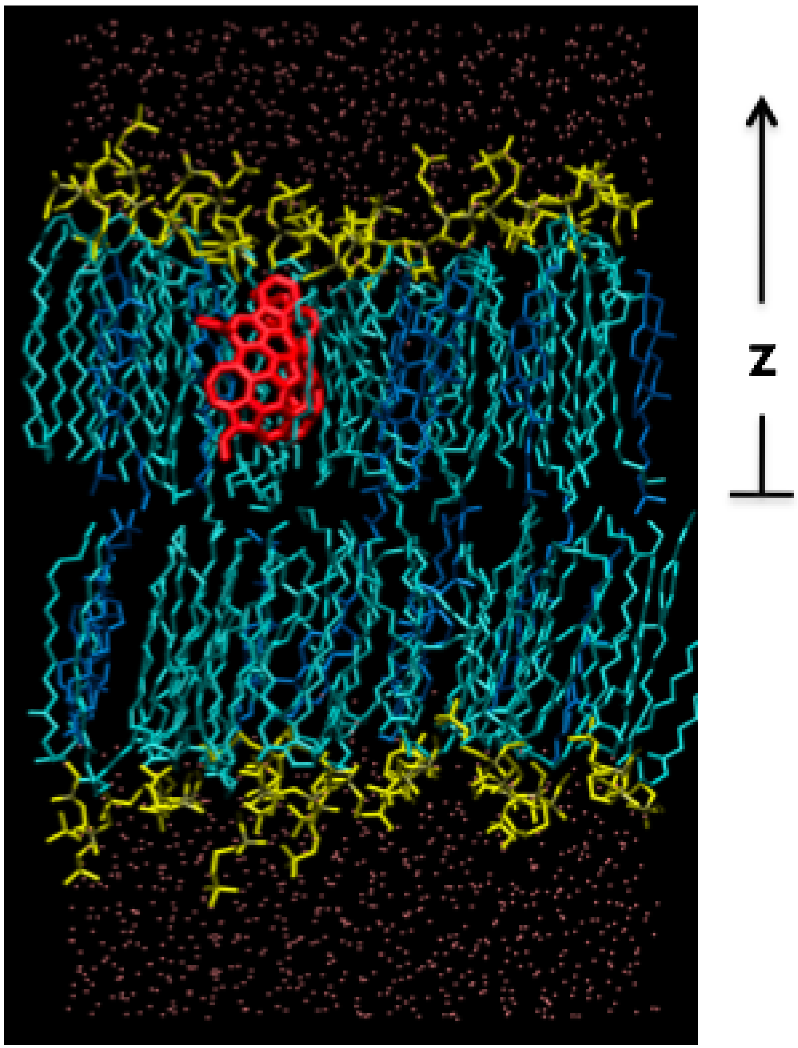


Normal Diffusion



Permeability



$$\frac{1}{P} = \int_0^{interface} R(z)\,dz$$

$$= \frac{1}{\int_0^{interface} \frac{\exp\left(\Delta G(z)/RT\right)}{D(z)}\,dz}$$

Stagnant water layer attenuation

$$\frac{1}{P} = \frac{2}{P_{UL}} + \frac{1}{P_M}$$

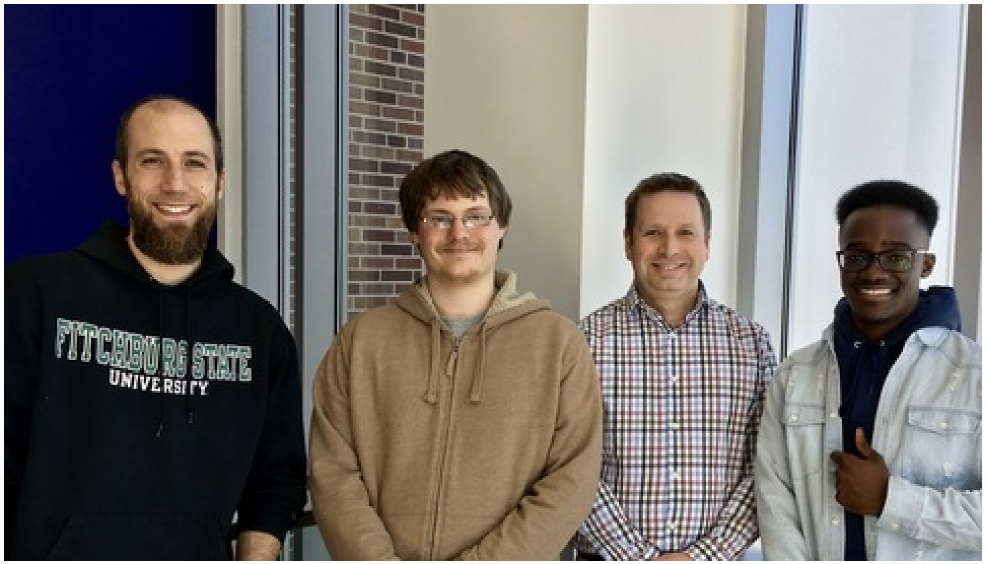
$$\frac{1}{P_1} = \frac{2}{P_{UL_1}} + \frac{1}{P_{M_1}}$$

$$\frac{1}{P_2} = \frac{2}{P_{UL_1}} + \frac{1}{P_{M_2}}$$

$$\frac{1}{P_3} = \frac{2}{P_{UL_2}} + \frac{1}{P_{M_1}}$$

$$\frac{1}{P_4} = \frac{2}{P_{UL_2}} + \frac{1}{P_{M_2}}$$

Acknowledgments



Lipid permeation

Ryan Hamelin

Alexander Steacy

Reginald Sarpong

Joshua Muzyk

Liquid Helium

Jussi Eloranta, CSUN

Nelly Bonifaci, G2ELab-Grenoble

S. Fiedler, A. Violi, Biophys. J. 99, 144 (2010)

N. Bonifaci, F. Aitken, V. Atrazhev, S. Fiedler, J. Eloranta, Phys. Rev. A 85, 042706 (2012)

S. Fiedler, J. Eloranta, J. Low. Temp. Phys. 174, 269-283 (2014)

N. Bonifaci, Z. Li, J. Eloranta, S. Fiedler, J. Phys. Chem. A 120, 9019 (2016)