Homework Assignment 1

Modeling Graphene Surface Properties

Due date: 15.Mar.2024

Graphene, a two-dimensional, one-atom-thick hexagonal lattice of carbon atoms, has received considerable attention due to its extraordinary properties. Research on wetting phenomena on graphene is the first step towards quantifying its surface properties, because the interfacial energies involved directly determine the macroscopic contact angle, θ of a liquid droplet on graphene. Using the concepts and methods that we discussed in class, we can approach this interesting system in a simple and insightful manner. Here are the assumptions used in the homework:

1. Graphene is a two-dimensional sheet with zero thickness, and the mass is uniformly distributed in the sheet.
2. Graphite is a lamellar structure of graphene with the interlayer distance of $d_0 = 3.35$ Å.
3. van der Waals (vdW) interactions are perfectly additive and pairwise.

Please answer the following questions to solve the problem step-by-step.

Q1 Surface tension of graphene and graphene stacks

In this question we will derive the surface tension of graphene and its stacks using the knowledge learned from the lecture. We assume the graphene sheets in graphite are dominated by the vdW forces. The vdW potential between two carbon atoms is given by: $V_{CC} = -\beta_{CC}/r^6$, where r is the distance between the two carbon atoms.

1. Please show that the surface tension of single layer graphene γ_{G1} is given by $\gamma_{G1} = \dfrac{\pi\sigma^2\beta_{CC}}{4d_0^4}$, where σ is the surface density of carbon atoms on graphene. Graphene has hexagonal unit cell with lattice constant $a = 2.49$ Å (Figure 1).
2. Assume two stacks of graphene A and B, both composed of parallel graphene sheets with interlayer distance d_0 separated by a distance δ (Figure 2). Stack A contains m layers of graphene, and graphene stack B contains n layers. Please derive the expression for the work of adhesion $\Delta W_{AB}(m, n)$ between A and B separated by a distance δ as function of m and n.
3. If we have $m \to \infty$ and $n \to \infty$, $\Delta W_{AB}(\infty, \infty)$ essentially becomes the work of adhesion for **graphite**. Assuming that the distance $\delta = d_0$, please write the expression for the surface tension of graphite $\gamma_{G\infty}$ using the variables given here.

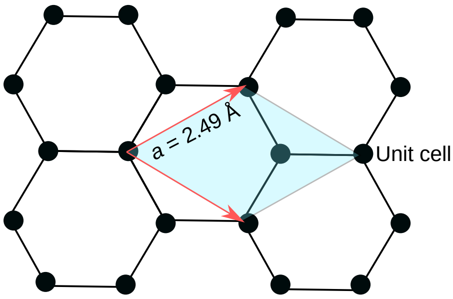

Figure 1: Structure of graphene. The unit cell and lattice constant are shown.

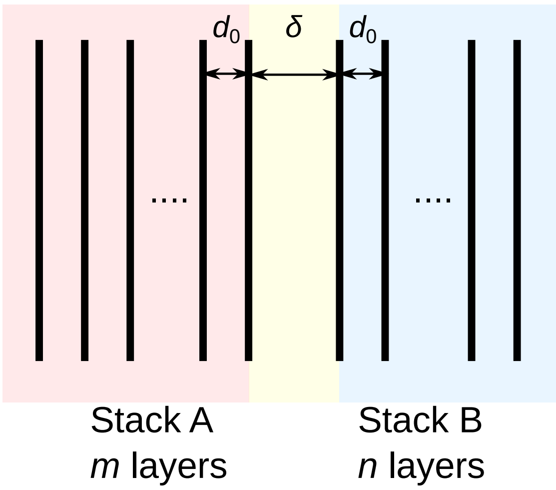

Figure 2: Scheme of graphene stacks A and B seperated by a distance δ with layer numbers m and n, respectively.

4. Experimentally, the surface tension of graphite $\gamma_{G\infty}$ has been found to be 129 $mJ \cdot m^{-2}$ [1].

   Using the expression you obtained in Q1.3, calculate the value of β_{CC}.

5. Using the value of β_{CC}, please calculate the energy required to cleave a sheet of 1-layer, 2-layer,.., to n-layer graphene (n up to 10) from graphite. Please plot the energy (in unit of $mJ \cdot m^{-2}$) as a function of n.

[1] Renju Zacharia, Hendrik Ulbricht, and Tobias Hertel. "Interlayer cohesive energy of graphite from thermal desorption of polyaromatic hydrocarbons". In: *Phys. Rev. B* 69 (2004), p. 155406.