Advanced Physical Chemistry
End-of-Year Portfolio

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1.   2-Dimensional to 3-Dimensional

1.1   Paper Cutting and Folding

The first part of the class consisted of changing how we think about objects. We began with paper, a two-dimensional object. With it, thought, nearly any three-dimensional object can be made. The instructor tested us on day to turn a piece of paper into a 3D representation of our name. This is where it all started.

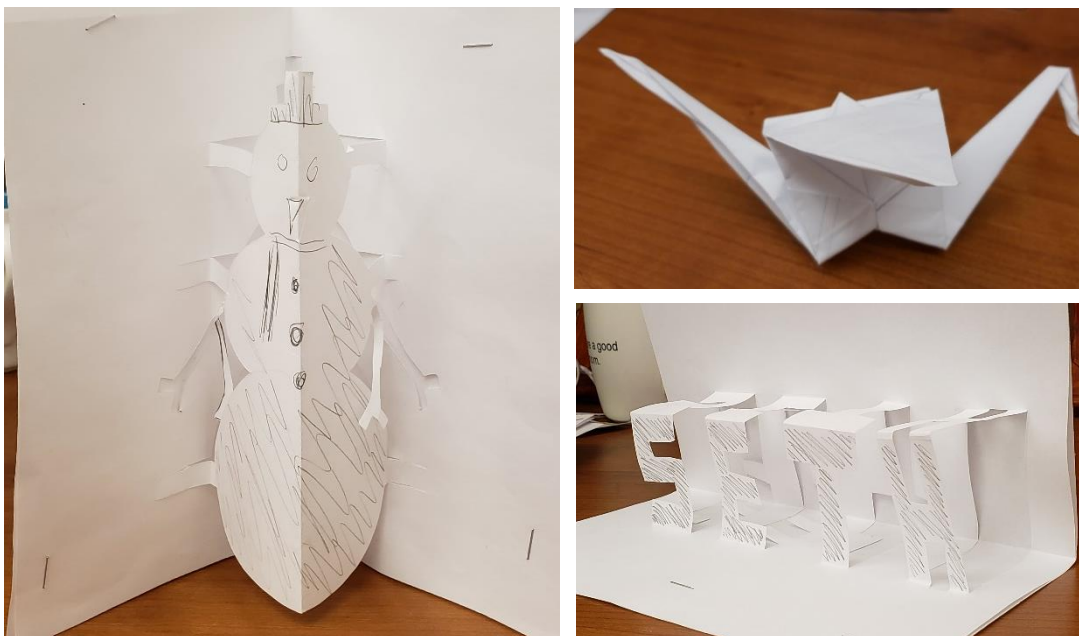Below are my first attempts of this: my name in 3D, a snowman, and then an origami crane.

Figure 1. Sample 2D to 3D paper cutting and folding projects

This idea of taking a two-dimensional object and making it 3D is all around us, and is commonly used in industry, such as making molds or parts for things. It is also used in 3D printing where a two-dimensional filament is heated and extruded onto a plate and moved in a specific way to create a three-dimensional object.

1.2   Bettendorf STEM Expo

With all of this in mind, the physical chemistry class traveled to Bettendorf Middle School to host a room filled with various displays and activities, most of which were focused on this idea of transforming a 2D object into a 3D object. We took with us 3D printers (SLA, FDM, and Ceramic), the paper cutting activity mentioned above, and the coffee roasting stuff.

This topic of 2D to 3D was talked about with the middle schoolers and their family and they were allowed to do the activity mentioned above. We also talked about how these "toys" such as the 3D printer can allow us to do research, such as printing mixing chambers or designing parts for microscopes. Some picture of the event are shown in *Figure 2*.

Figure 2. Pictures from the STEM Expo at Bettendorf Middle School

2. Raspberry Pi and Arduino

2.1 Setting Up the Raspberry Pi

After the STEM Expo, the class shifted the focus towards another maker topic, the Raspberry Pi. A Raspberry Pi (*Figure 3*) is a small, low-cost computer that runs on a Linux-based operating system called Raspian.

Figure 3. A Raspberry Pi 3 Computer

To setup the Raspberry Pi, we had to install the operating system by downloading a NOOBS file (New Out Of the Box Software) and unzipping it onto a micro SD card, which is the entire storage for the computer. Once finished, the Pi was then updated via the Command Terminal with the following script: sudo apt-get update && sudo apt-get install. Software was then downloaded to interface with an Arduino using the following script: sudo apt-get install Arduino. The Pi was then placed into an acrylic case and connected to a monitor, keyboard, and mouse via the equipped HDMI and USB ports. The Raspberry Pi setup was then used to create a display of various molecules and amino acid sequences at the end of the year for Scholars Day; this will be talked about in more detail in *section 3*.

2.2 Interfacing/Coding with Arduino

Once the Pi was setup, the class connected an Arduino Esplora (*Figure 4*) to it. The Arduino Esplora is a microcontroller and has several integrated sensors and controls which can be

controlled through the Arduino software installed earlier called Arduino IDE. Through this software, code can be written to control every aspect of the Esplora. My project with the Esplora was to control an external servo motor using the Esplora's slider and then output a specific color on the LED on the Esplora depicting about what degree the servo had moved to.
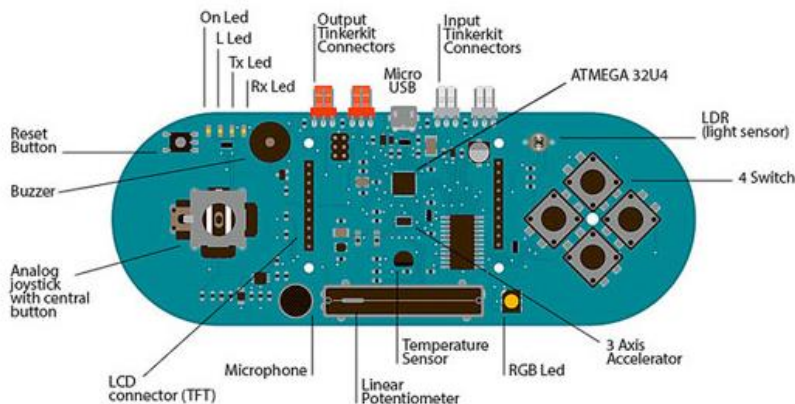

Figure 4. Diagram of an Arduino Esplora along with labels for each of its sensors and controls.

3. Computational Chemistry

3.1 WebMO Pro

After using the Raspberry Pi and Arduino for a few weeks, we shifted our focus to computational chemistry. The medium through which we would perform our computations was WebMO Pro. WebMO Pro is a computational chemistry package that is ran on the Monmouth College Chemistry Department's Server. The interface of the software is shown in *Figure 5*.
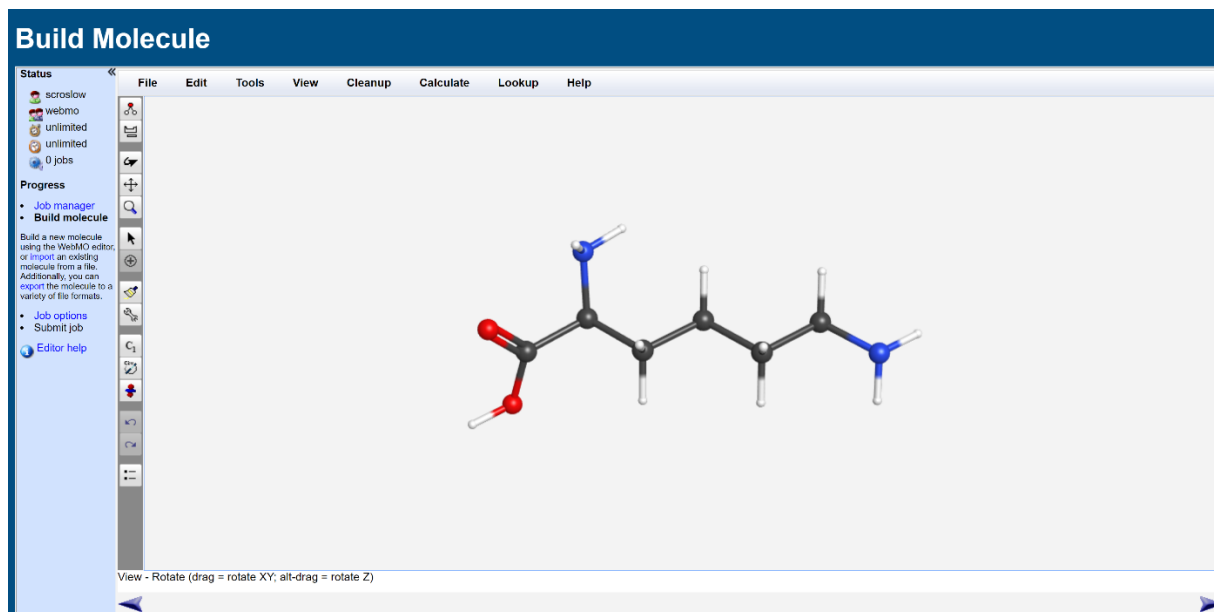

Figure 5. The interface for WebMO Pro with a structure of lysine

WebMO allows users to run several computational calculations such as molecular energy, molecular orbital, geometry optimization, vibrational frequencies, and coordinate scans. The three calculations that we focus on were molecular energy, geometry optimization, and coordinate scans.

3.1.1   Molecular Energy

The molecular energy calculation calculates the energy and properties of whatever atom or molecule is loaded into the software. This was typically calculated using a Hartree-Fock method which is a method to determine the wave function and energy of the system.

3.1.2   Geometry Optimization

The geometry optimization calculates the energies of the molecule at different geometries and tries to reduce the energy. The geometry with the lowest energy is then "spit-out" and then that molecule can then be used to run other calculations on.

3.1.3   Coordinate Scan

The coordinate scan calculates the bond length, angle and dihedral angle through a series of steps and calculates an energy for each of them. We can then get a graph of the angles and the energy for each respective angle to determine which angle is the most energetically favorable.

3.1.4   My Projects

To get used to WebMO, I began do a molecular energy calculation for a single atom, lithium. I then moved on to a diatomic molecule, fluorine. Once I got those calculations to work, I moved on to larger molecules, including benzene. We then started to relate the calculations to proteins, so I began to build a lysine protein and rand the geometry optimization on it; this took about 30 minutes to calculate. Once it was finished, I made a dipeptide bond between two lysines, and performed a coordinate scan on them. After doing a simple amino acid like lysine, I moved on to do a larger dipeptide, diproline. I followed the same process mentioned above on it, then did the same for a tripeptide, triproline, and got the following coordinate scan (*Figure 6*).
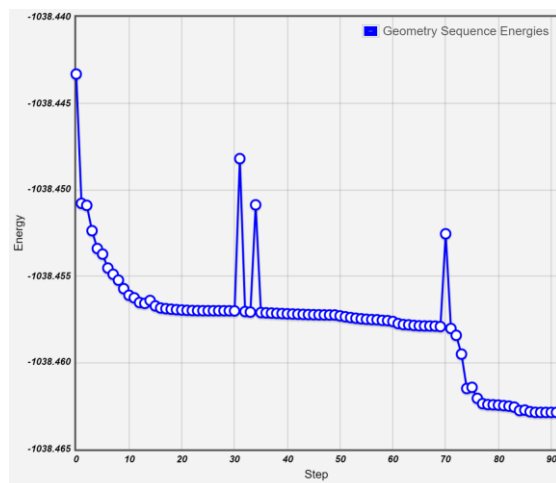

Figure 6. Coordinate Scan of triproline on a peptide bond

3.2   I-TASSER

Another software that was used was I-TASSER (Iterative Threading ASSEmbly Refinement), which is a protein folding software made by the Zhang Lab at the University of Michigan. I used this to predict the folding pattern for a sequence of amino acids from insulin. The amino acid sequence was FVNQHLCGSH and its predicted folding pattern is shown below (*Figure 7A*). This was then mutated by one amino acid to form the following sequence: FVNQHLCGS<u>S</u>, which is shown in *Figure 7B*.
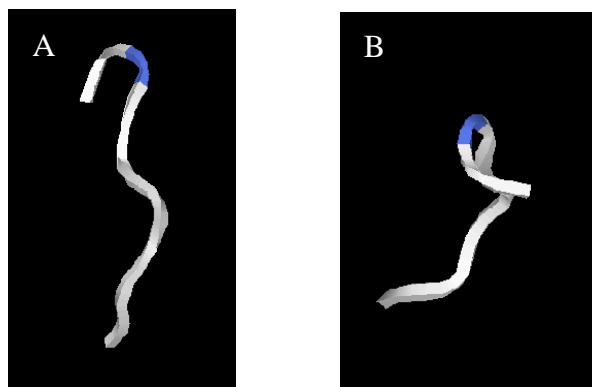

Figure 7. I-TASSER structures for insulin peptide chains where B is a mutated form of A

3.3   PYMOL/JMOL

Once the amino acid sequence was folded, it could be opened and modified using software called PYMOL or Jmol. We started using PYMOL, which wouldn't download onto the Raspberry Pi, so changed to Jmol which could be downloaded onto the Pi. This software loads a pdb, or protein database, file. Once loaded into the software, we were able to manipulate it and change how it looks, such as ball and stick or ribbon. A sample of Jmol is shown in *Figure 8* to show the overall environment of the software. Once we had made our files on Jmol, we made them rotate and displayed them on a large monitor array, 3x3, that displayed everyone's sequences.
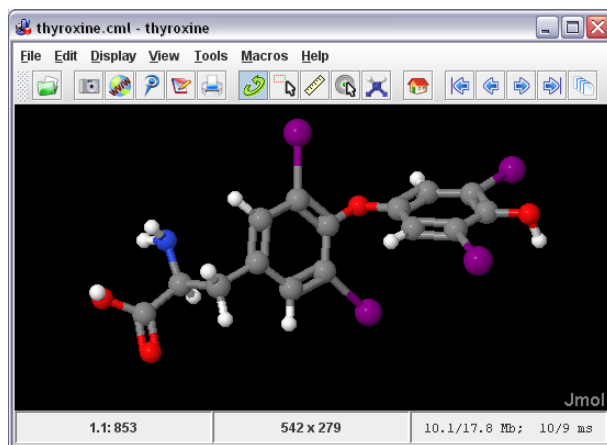

Figure 8. Environment of Jmol showing thyroxine molecule

4.   Scientific Discussion

As students who are bound for scientific futures, whether that be industry, graduate school, or medical school, we all need to know how to read scientific articles. Another topic covered in the class was the process by which scientific manuscripts are reviewed. We had to opportunity to review an actual manuscript and give our input on whether or not the manuscript should go on to be published, published with corrections, or rejected. This was a very interesting aspect of the class as I had never had to opportunity to do this before and had no idea how scientific journal articles were published. I did not think that the manuscript was good enough to publish; the figures were way to cluttered and were hard to read and there were several grammatical errors throughout the entire paper. For these, and other, reasons we as a class "rejected" the paper from being published right away and decided that they would need to make revisions.

5.   Maker Movement

Throughout the entirety of the class, one of the primary things we focused on was the idea of the "Maker Movement". In previous years leading up to today, people have began this maker movement where instead of buying certain things or asking people to make it for them, they make it themselves.

This movement was a core idea of the class, so a focus on building was established. One of the larger projects we did during the class was the creation of flag holders for staff at Monmouth College. During this, we created a process to make the flag holders and each took part in every aspect of it. The first step was to take a piece of wood, we used a 2x4, and cut it to a specified length. We did this using either a chop saw or a band saw. Then, using a laser-cut stencil, we marked where holes should be drilled. Using a drill press, we precisely drilled holes into the specified spots. After that, the entire piece was sanded using a belt sander. Once sanded, we used a tabletop router to cut out a decorative design into the wood block to make it more aesthetic. Finally, the wood blocks were stained and a coat of primer was added. These block were given to a faculty member to give out to other members of the Monmouth College staff to represent nations of interest to them, either due to nationality or from trips abroad.

Additional side projects were performed such as making robotic arms or helping to put together the electronic stand for the "wall-of-monitors" for Scholars Day.