

Tutorial: BD Exercises

February 06, 2026

Note: Read the entire question paper carefully, before attempting to solve the problems to avoid any mistakes, and possible marks reduction.

Maximum marks: 70

Answers

1. Verification of the Einstein Diffusion Equation

The Einstein diffusion relation for Brownian motion is

$$D = \frac{k_B T}{\gamma},$$

which predicts a linear dependence of the diffusion coefficient D on temperature T , inverse friction γ^{-1} , and inverse mass m^{-1} .

- Step 1: Dependence on friction coefficient

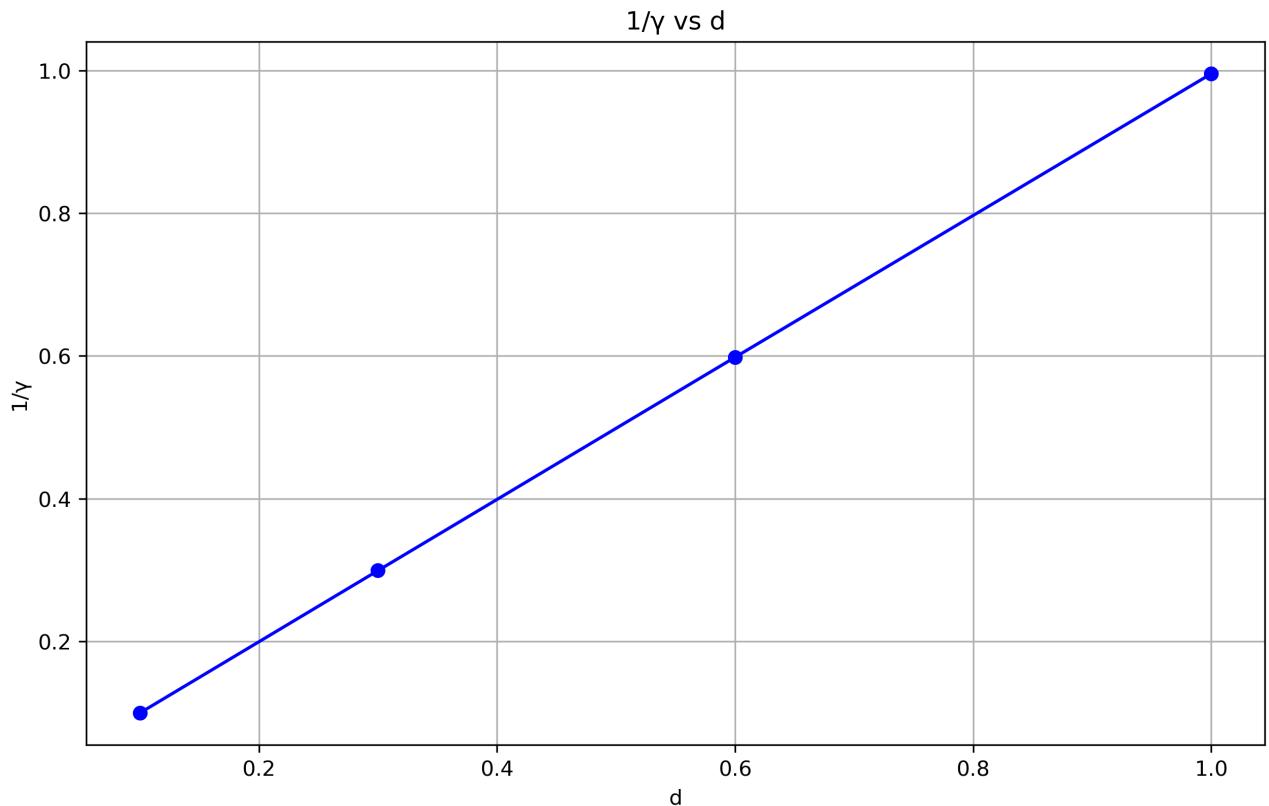


Figure 1: Graphene sheet.

The diffusion coefficient was computed for $\gamma^{-1} = 0.1, 0.3, 0.6, 1.0$, while keeping the mass $m = 1$ and $k_B T = 1.0$ fixed. Figure 1 (`gamma_vs_d.png`) shows that D increases linearly with γ^{-1} , indicating reduced dissipation at lower friction.

This result is in excellent agreement with the Einstein diffusion equation.

- **Step 2: Dependence on temperature**

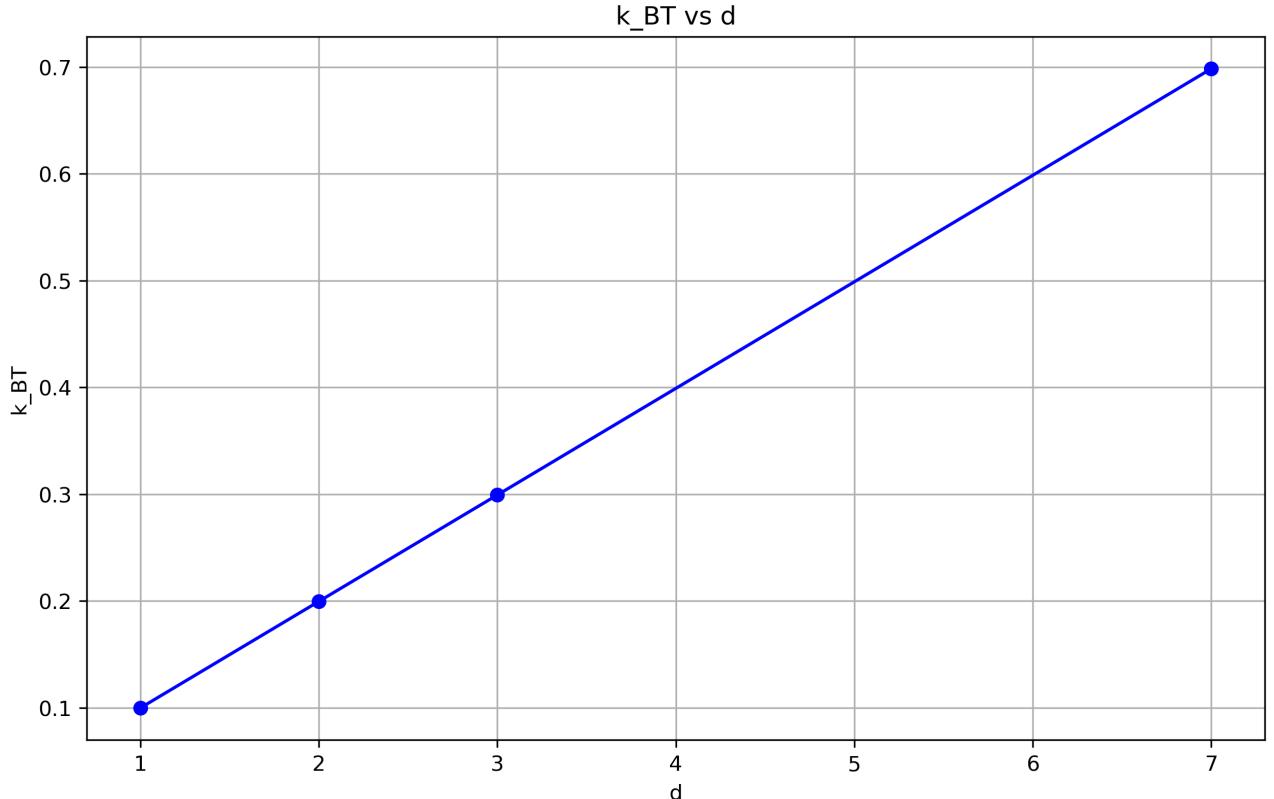


Figure 2: Graphene sheet.

Simulations were performed at temperatures $k_B T = 1, 2, 3, 7$, with fixed $\gamma^{-1} = 0.1$ and $m = 1$. The plot shown in Figure 2 (`t_vs_d.png`) demonstrates a linear increase of the diffusion coefficient with temperature.

This confirms the proportionality $D \propto T$, as expected from theory.

- **Step 3: Dependence on mass**

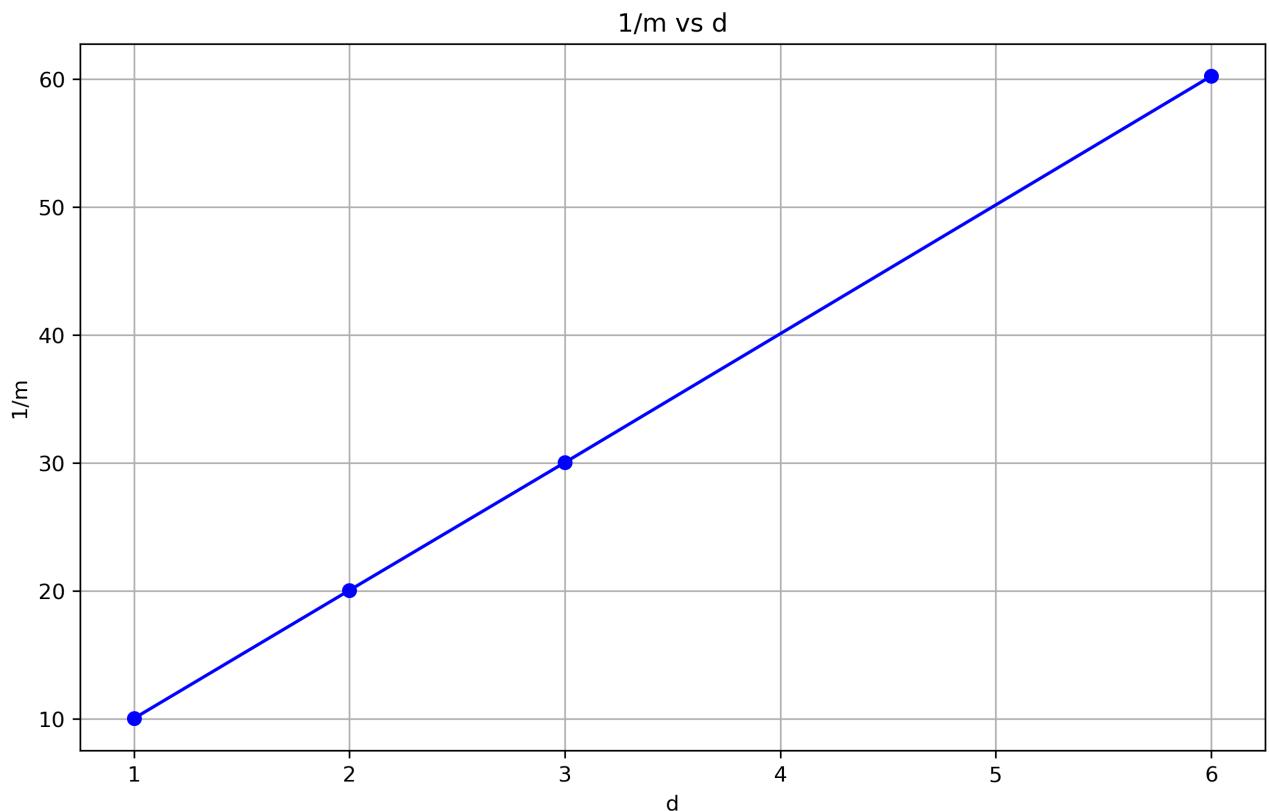


Figure 3: Graphene sheet.

The diffusion coefficient was evaluated for particle masses $m = 1, 2, 3, 6$, while keeping $k_B T = 1.0$ and $\gamma^{-1} = 0.1$ fixed. Figure 3 (`m_vs_d.png`) shows that the diffusion coefficient decreases with increasing mass, consistent with inertial effects in Brownian dynamics.

- **Step 4: Discussion**

From Figures 1â3, the following relations are observed:

$$D \propto \gamma^{-1}, \quad D \propto k_B T, \quad D \propto m^{-1}.$$

All three dependencies are approximately linear within numerical uncertainty, thereby validating the Einstein diffusion equation for the simulated system.

2. Viscosity of a Lennard-Jones Fluid Using the Green-Kubo Method

- **Step 1: Simulation box modification and density control**

To simulate a Lennard-Jones fluid at the target number density $\rho = N/V = 0.5$, the simulation box size and lattice density were appropriately adjusted.

The relevant section of the modified LAMMPS input file is shown below:

```

region          box block 0 23 0 23 0 23
create_box      1 box
lattice         fcc 0.5
create_atoms    1 box
mass            1 1.0

```

Justification: The number density is defined as

$$\rho = \frac{N}{V}.$$

Using an FCC lattice minimizes initial particle overlaps and provides a uniform initial configuration suitable for dense fluids. In LAMMPS, the command `lattice fcc 0.5` specifies a reduced lattice density parameter that directly controls the number of atoms created per unit volume.

The simulation box dimensions were chosen as $23 \times 23 \times 23$, yielding a total volume

$$V = 23^3.$$

With this box size and lattice density, the generated number of atoms results in a measured density close to the target value $\rho = 0.5$, verified using

$$\rho = \frac{\text{count(all)}}{\text{vol}}.$$

Minor deviations (within 10%) are acceptable due to the discrete nature of lattice-based particle generation under periodic boundary conditions. The final density was printed and verified at the end of the simulation.

[5 marks]

- **Step 2: Choice of timestep, thermostat, and integrator**

The Lennard–Jones fluid was equilibrated using a combination of a small timestep, a Langevin thermostat, and an NVE integrator. The relevant equilibration section of the input script is shown below:

```
variable dt      equal 0.00001
timestep        ${dt}

velocity        all create ${Tinit} 12345 dist gaussian
velocity        all scale ${T}

fix thermostat  all langevin ${T} ${T} 0.1 34300
fix integrator  all nve

run             100000

variable dt      equal 0.001
timestep        ${dt}

run             50000
unfix           thermostat
unfix           integrator
```

Justification: A very small timestep ($\Delta t = 10^{-5}$) was initially chosen to safely relax the dense LJ system and avoid numerical instabilities caused by large repulsive forces during early equilibration. Particle velocities were initialized from a Maxwell–Boltzmann distribution at a slightly higher temperature $T_{\text{init}} = 1.2$ to accelerate equilibration and then rescaled to the target temperature $T = 1.0$.

A Langevin thermostat was applied during equilibration to efficiently control the temperature and remove excess kinetic energy. The damping constant ($\tau = 0.1$) ensures rapid thermalization without overdamping particle dynamics. Time integration was performed using the velocity-Verlet scheme via `fix nve`.

After initial equilibration, the timestep was increased to $\Delta t = 0.001$ to improve computational efficiency while maintaining energy stability. All thermostats were removed before the production run to ensure that equilibrium stress fluctuations required for the Green–Kubo viscosity calculation are not artificially damped.

[5 marks]

- **Step 3: Density dependence of viscosity**

The shear viscosity was computed for densities

$\rho = 0.05, 0.1, 0.3, 0.4, 0.5$ using the Green–Kubo formalism.

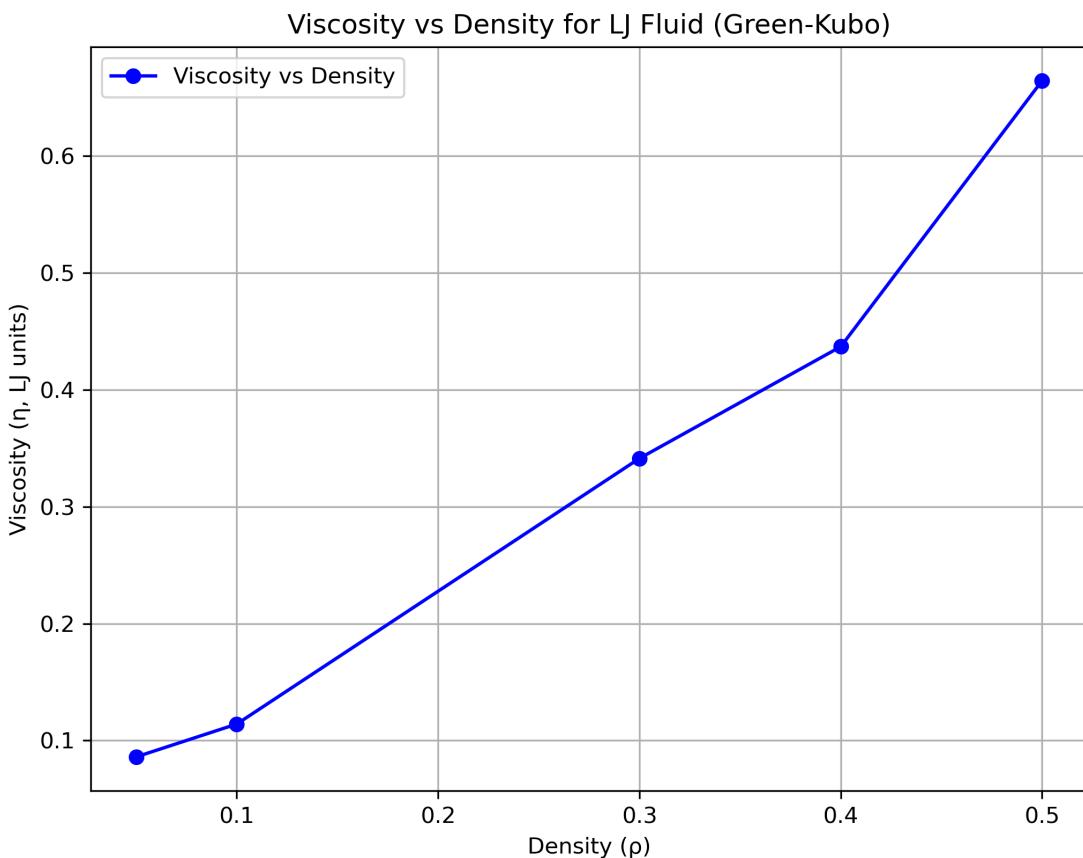


Figure 4: Graphene sheet.

Figure 4 shows that viscosity increases monotonically with density.

This trend is physically reasonable, as higher densities lead to stronger interparticle interactions and enhanced momentum transport.

- **Step 4: Conversion of viscosity from LJ to SI units**

In Lennard–Jones (LJ) reduced units, viscosity is expressed in terms of the fundamental LJ units of mass m , energy ϵ , and length σ . The dimensional form of viscosity

is

$$[\eta] = \frac{\text{mass}}{\text{length time}}.$$

In LJ units, the characteristic time scale is defined as

$$\tau = \sigma \sqrt{\frac{m}{\epsilon}}.$$

Therefore, the LJ unit of viscosity can be written as

$$\eta_{\text{LJ}} = \frac{m}{\sigma \tau} = \frac{m}{\sigma^2} \sqrt{\frac{\epsilon}{m}} = \frac{\sqrt{m \epsilon}}{\sigma^2}.$$

Hence, the conversion factor from LJ viscosity units to SI units (Pa·s) is

$$\eta_{\text{SI}} = \eta_{\text{LJ}} \frac{\sqrt{m \epsilon}}{\sigma^2}.$$

(a) Substitution of physical values The LJ parameters are mapped to physical units as follows:

$$\begin{aligned}\sigma &= 1 \times 10^{-10} \text{ m}, \\ \epsilon &= k_B T, \quad T = 300 \text{ K}, \\ k_B &= 1.380649 \times 10^{-23} \text{ J K}^{-1}, \\ m &= 12 \text{ amu}, \quad 1 \text{ amu} = 1.660539 \times 10^{-27} \text{ kg}.\end{aligned}$$

First, convert the mass into SI units:

$$m = 12 \times 1.660539 \times 10^{-27} = 1.99265 \times 10^{-26} \text{ kg}.$$

Next, compute the energy scale:

$$\epsilon = k_B T = 1.380649 \times 10^{-23} \times 300 = 4.14195 \times 10^{-21} \text{ J}.$$

Now evaluate $\sqrt{m \epsilon}$:

$$\sqrt{m \epsilon} = \sqrt{(1.99265 \times 10^{-26})(4.14195 \times 10^{-21})} = \sqrt{8.25 \times 10^{-47}} = 9.08 \times 10^{-24}.$$

Finally, divide by σ^2 :

$$\frac{\sqrt{m \epsilon}}{\sigma^2} = \frac{9.08 \times 10^{-24}}{(1 \times 10^{-10})^2} = 9.08 \times 10^{-4} \text{ Pa} \cdot \text{s}.$$

(b) Final conversion factor

$1 \eta_{\text{LJ}} = 9.1 \times 10^{-4} \text{ Pa} \cdot \text{s}$

Thus, the viscosity obtained from LAMMPS in LJ units can be converted to SI units by multiplying it with $9.1 \times 10^{-4} \text{ Pa} \cdot \text{s}$.

3. Dumbbell-Shaped Patchy Particle System

- **Step 1: Constructing a dumbbell-shaped molecular template**

The dumbbell-shaped molecule consists of three atoms:
- One central hard-core atom (core)
- Two patch atoms located on opposite ends of the core

The complete .mol file is provided below:

```
# Dumbbell-shaped molecule template

3 atoms          # Total number of atoms in the molecule

# ----- COORDINATES -----
# Format: atom_index    x    y    z (in reduced LJ units)
Coords
1  1.0  1.0  1.0    # Core atom at the center
2  1.0  1.0  1.5    # Patch atom on +z direction (bond length 0.5)
3  1.0  1.0  0.5    # Patch atom on -z direction (bond length 0.5)

# ----- ATOM TYPES -----
# Format: atom_index    type
Types
1   1    # Core atom
2   2    # Patch atom
3   2    # Patch atom
```

Justification: - The molecule is symmetric along the z-axis to form a dumbbell shape.
- The central core atom (type 1) is bonded to both patch atoms (type 2) with fixed bond length 0.5 LJ units.

[5 marks]

- **Step 2: Phase behavior**

Simulations were performed over a range of temperatures. At lower temperatures ($k_B T < 0.15$), the system exhibits liquid-like chain-forming behavior, as shown in Figure 5.

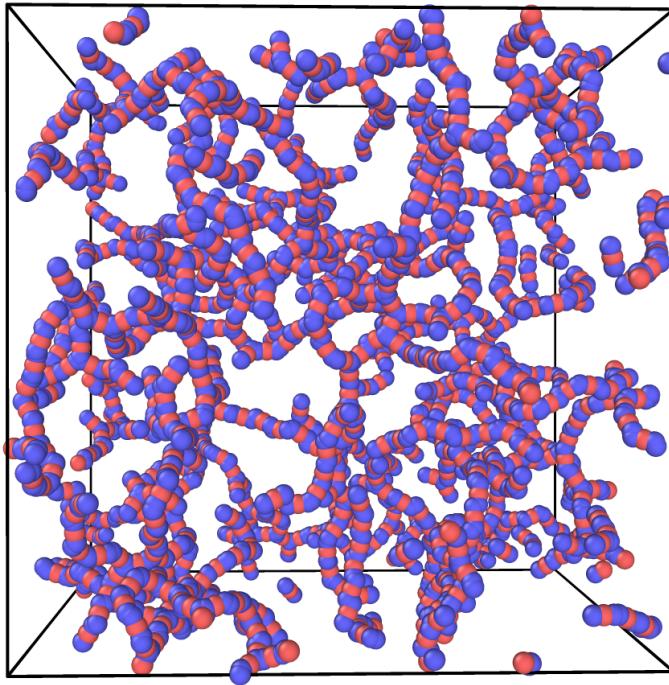


Figure 5: Graphene sheet.

Core and patch particles are clearly distinguishable by color and size. The corresponding temperature at which stable chains are observed is reported.

- **Step 3: Stability discussion**

The chain structures are metastable and persist over long simulation times at lower temperatures.

At low temperatures, thermal motion is insufficient to break directional patch bonds, leading to metastable chains.

At higher temperatures, thermal fluctuations dominate, resulting in chain breakup which leads system to the lowest potential energy state, which has more than one bond per patch (where a chain can have only one bond per patch). Compared to globular structures observed at $k_B T = 1.0$, chain phases are stabilized by directional interactions and anisotropic bonding and therefore not an equilibrium structure, especially at higher temperatures.

4. Topology Verification of a Carbon Nanotube

We consider a carbon nanotube (CNT) consisting of a total of 288 carbon atoms, divided into 264 bulk atoms and 24 edge atoms. Bulk atoms are bonded to three neighbors, while edge atoms are bonded to only two neighbors.

- **Number of bonds**

Each bond connects two atoms, so double counting must be avoided. The total bond contributions are

$$264 \times 3 + 24 \times 2 = 792 + 48 = 840.$$

Dividing by two to remove double counting, the total number of unique bonds is

$$N_{\text{bonds}} = \frac{840}{2} = 420.$$

- **Number of bond angles**

A bond angle is formed by two bonds sharing a common central atom.

A bulk atom with three neighbors forms

$$\binom{3}{2} = 3$$

bond angles, while an edge atom with two neighbors forms

$$\binom{2}{2} = 1$$

bond angle.

Thus, the total number of bond angles is

$$N_{\text{angles}} = 264 \times 3 + 24 \times 1 = 792 + 24 = [816].$$

- **Number of dihedral angles**

A dihedral angle is defined by four sequentially bonded atoms $A-B-C-D$, with the bond $B-C$ acting as the central bond. For a bond between atoms with coordination numbers n_B and n_C , the number of dihedrals is

$$(n_B - 1)(n_C - 1).$$

In the CNT, there are two types of bonds:

- Bulk–bulk bonds: $n_B = n_C = 3 \Rightarrow 4$ dihedrals per bond
- Bulk–edge bonds: $n_B = 3, n_C = 2 \Rightarrow 2$ dihedrals per bond

Each of the 24 edge atoms has two bonds, giving

$$24 \times 2 = 48$$

bulk–edge bonds. Therefore, the number of bulk–bulk bonds is

$$420 - 48 = 372.$$

The total number of dihedral angles is then

$$N_{\text{dihedrals}} = 372 \times 4 + 48 \times 2 = 1488 + 96 = [1584].$$

- **Number of improper dihedral angles**

An improper dihedral is defined for each atom bonded to exactly three neighbors, with that atom acting as the center. Only bulk atoms satisfy this condition.

Thus, the total number of improper dihedrals is

$$N_{\text{impropers}} = 264.$$

The calculated numbers are consistent with the expected topology of a hexagonal sp²-bonded carbon nanotube and provide a reliable verification of the generated molecular topology.

5. Martini Force-Field Representation of Carbon Nanotubes

- Since we have a chain configuration and each Martini carbon particle represents four real carbon atoms, the effective bond length between two Martini beads is approximately four times the real C–C bond length:

$$d_{\text{Martini}} \approx 4 \times 1.2 \text{ \AA} = 4.8 \text{ \AA}.$$

- On the provided graphene lattice (Fig. 5), Martini beads are placed such that each bead overlays four carbon atoms, forming a coarse-grained lattice that perfectly superimposes the real structure without voids or defects. To do so, there are several ways and each of them are correct answer.

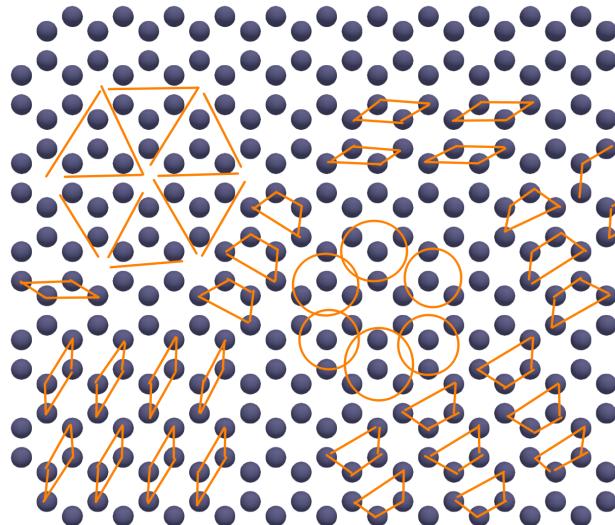


Figure 6: Caption