Using Molecular Simulation to Understand the Interactions Between DNA-Coated Graphene Sheets and Phospholipid Bilayers

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UMBC University of Maryland Baltimore County 1966

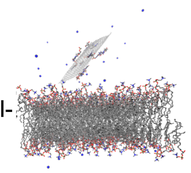
MUMS Multiscale Modeling and Simulation

Background

- Graphene is a nanocarbon made up of two-dimensional layered hexagonally arranged carbon atoms and derived from the parent material graphite. Its unique structure enables its usefulness for various applications, including drug and gene delivery.[1]
- Some of these applications require interactions between graphene and lipid bilayers, which can be studied using molecular simulation.
- Phospholipids bilayers compose cell membranes, which are frequent targets for drug delivery.
- Simulations allow the study of how DNA-coated graphene inserts into bilayers using harmonic springs by observing the work and force applied as a function of the angle of insertion and harmonic force constant.

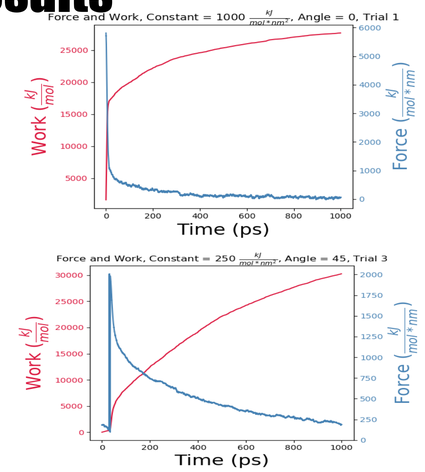
Methods

- GROMACS 2018 software as well as the CHARMM force field conduct a molecular dynamics simulation using these force constants: 125, 250, 500,and 1000 $\frac{kJ}{mol*nm^2}$, as well as these angles: 0, 15, 30, and 45 degrees.[2,3,4]
- Harmonic springs are used to pull the graphene sheet into the bilayer
- The phospholipid bilayer is composed of two main lipid molecules:1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) and cholesterol (CHOL)

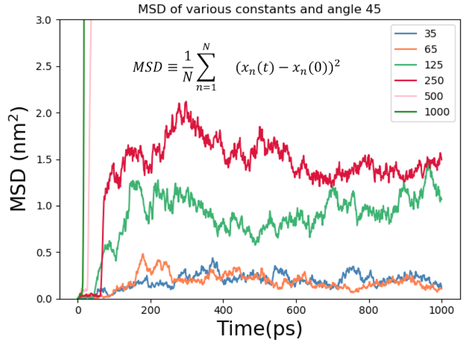


- DNA can possibly modulate the graphene-bilayer interactions, and four single-stranded DNA is chosen as the model for these tests
- Initially the graphene sheet, which is 5 nm x 5 nm, is situated 0.5 nm above the bilayer with the corner closest to the bilayer. The sheet is tilted such that 90 degrees corresponds to the sheet being parallel to the bilayer surface

Results



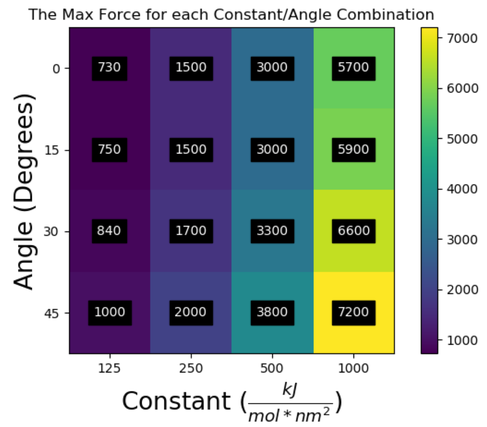
- Force peaks early due to the distance between the graphene and the center of the bilayer, but quickly decreases to zero as the graphene gets closer to the center and the harmonic spring weakens.
- As the force diminishes, work approaches a steady-state value

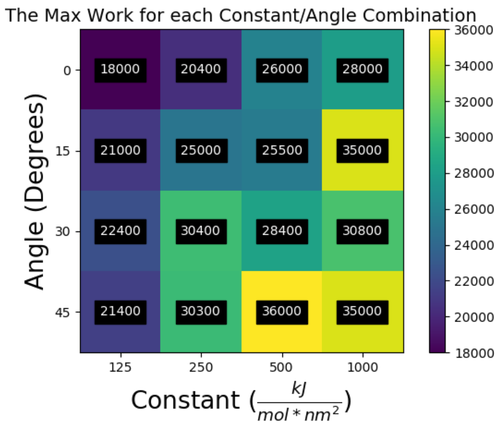


Units of force constants = $\frac{kJ}{mol*nm^2}$

- Using mean squared displacement indicates that DNA remains better mounted on the graphene sheet with lower force constants

Max Force and Work





- In general, the max work increases as the force constant and the angle of insertion increases.
- The max force follows the same trend.

Conclusion

- The max work and force increase when the angle and force constant increase
- A lower force constant also better allows for DNA to remain on the graphene.

Future Work

- Examine bilayer structure to observe graphene effects
- Find the lowest force constant for each angle that allows for insertion
- Implement different pulling forces to draw graphene into the bilayer

Acknowledgements

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