As for the measurement of the interaction between gold surface and alkyne.

The thought of this work came from the research of a foreign chemical group published. They theoretically proposed four possible structures of the interaction between the Au nanoparticle and alkyne. We can see them on the sketch map. Our ultimate goal is to experimentally determine which form of the Au-C bond do existed. To do this, we need to do single molecular experiments.

The principle of our SMFS(single molecule force spectroscopy) testing is shown on the right side. In 2015, a research about the interaction between the sulfydryl and gold nanocluster with long chain molecule and sulfydryl. A long chain alkyne is attached to the AFM tip. Then the tip contact with the gold base. The alkynyl group is pressed toward the Gold atom and thus form the Au-C interaction. When the tip is raised again and apply tension on the long PEG chain, the rupture force of the bond can be recorded on the force spectra.

This is how we made our long chain modified AFM tip.

First, we need to modify the tip with APTES molecule and ALK-PEG-NHS. The APTES molecule is showed on the picture. The APTES can form Si-O bond with the silicon AFM tip. While the ALK-PEG-NHS, a long chain molecule with alkenyl on one side and N-Hydroxysuccinimide(羟基丁二酰亚胺) on the other side, and act with the amino-group on the APTES. Thus, form the long chain alkyne we need.

To calculate the strength of the Au-C bond, we need to first model the long PEG chain. The model used is the worm like chain model, a spring that based on entropy effect. It eventually comes to two formulas like this.

The first formula is the partition function which is simplified through the solution of the Schrodinger equation. The second formula shows the relationship between the tension F, end to end length z of the polymer, and the temperature T.

These is how we analyze our data. The two graphs are single molecule force spectroscopy and the statistic result of the rupture force.

As we can see in the force spectra, there are two peaks. The first peak is the Van Der Waals interaction between the AFM tip and the gold base. The second peak is what we were interested about, the interaction between the gold surface and the alkenyl. We used the formula mentioned above to fit it, and get the statistic result. The result is then fitted with Gauss pulse, and average rupture force as well as the half-width of the Gauss pulse are calculated.

Here comes our experiment results.

This formula is calculated by quantum physics method. It shows the relationship between the tension f and the force-applying rate rF (also represent the speed of the tip). Here P is the persistence Length Lp, and fβ is a thermal force parameter related to the temperature and the width of the energy gap xβ.

In order to fit our result with this formula, the experiment is carried out with different force-applying rate rF. We can see from graph, as the force-applying rate increases, the rupture force also increased. And if we prolong this line, when the rupture force comes to zero, then the force-applying rate rF represents the dissociation rate of the Au-C bond. (the time that it takes for the alkynyl to detach from the gold base)