纳米液滴在不同表面的浸润行为

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Brief Introduction

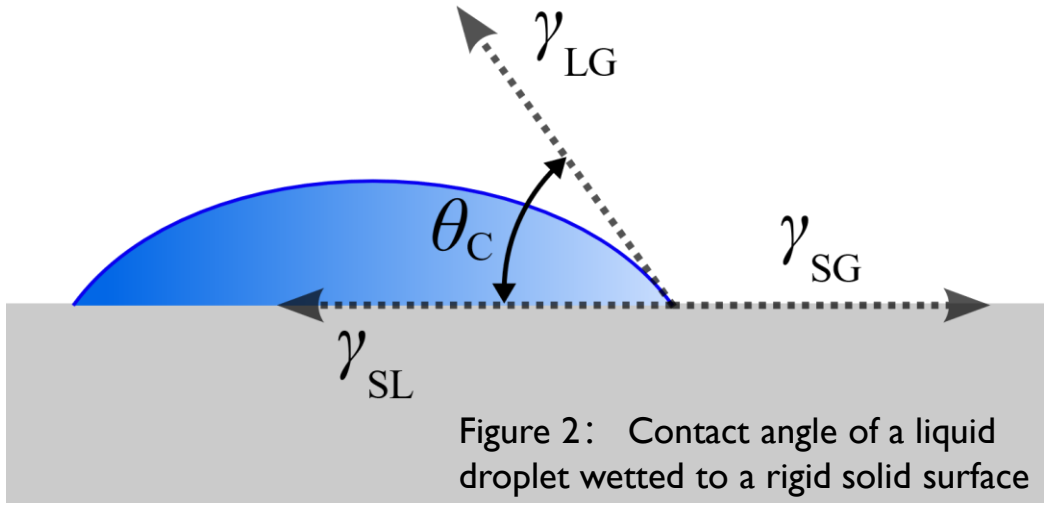


Figure 2： Contact angle of a liquid droplet wetted to a rigid solid surface

Young′s relation:

$$\gamma_{SG} = \gamma_{SL} + \gamma_{LG} \cdot cos\theta$$

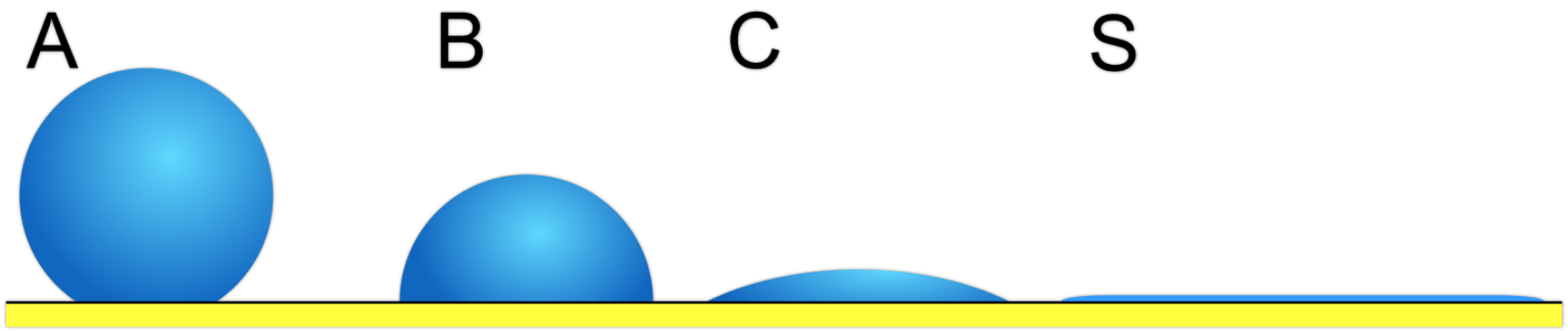
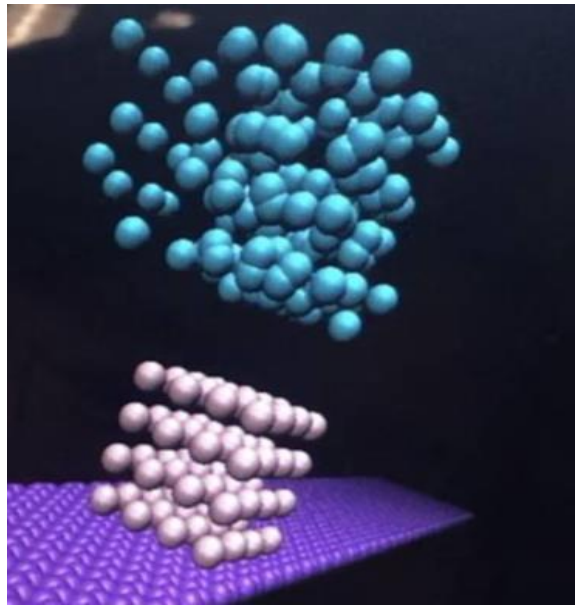
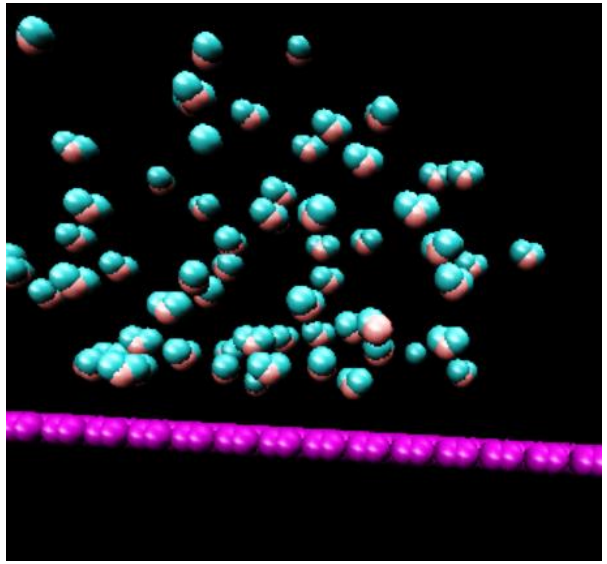


Figure 1： Wetting of different fluids: A shows a fluid with very little wetting, while C shows a fluid with more wetting. A has a large contact angle, and C has a small contact angle.as a large contact angle, and *C* has a small contact angle.

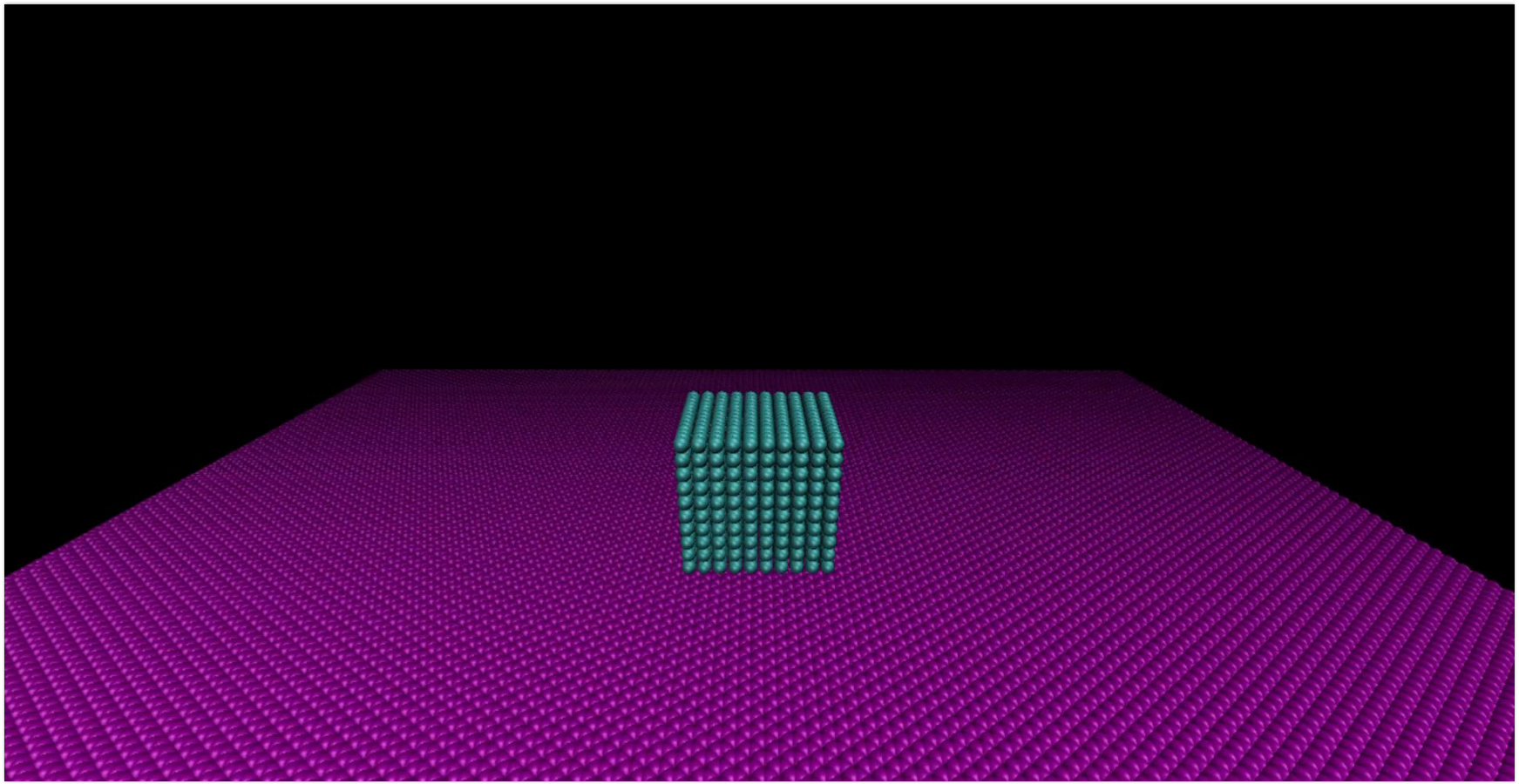
https://en.wikipedia.org/wiki/Wetting

MD Simulation





MD Simulation



MD Simulation

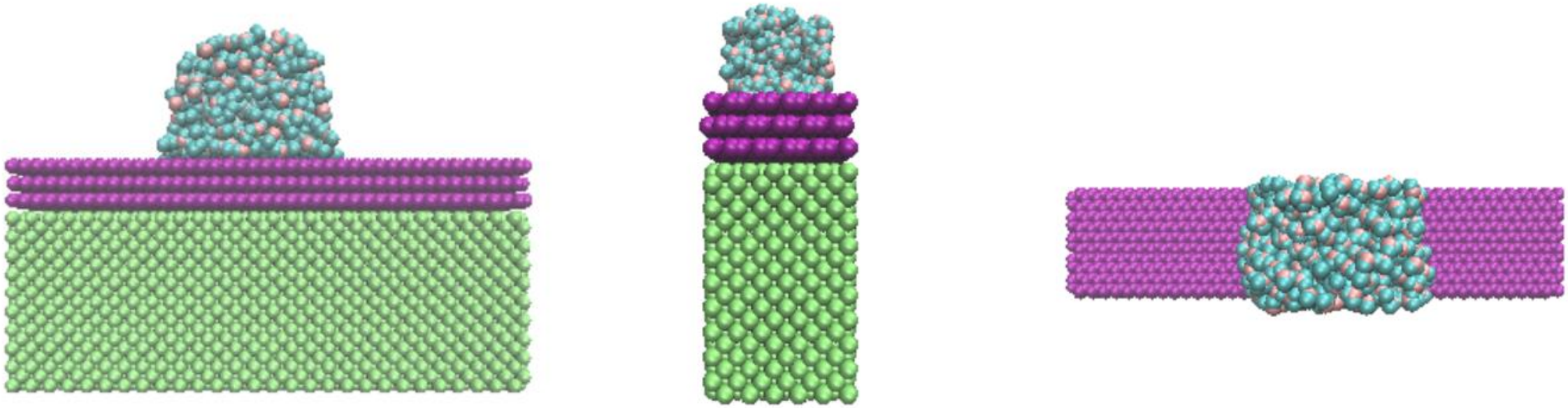


Figure 3 : Elevation view, top view and side view of the model

MD Simulation

Pair	ε(kcal/mol)	σ(Å)
O-O	0.1020	3.1880
O-H	0.0836	1.7753
H-H	0.0460	0.4000
O-C/H-C	0.1143	3.2751
O-Cu	0.1700	3.1900
C-C	0.0860	3.400

Table.1. LJ parameters of different pairs.
https://youtu.be/VGBzGGgnnTI

```
pair_style lj/cut/coul/cut 10.0
bond_style harmonic
angle_style hybrid charmm harmonic
dihedral_style charmm
```

MD Simulation

```
fix 11 water langevin 300 300 1000 212894
fix 12 water nve/limit 0.1

run 5000
unfix 12

fix 21 water nve
run 50000
```

$$Langevin\ equation:$$
$$ma = -\xi v + f(v) + f'$$

Equilibrium Analysis

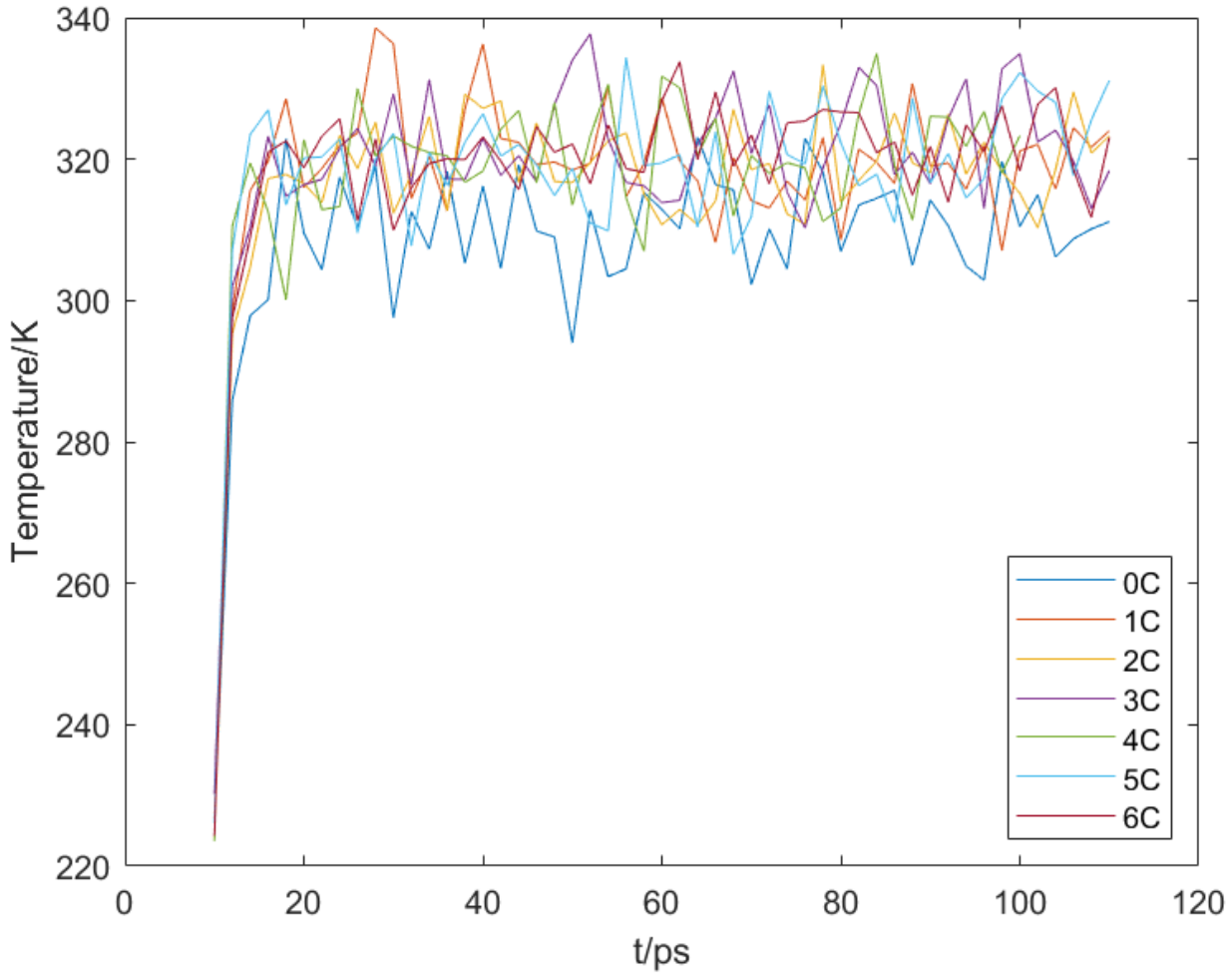


Figure.4. The structures with different number of graphene layers reached dynamic equilibrium within 20ps.

Structure Analysis： RDF

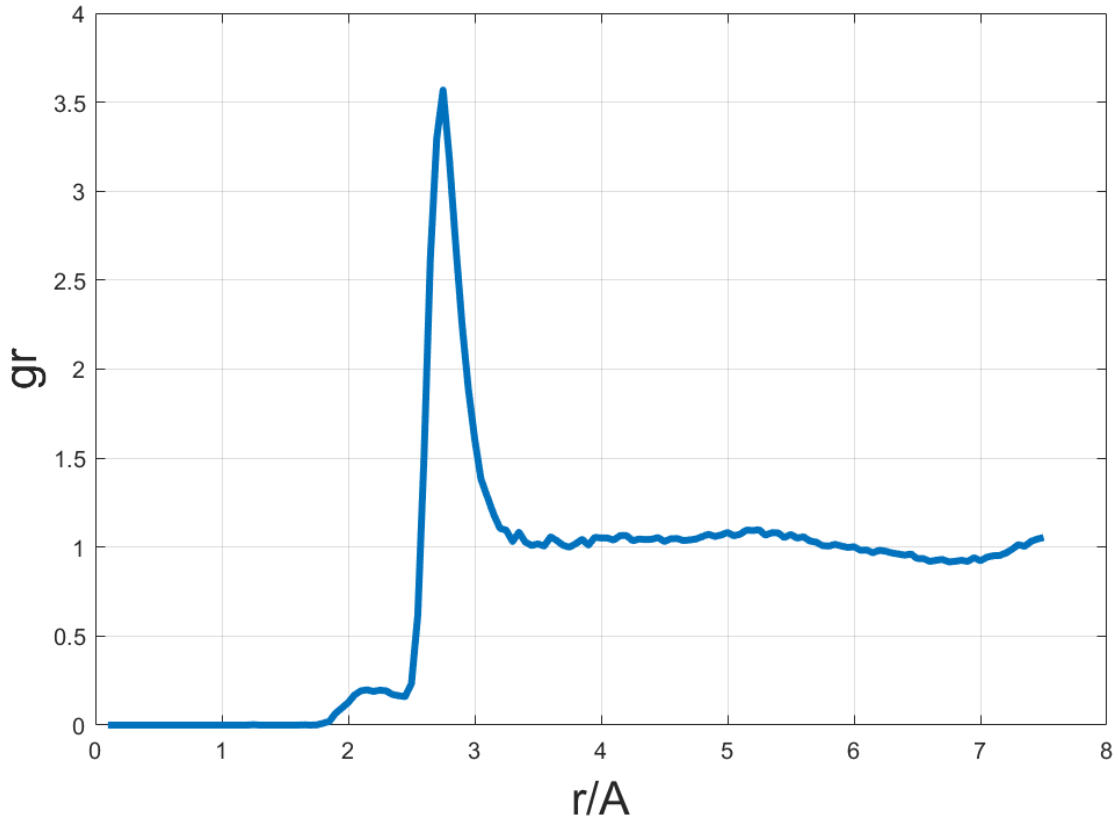


Figure.5. Radial distribution function of oxygen atoms

Structure Analysis : Q6

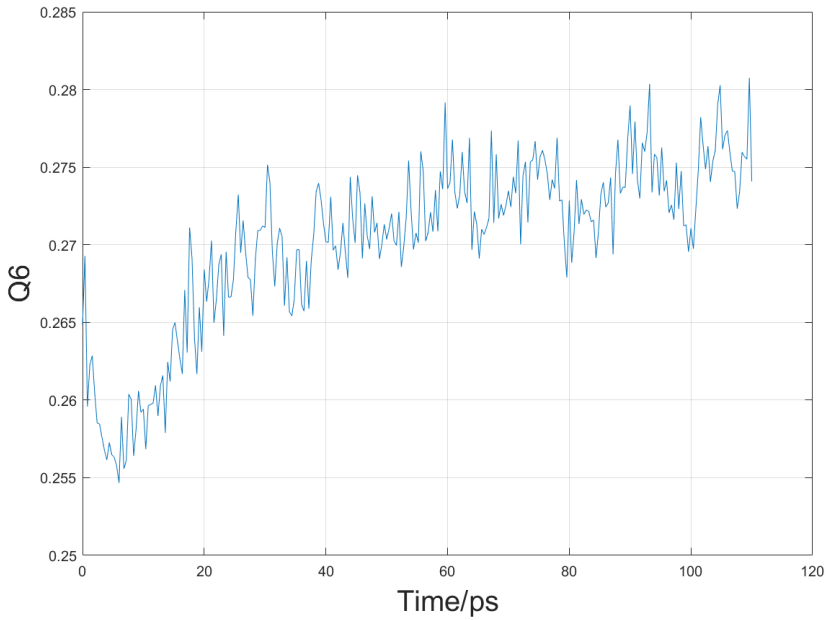


Figure.5. Q_6 of the water droplets when there are 6 layers of graphene.

	fcc	hcp	random
Q_6	0.574	0.485	0.289

Table.2. Q_6 in different lattice structure.

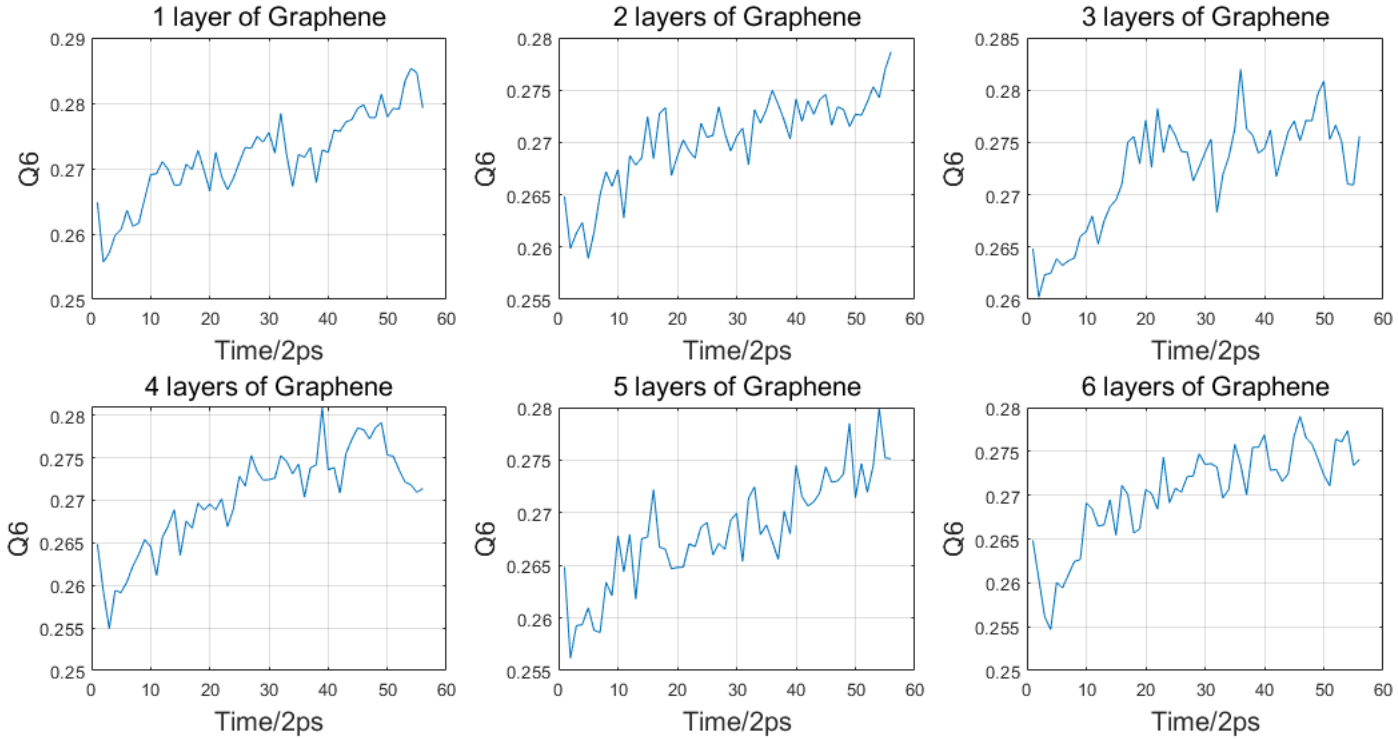
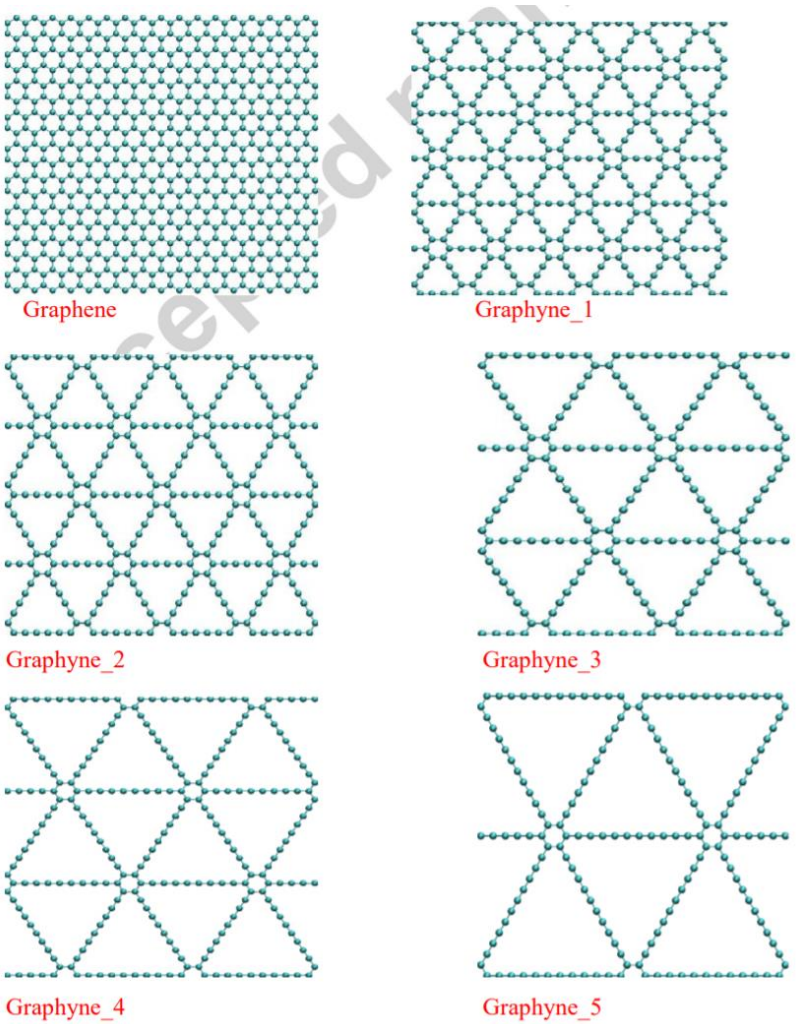


Figure.6. Q_6 of water droplets when there are different number of graphene's layers. Q6 ascends with fluctuation, but eventually falls within the range of 0.27~0.28, indicating that the structure of water droplets is random all the time.

Structure Analysis : Density in z direction



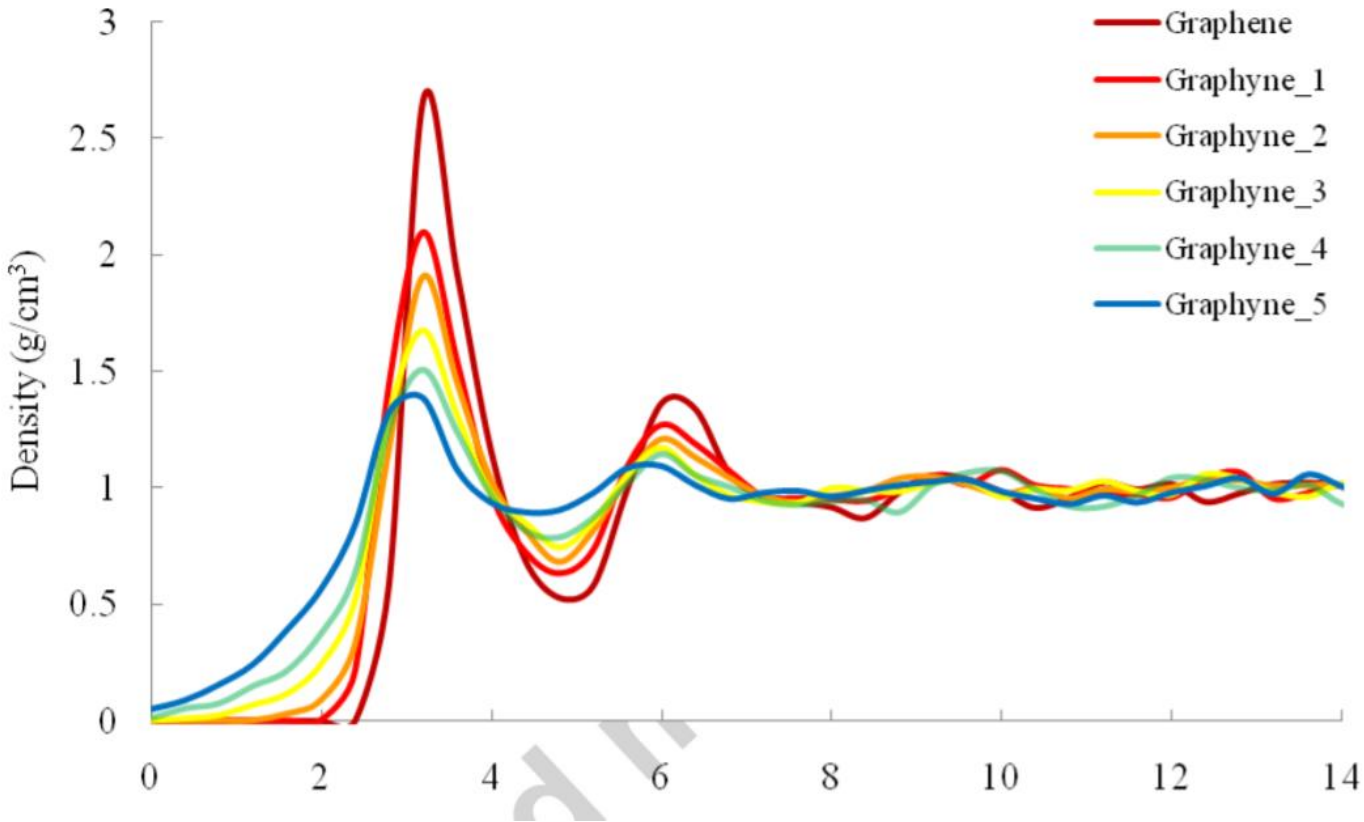


Figure.7. Saleh Bagheri, Abolghasem Shameli, Mehdi Darvishi, Ghasem Fakhrpour, Molecular investigation of water adsorption on graphene and graphyne surfaces, Physica E: Low-dimensional Systems and Nanostructures, Volume 90,2017, Pages 123-130, ISSN 1386-9477.

Structure Analysis： Density in z direction

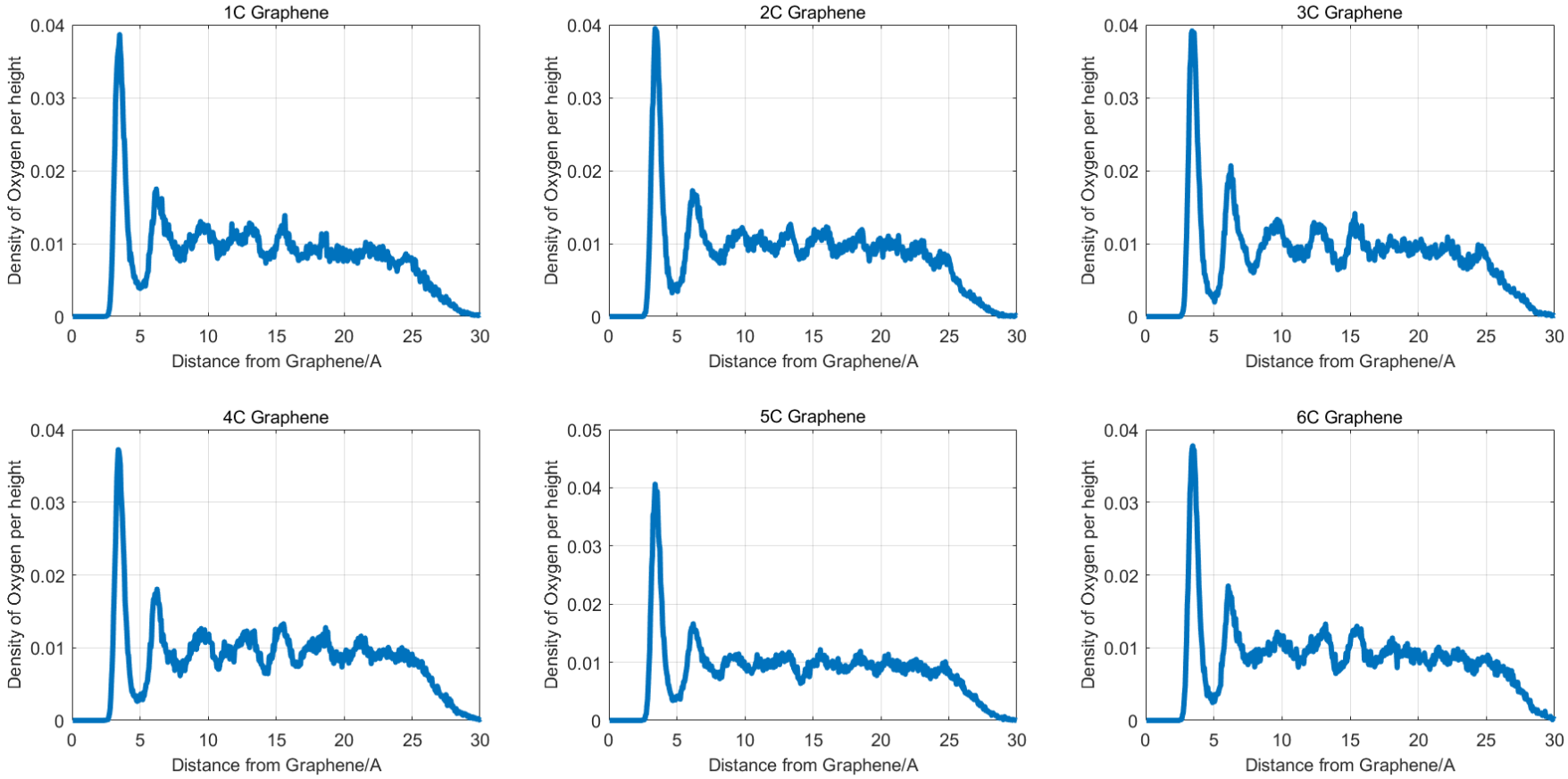


Figure.8. Density in z direction basically invariant with the layer's number of Graphene .

Dynamic Analysis： MSD

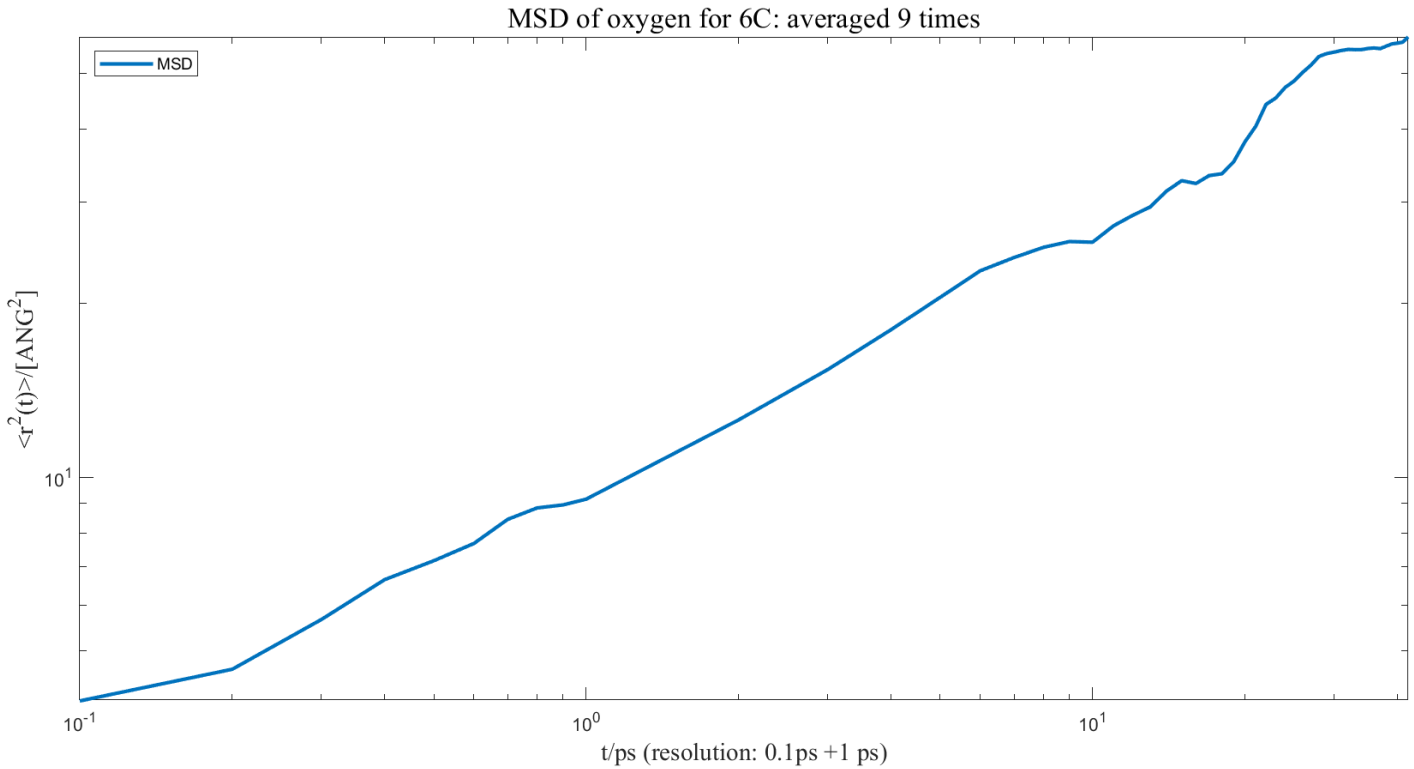


Figure.9. MSD curve in this simulation when there are 6 layers of graphene.

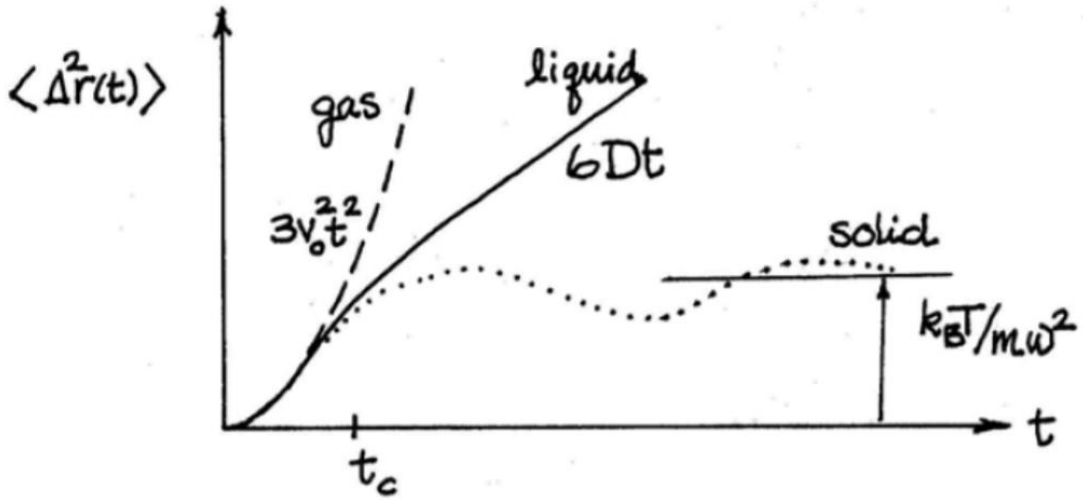
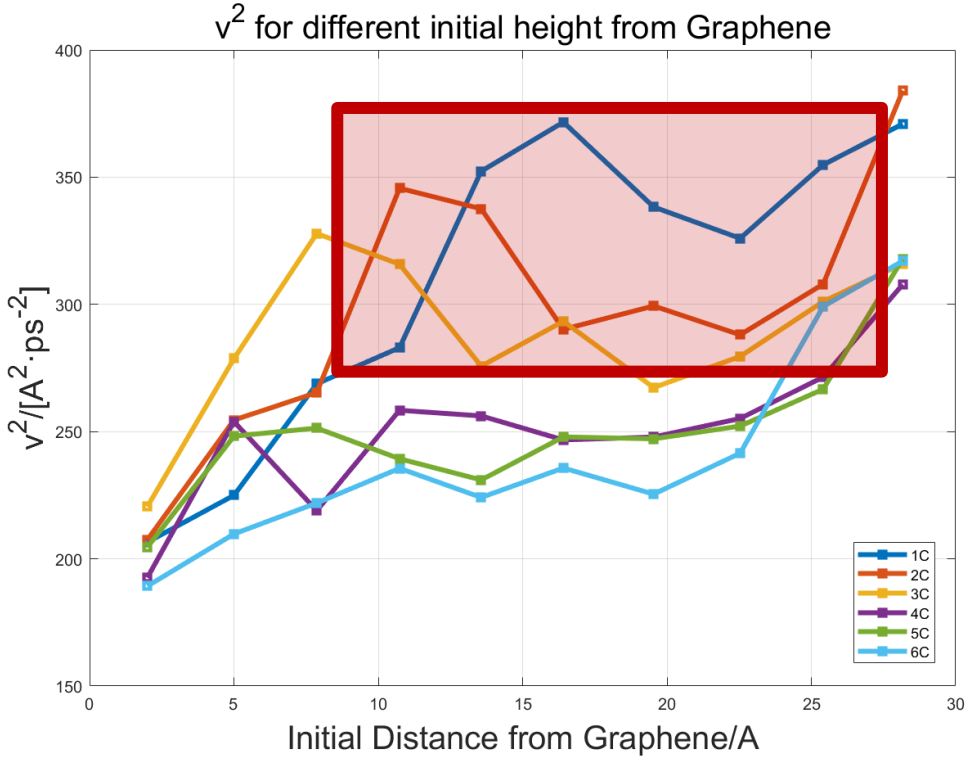


Figure.10. MSD curve in different phase.

Dynamic Analysis : E_k



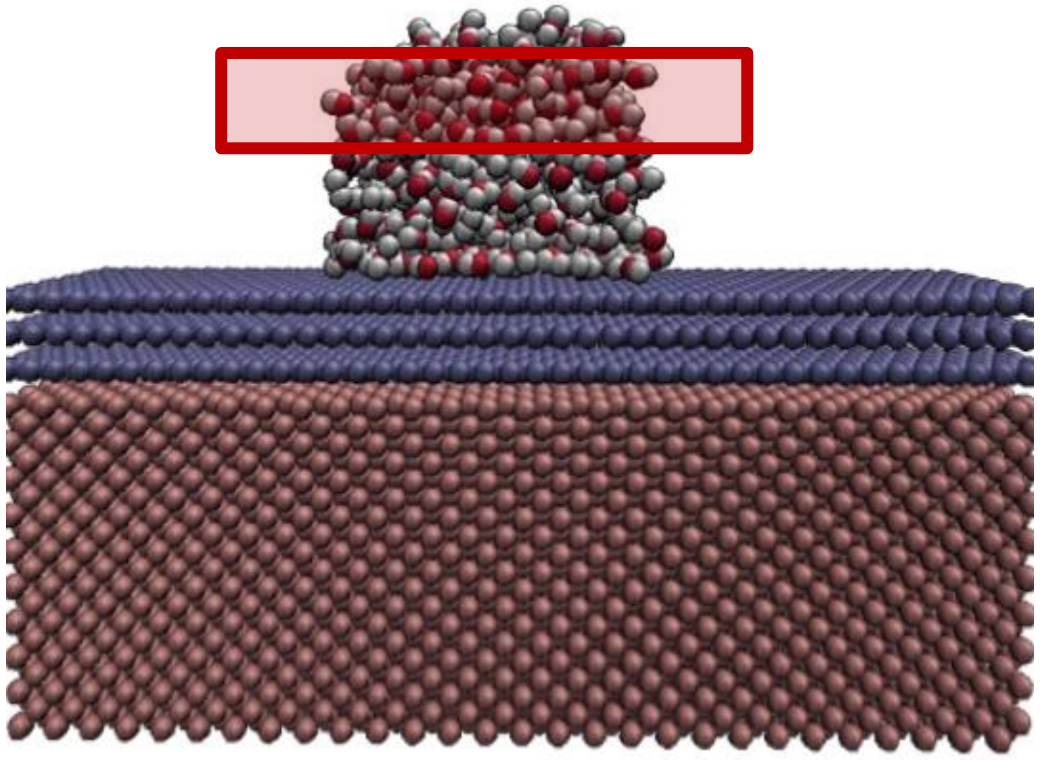
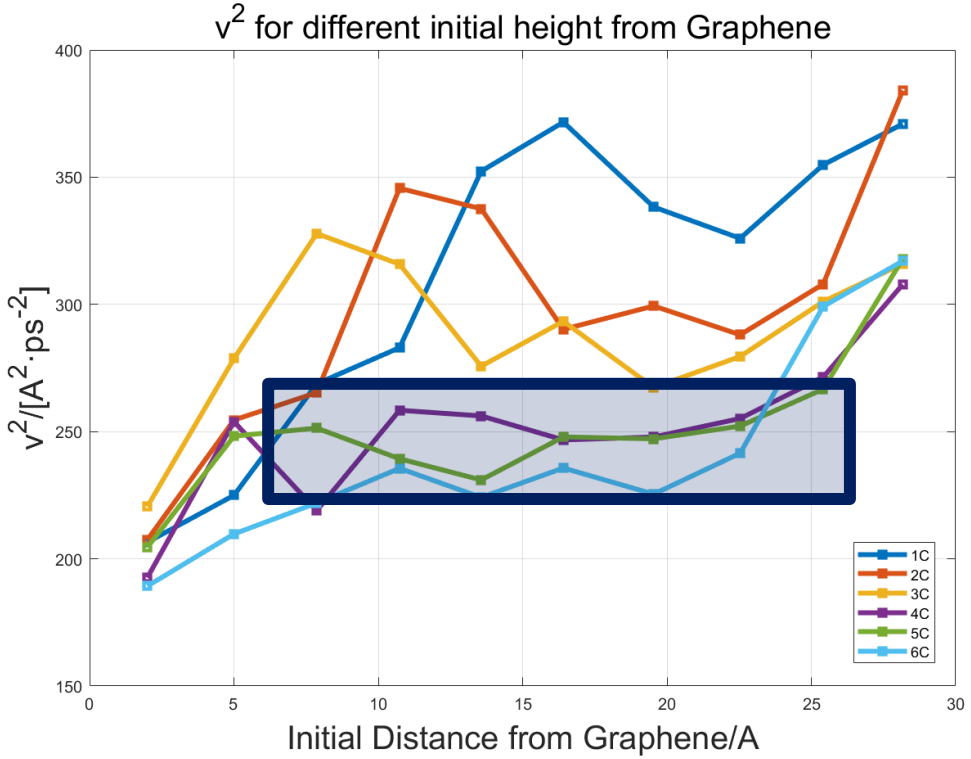


Figure.11. v^2 for different initial height from graphene.

Dynamic Analysis : E_k



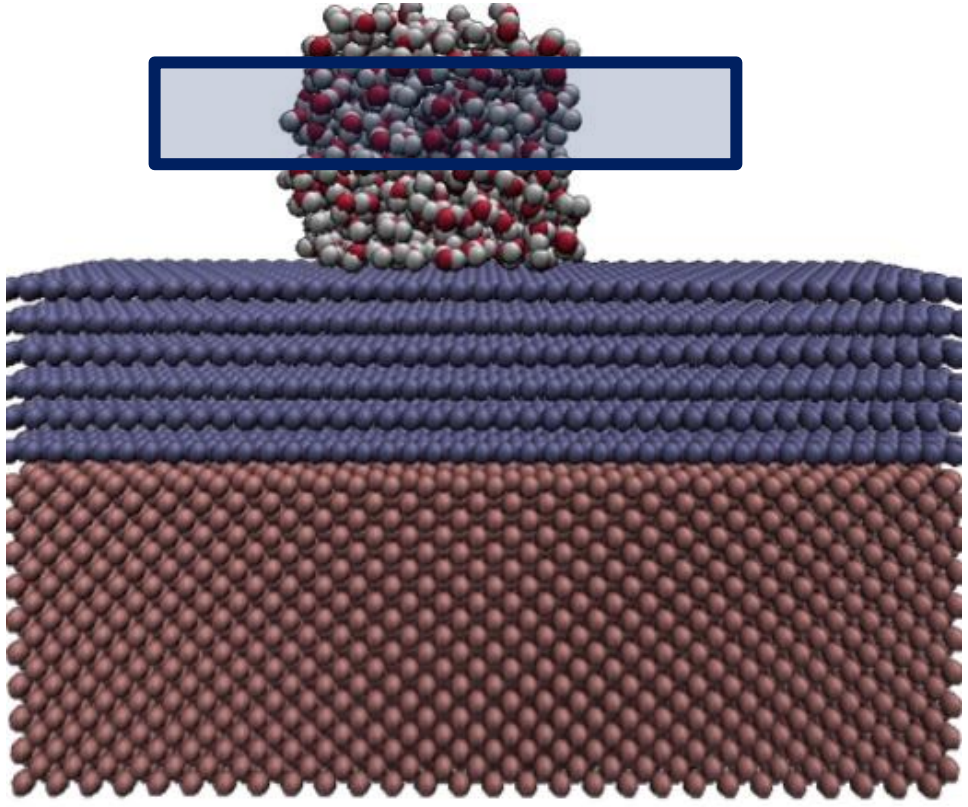
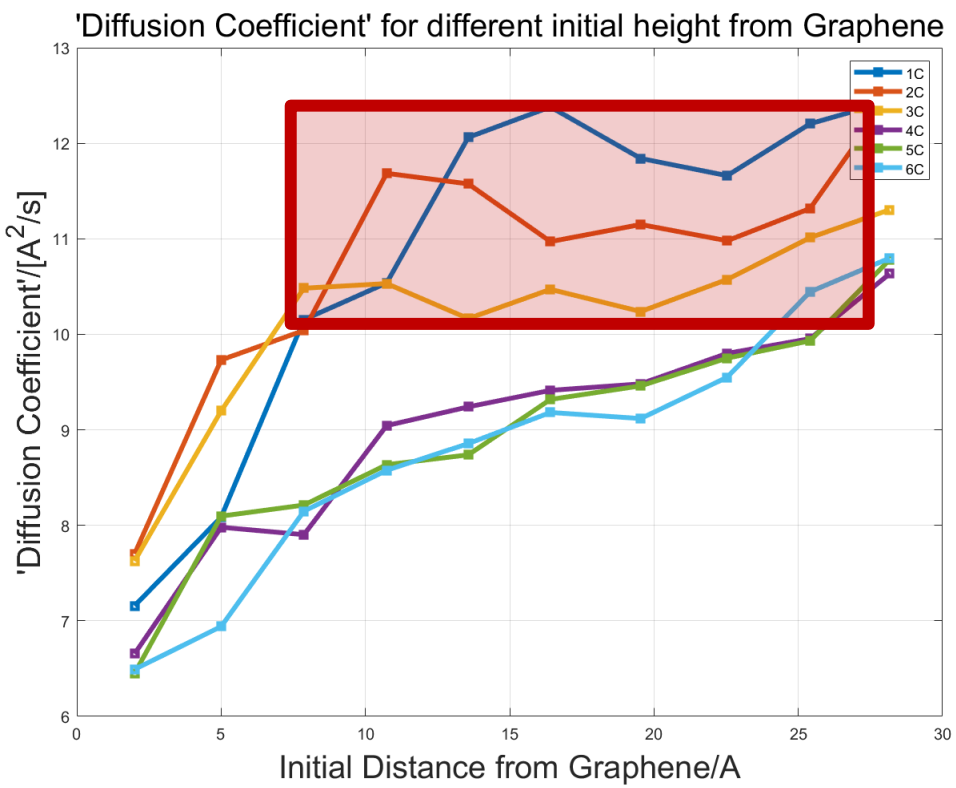


Figure.12 v^2 for different initial height from graphene.

Dynamic Analysis： D’



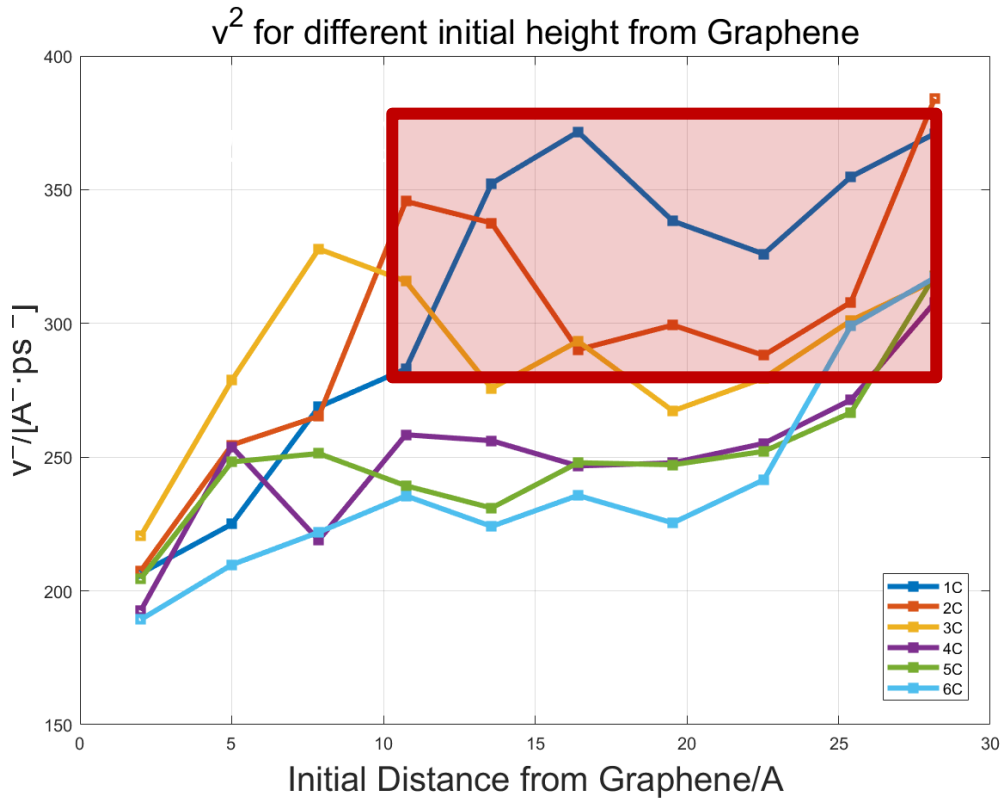
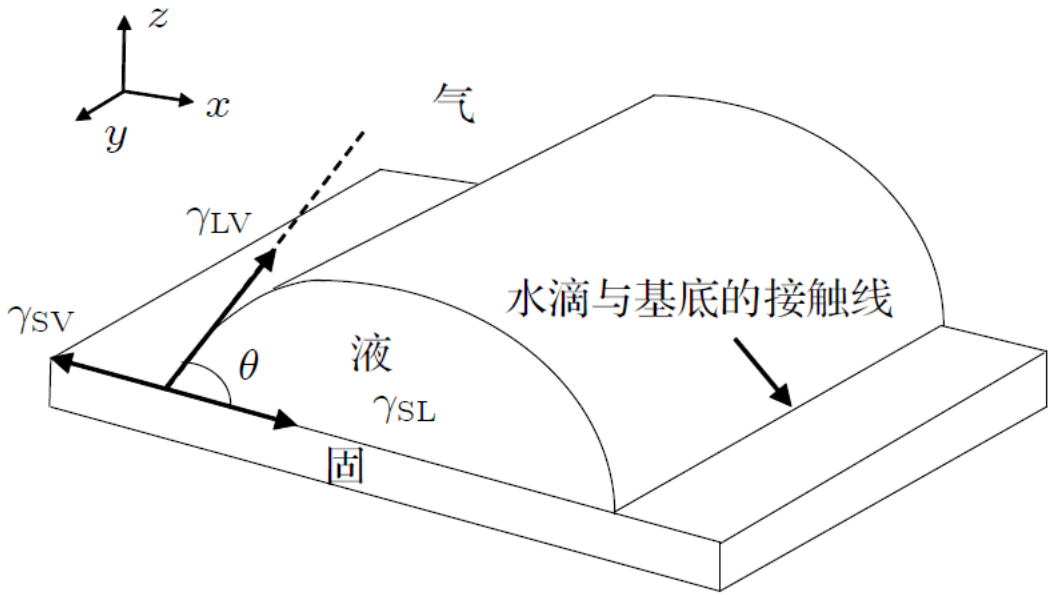


Figure.13. “Diffusion Coefficient” for different initial height from graphene

$$"Diffusion\ Coefficient": D' = \frac{1}{\mathrm{t}} \sum_{i=1}^{N_\alpha} \langle |r_i(t) - r_i(0)|^2 \rangle$$

Contact Angle Analysis

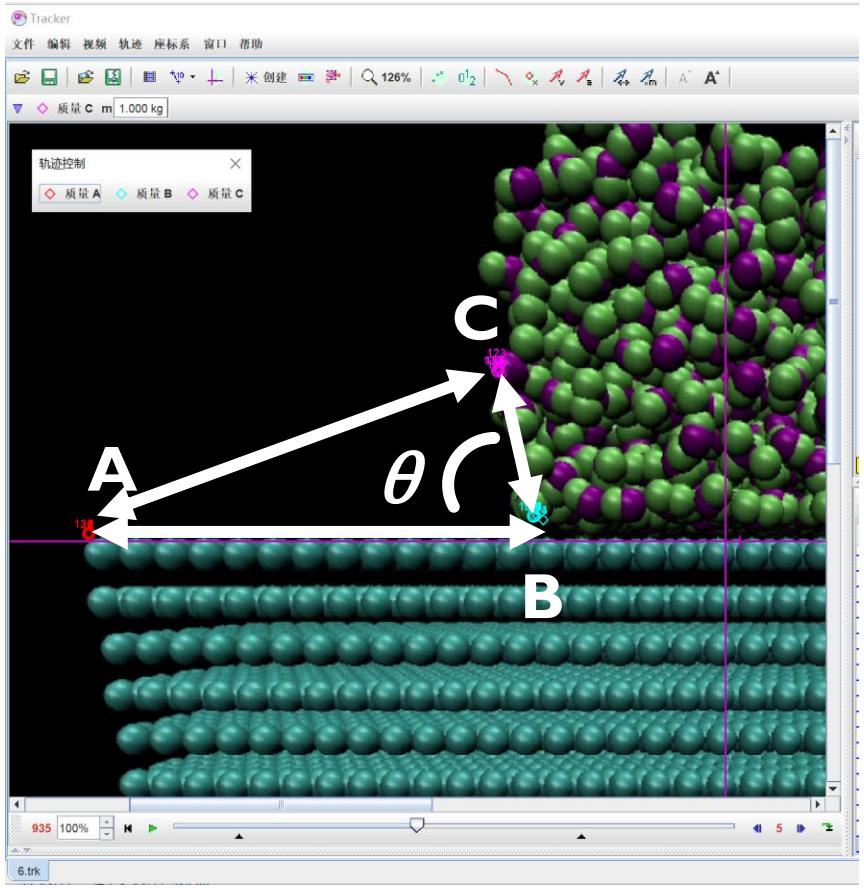


$$cos\theta = cos\theta_{\infty} - \frac{\tau}{\gamma_{LV}} \times \frac{1}{r_B}$$

$$cos\theta_{\infty} = \frac{\gamma_{SV} - \gamma_{SL}}{\gamma_{LV}}$$

Figure.14. Schematic diagram of infinite long liquid column simulation system.
DOI: 10.7498/aps.68.20182307

Contact Angle Analysis



$$|\mathrm{AB}| = \sqrt[2]{(x_A - x_B)^2 + (y_A - y_B)^2}$$

The same for **BC, AC**

$$\theta = \sum_{t1}^{tN} \arccos\left(\frac{|AB|^2 + |BC|^2 - |AC|^2}{2|AB||BC|}\right) / N$$

Where **N** is frame numbers

Figure.15. Contact angle measurement in Tracker.

Contact Angle Analysis

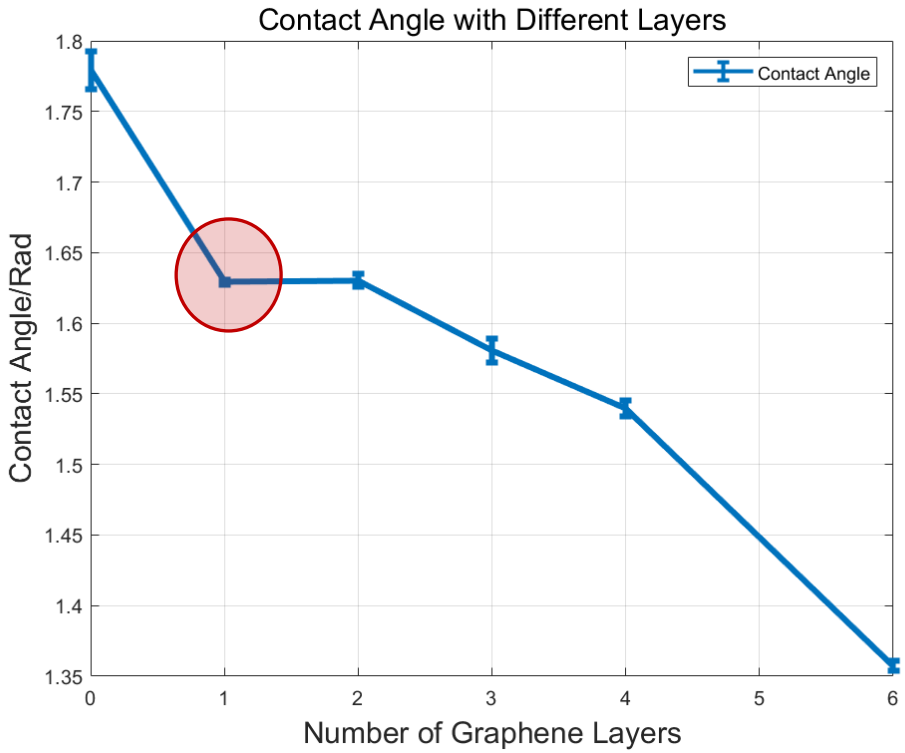
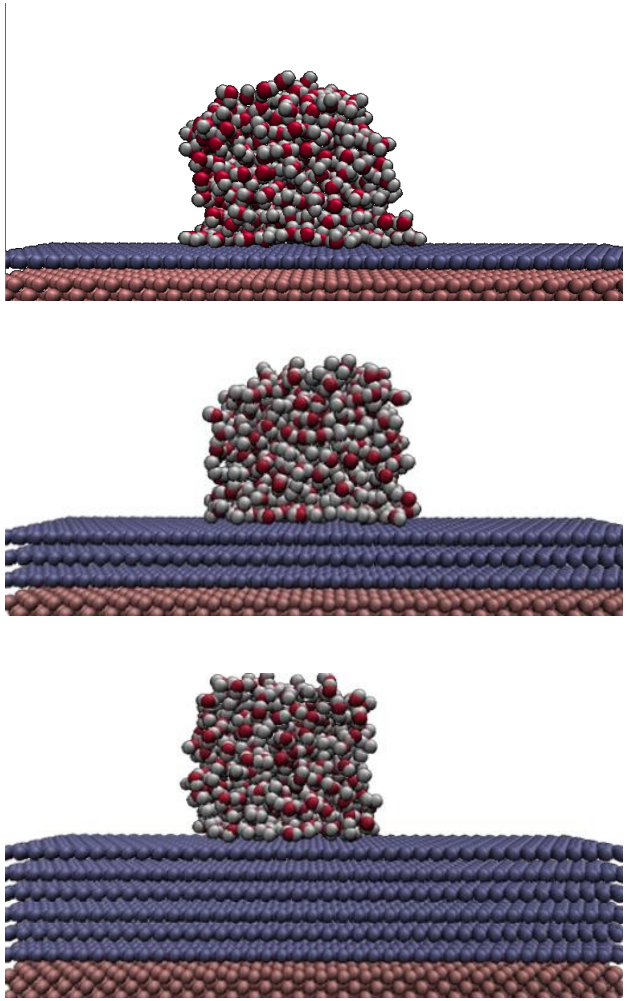


Figure.16. Contact angle with different layers.



One layer

Three layers

Six layers

Reference

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