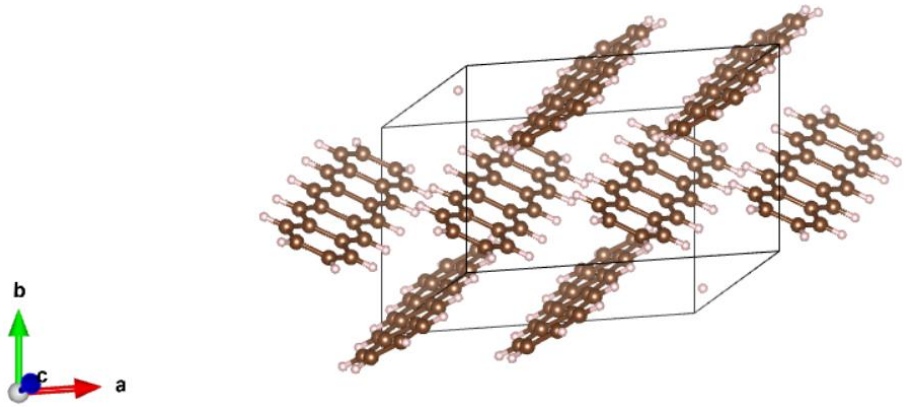
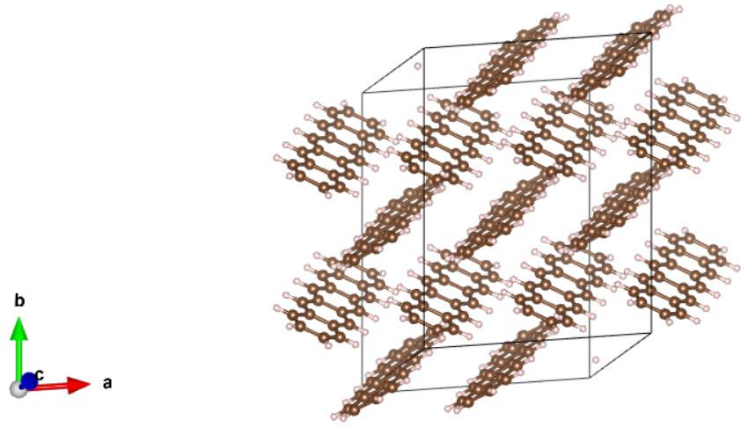
I am Qingxin Zhang, a first-year Ph.D. student in chemistry from the university at buffalo. I am working in Dr. Akimov's lab on the modeling of electron transfer in photocatalytic process. I will discuss in this report how I can take advantage of the computational chemical packages discussed in this workshop. On the 7/12 afternoon, tutorial_of_eQE_and_QE provide the new idea for me. I use the relevant code and software VESTA to cut and split pentacene. The reason I chose pentacene because organic semiconductors have more flexibility compared to inorganic semiconductors, such as the ability to mass produce at low cost. But organic semiconductors are far less efficient at converting solar energy into energy than inorganic semiconductors. Getting the photochemical efficiency of organic semiconductors up is an interesting challenge.

In the workshop, I found that cutting the cell in x, y, and z axes or dividing the cell into fragments may increase the computational efficiency and better convergence. I chose two different sizes of crystals, 2x1x1 and 2x2x1.





I performed four different sets of energy calculations on the two different cells.

2x1x1			fragments	split direction	energy(ry)
	e	QE	one piece	z axis	-1074.11019152
			two pieces	z axis	-1074.15577136
			one piece	x,y,z axis	-1074.11019152
		QE	one piece	no split	-1074.11050934
2x2x1			fragments	split direction	energy(ry)
	e	QE	one piece	z axis	-2148.22179864
			two pieces	z axis	-2148.35493835
			one piece	x,y,z axis	-2148.22179864
		QE	one piece	no split	-2148.22244215

I found that cutting in z-axis or cutting in x-axis, y-axis, z-axis, all three axes, the final calculated energy magnitude is the same. But after dividing the cell into two fragments and then cutting in the z-axis, the final calculated energy obtained is the lowest, that is, the most stable. My next step is dividing the cell into more fragments and exploring if the calculated energy would be lower. Since pentacene has one or two hundred cell atoms, it may not be convenient to modify the atomic parameters in the python file to draw the pdos diagram. The molden.file obtained by calculating the energy with software like CP2K or SHARC can provide a convenient way to draw pdos diagrams.