Comparative Studies on Water Self-Diffusivity Confined in Graphene Nanogap: Molecular Dynamics Simulation

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Motivation and Objectives

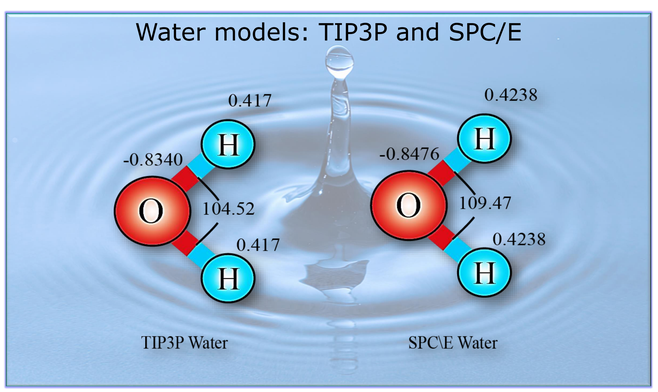
Motivation
- Graphene is being used to enhance desired transport properties and energy conversion efficiency in various renewable energy applications including fuel cells.
- However, water behaviors in presence of graphene are not well understood.

Objectives
- To articulate confined water behaviors (self-diffusivity) in graphene different graphene nanogap sizes using molecular dynamics simulations with various graphene-water interatomic potentials.
- To provide a guideline to optimally design the graphene structures for the desired water transport properties.

Background

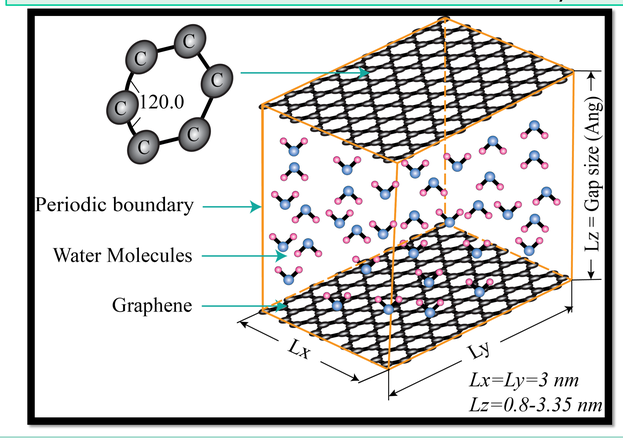
- Diffusivity as a one of the most important behaviors of water in a confined region is investigated is different studies.
- Some studies have reported higher water self-diffusivity under confinement.
- Some studies have reported lower water self-diffusivity which does not match the other studies.
- Effect of Nanogap size on water self-diffusivity is not studied much.
- The Effect of different water-carbon potentials on water self-diffusivity is poorly understood.

Methodology: Water Model



Methodology: Water in Graphene Nanogap

- Graphene nanogap structure filled with water: different gap size in z direction are used to examine their effect on water self-diffusivity under confinement.



Potential Equations, Lenard-Jones Potential (LJ), and water self-diffusivity:

$$\varphi_{total} = \varphi_{bond} + \varphi_{angle} + \varphi_{van\ der\ walls} + \varphi_{coulombic}$$

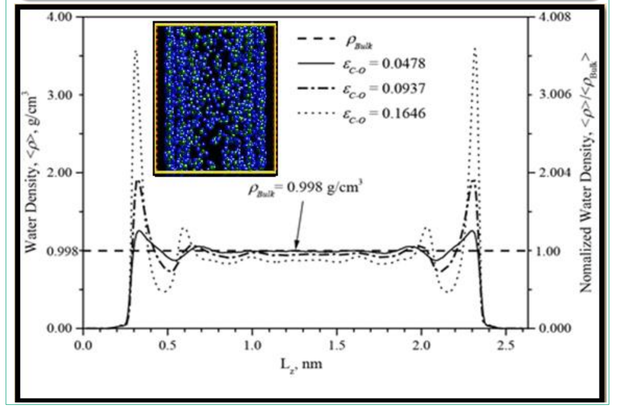
$$\varphi_{bond} = \frac{1}{2}k_b\left(r - r_0\right)^2, \quad \varphi_{angle} = \frac{1}{2}k_\theta\left(\theta - \theta_0\right)^2$$

$$\varphi_{ij} = 4\varepsilon_{ij}\left\{\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right\} + \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r_{ij}}$$

$$D = \lim_{n\to\infty}\frac{1}{6N_m t}\left\langle\sum_{j=1}^{N_m}\left[r_j(t) - r_j(0)\right]^2\right\rangle$$

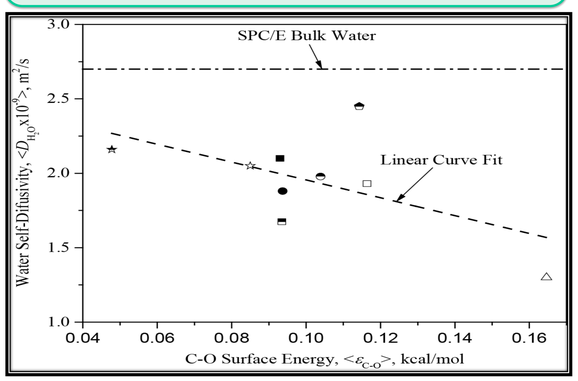
Results: Local Water Density

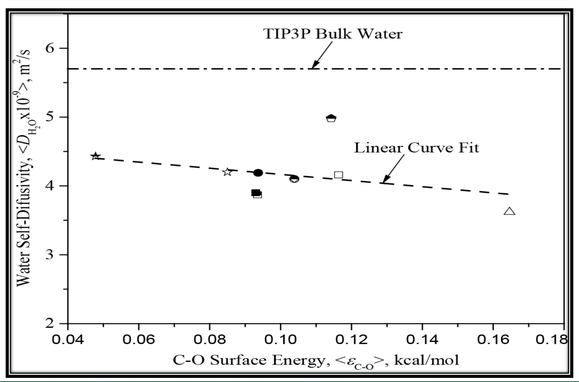
Local Water Density Distribution:
- Higher density close to the surface
- Two density peaks



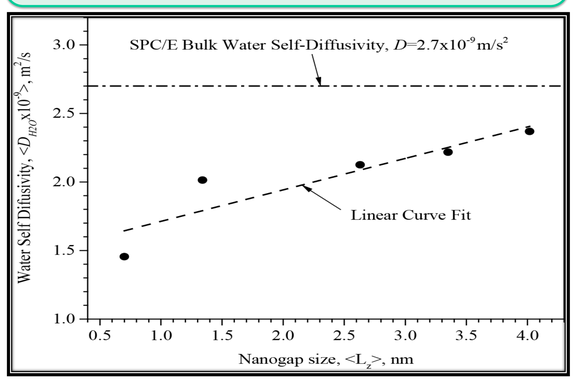
Results and Discussions: Water Self-Diffusivity

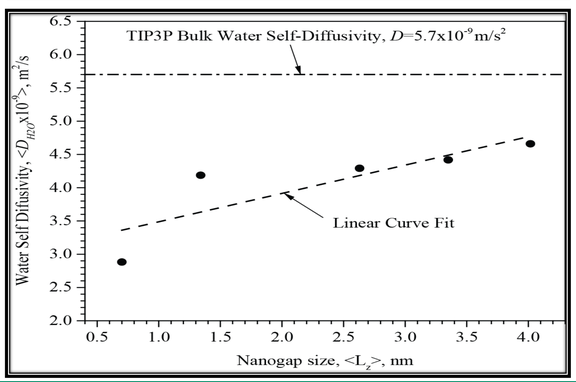
Water-carbon potentials effect:
- Lower water self-diffusivity in all cases
- Strong interaction ⟹ Lowest diffusivity





Nanogap size effect:
- Lower water self-diffusivity in all cases
- Smaller size ⟹ Lowest diffusivity





Conclusion

- Confinement decreases diffusivity in all cases.
- Strong interaction ⟹ Lowest diffusivity
- Smaller size ⟹ Lowest diffusivity
- Surface energy results in slower water mobility in z direction.

Acknowledgment

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