Hey guys, sorry for missing today’s meeting, I’m just not well enough to make it. I contacted everyone I could so hopefully they have made arrangements for you during that time. I am well enough to type, though, so here’s some notes to hopefully help you with your paper:

The ‘birch\_murnaghan.png’ shows a series of energy calculations vs cell separation distance cubed. The Birch-Murnaghan equation of state relates the volume of a material to the energy of the material. The VASP program calculates the total energy, and by varying the distance between the graphene and silicon layers and cubing the distance a volume can be calculated. The five points are then fit to the Birch-Murnaghan via python script. The minimum point on that black curve line is the point of lowest total energy, i.e. the most stable point. By taking the x-value at that point and raising it to the 1/3 power the stable layer spacing can be estimated. For graphene and our crystalline silicon layer the fitted stable layer spacing was calculated to be **2.171513 Angstroms.**  I used that estimated separation distance for each of the glassy phases in the series, though it would have been more precise to perform a layer spacing fit for each glassy phase separately.

The excel sheet in the Dropbox folder shows the summary of the calculated data for the series of glass silicon layers. In this case ‘glassiness’ is equal to the maximum possible distance, in Angstroms, an atom may be displaced from the crystalline position (something to think about is what would the maximum displacement distance be? It’s not equal to the glassiness parameter!) E.g., if the glassiness paremeter is equal to 0.4, that means each atom may be shifted up to 0.4 Angrstroms from its initial crystalline position in the x and y direction. A glassiness parameter of zero would be the crystalline phase. This roughly approximates a glassy phase of silicon.

Several energy calculations were performed:

A single layer of graphene was calculated. Since the graphene layer remains undisturbed, only a single calculation needed to be performed. That energy is in the ‘graphene only’ column.

Each of the 5 silicon glassy layers were calculated. Those energies are in the ‘silicon only’ column.

The energies of the combine graphene and silicon layers were calculated, those are in the ‘graphene and silicon layered’ column.

The following experimental details would typically be written in a scientific publication

Program used: The Vienna Ab initio simulation package (VASP)

Functional: vdW-optB88 (This functional is meant specifically for calculations with van der Waals forces, which we have in our system since van der Waals is what adheres the two layers to each other.)

**Interpreting the data:**

The purpose of these calculations is to measure the binding energy, which is a quantified measure of how much the two materials stick together via the van der Waals force. If you take the two layers alone, then stick them together, the energy difference should be negative. This means the bonded layers stuck together have a lower total energy than the two separate layers. Phrased another way, it means it would require energy to break the two layers apart. The more negative the binding energy, the more energy it takes to separate the two layers, so the stickier the bond is.

The equation for binding energy is below:

[g\_s] – ([s] + [g]) = [binding energy]

where ‘g\_s’ is the energy of the combined graphene and silicon system where they’re stuck together, ‘s’ is the energy of the silicon layer alone, and ‘g’ is the energy of the graphene layer alone. For this series the graphene energy remains the same, so it’s only the combined system and the silicon layers by themselves that determine the binding energy. If the binding energy is negative, the layers are bonded, but if the binding energy is positive that means it takes energy to force them together, so not only are they not sticky, they are repellent,

**Forming a hypothesis:**

If a hypothesis is necessary, try to use the above equation to form one along with the information that the energy of the silicon layer will be the greatest factor in determining binding energy. My thinking was that the glassy systems would have higher total energy, therefore be less stable on their own, and so by the above equation they would be more sticky than the crystalline phase. However, my previous experience tells me crystalline phases tend to form better bonds with other crystalline phases, so I assumed the combined ‘g\_s’ energy value would change such that the glassy phases were overall less sticky.

**Analysis of the data:**

The data is strange, not what I expected. Well, the outcome is expected, but not the reason why. It appears the energy of the combined system hardly changes. Only the solo silicon layer varies much at all, and it varies in the opposite way I would expect. Oddly enough the glassier the silicon phases get, the lower their total energy. The 2D silicon wafer is actually more stable in a glassy phase. If we were able to fully simulate bulk silicon, rather than a single layer, the energy difference may not be as large.

As it stands, the data indicates graphene sticks to crystalline silicon stronger than glassy silicon. By this very rough estimation we have calculated, it would take more than twice as much energy to separate pure crystalline silicon from graphene than it would to separate glassy silicon from graphene.

**What you guys should do:**

Divide the binding energy (the last column) by the area to get the binding energy per unit area. The units for that will be [eV/Angstrom^2]

Take that data I’ve given you and make a good-looking plot from it. On the y-axis you should plot binding energy per unit area, and on the x-axis you should plot glassiness.

Bonus: use Excel, or some other program, to fit an equation to the data that allows you to relate the glassiness parameter with binding energy.

You may also want to attempt to find publications online that do similar work to compare ours with.

Think of ways to improve the experiment, if you can. We won’t do any of it since we have limited time, but it’s a good idea to always think about how something could be done better. Consider that we are testing a very small section, only a square nanometer, of glassy phases that are randomly distributed. It could be our data is just an artifact of randomness, rather than a real phenomenon. How might we determine if it’s merely randomness?

It’s likely I won’t be available for the rest of the day, but whatever progress you make on the paper I’ll check once I’m able and I’ll provide feedback. Email me with any thoughts or questions, I’ll get back to you as soon as I can.