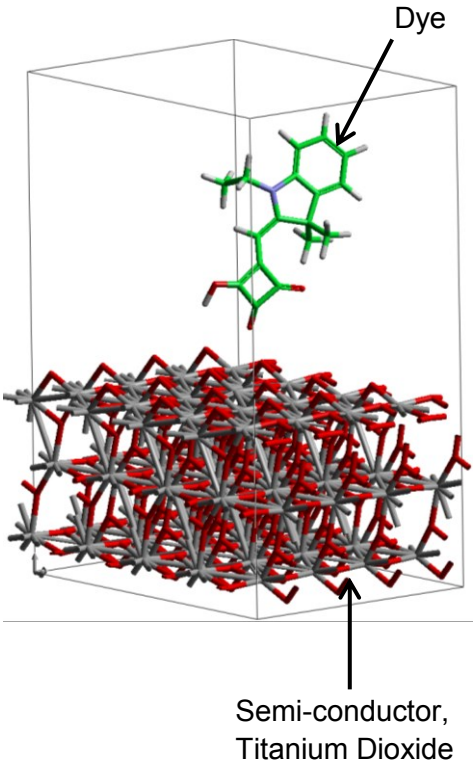
Solar Cell Results

21 July 2016

This is a project I carried out after a school's day on the 7th July 2016 as part of the Daresbury Careers Academy. I worked alongside people from the computational chemistry department and this project lasted for 2 weeks.

From a Key stage 5 schools day on the 7th July 2016, students were exploring Solar Cell materials that use a dye and a metal oxide instead of the conventional method that is being used today. They used visualisation software called Aten to visualize the dye and the metal. When light is absorbed by the dye, an electron is excited or ionised and then passes through the semiconductor (Titanium dioxide – TiO_2) and then goes back to the system of the dye and metal oxide. This creates an electrical circuit as only electrical energy is taken out of the system, no matter.

As the dye is in solution this solar cell concept is completely different to methods in current use. Panels are solid and have to be fixed to places where there is a large concentration of light most of the time to get the most amount of electricity. However, this concept will have a dye in solution, it is dissolved in water. This could mean that many of these solar cells can be made into a paint that will generate electricity, and by being painted onto places that panels could not be fixed, such as roads or complex buildings, we can increase the amount of energy captured by sunlight.



These visualisations help us to see how electrons will pass from the dye to the semi-conductor. There are 4 dyes that are currently being looked into with minor differences between them, but these minor atomic differences could mean large differences in electron transfer. One theory is that the rotation of the dye to the surface of the metal oxide will make a difference in terms of energy; this is one of the first areas being researched here at Daresbury Laboratory to help experimentalists when they are doing a real-time experiment.

Students then helped create input files for this simulation that subsequently have been run on a supercomputer, as each rotation (of the organic dye) can be different (with respect to the TiO_2 surface) and it is hard to predict what the best angle will be. When these files ran on the supercomputer *Blue Wonder,* they took about 2 and a half hours to get a result outputted. This can be seen as a fast calculation even for a supercomputer as it is doing very complex equations for approximately 300 atoms, if this were to be done on your desktop computer it would take at least a week!

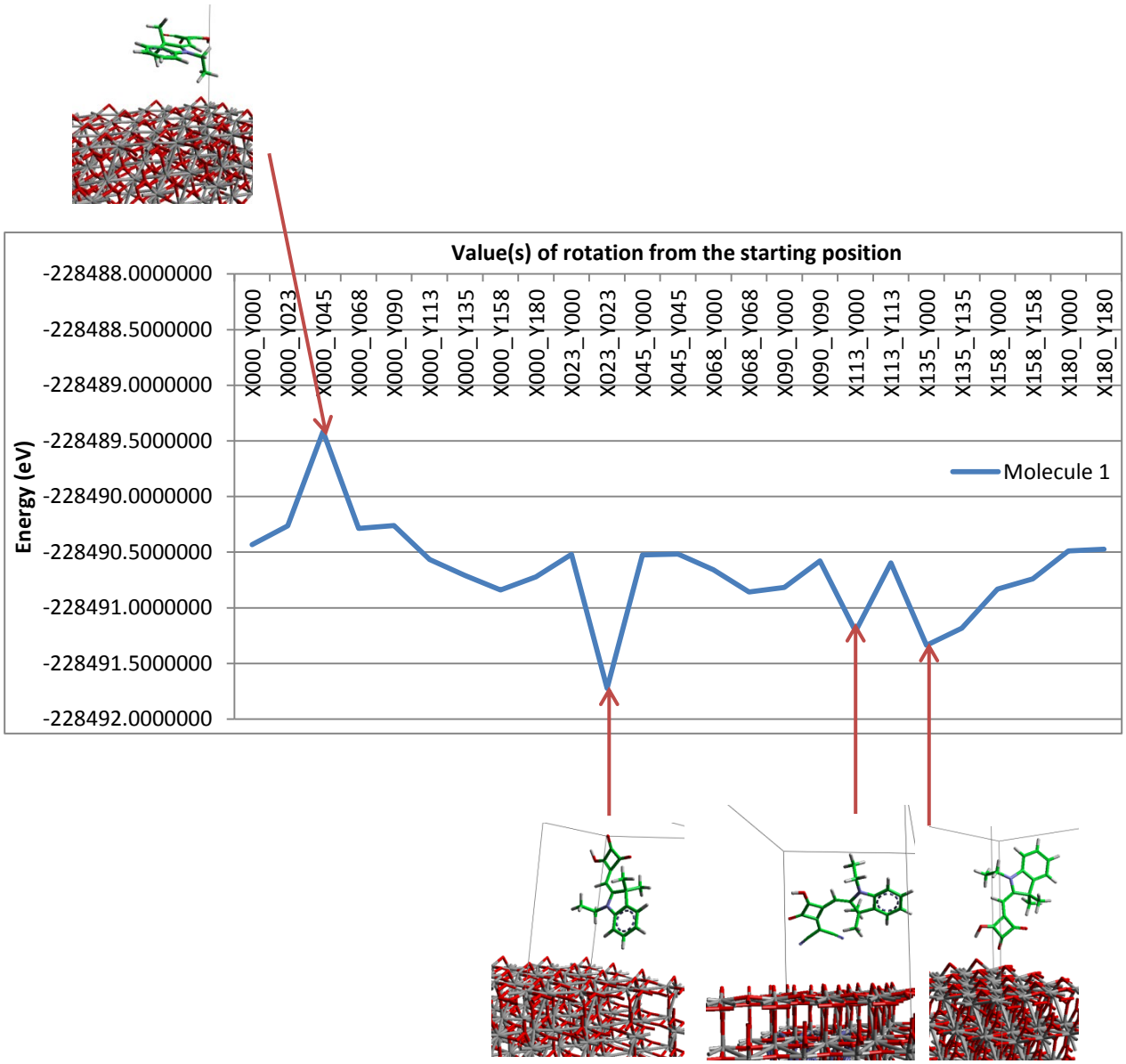


Figure 1: This is the graph of the energies the first dye has when the rotation from the original point increases. Each value will mean a small change in the angle from its starting position; therefore different parts of the molecule are closer to the semi-conductor surface. Each peak found will

correspond to a specific rotation made from the visualisation software; the rotations are made in regular increments.

No specific trend can be seen in Figure 1, but peaks help show that rotating the dye does have an effect on the energy of the whole system. Future work will involve further research into these peaks to see whether they become more distinct and stand out more, or if they decrease and fit more into the line with the rest of the data.

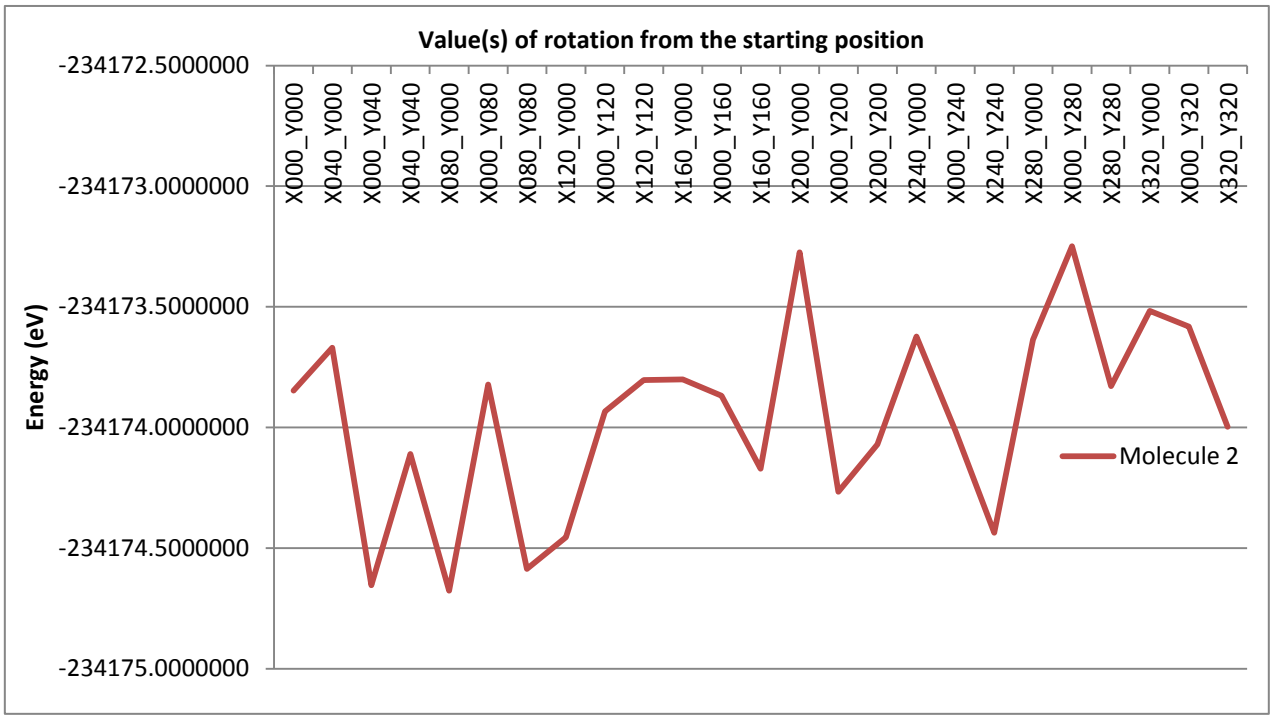
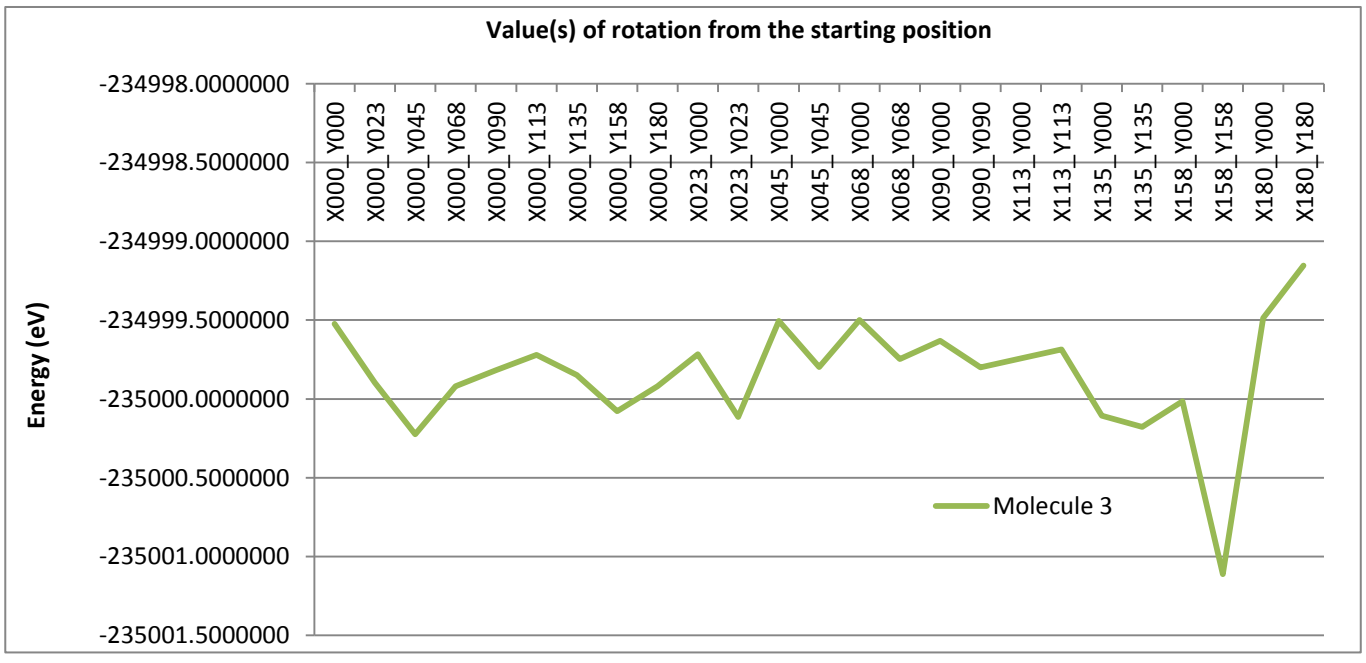


Figure 2: Molecule 2 has even more peaks than the first but the range of the data is smaller, so even though they are peaks they do not stand out by a large difference to the rest of the data.



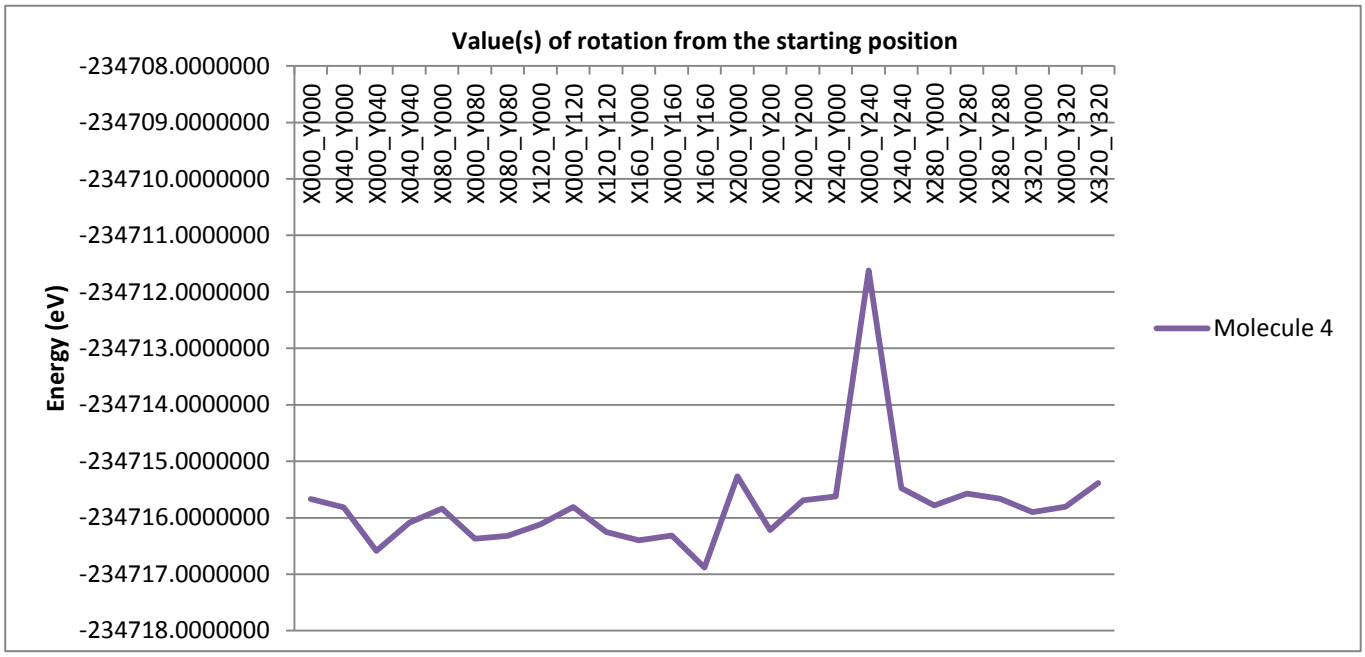


Figure 3, 4: Then with the dyes 3 and 4 we have some consistent data with a few significant peaks.

This generated data will be further processed to see what the best conditions (i.e. orientation of molecule with respect to TiO_2 surface) should be to find the lowest energy state, so that the most energy efficient solar cell dye paint is made.

For more information, please look at the following links:

Bangor University Solar Cell Research Group:

https://www.bangor.ac.uk/chemistry/pjh/index.php?subid=1278

Supercomputers at the Hartree Centre:

http://community.hartree.stfc.ac.uk/wiki/site/admin/home.html