Simulation of the Resonant X-ray Emission Spectroscopy (RXES) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectra of monolayer and bulk films of 3,4,9,10-perylene tetracarboxlylic dianhydride (PTCDA)

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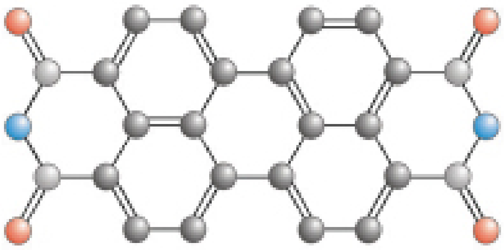

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7. Apendix

1. Abstract

We present an investigation into the electronic structure of 3,4,9,10-perylene tetracarboxlylic dianhydride (PTCDA), followed by a computational analysis of the Near Edge X-Ray Absorption Fine Structure (NEXAFS) through simulation of X-ray spectroscopies using the StoBe software package. Using detailed Density Functional Theory (DFT) calculations, the core binding energies were determined to be shifted in energy from other experimental and theoretical determinations, though plots of these energies had similar structure and shape. Precise NEXAFS spectra of the p and s-polarised C1s and O1s ionisation states of PTCDA were produced for comparison with experimental data. These computational spectra yield very close agreement with past experiments and this data has since been used to determine an approximate 4:10 ratio of p to s polarisations in an experimental NEXAFS output.

2. Motivation

2.1 Understanding Large Organic Molecules

A detailed knowledge of large organic molecules is an important aspect of solid state physics. For instance, knowing the orientation of molecules in a thin film can be used can be used to improve the electron transport properties of semiconductors used in modern applications such as solar cells.

Variable energy, linear polarised X-ray spectroscopy can be used to probe the electronic structure and molecular growth of molecules on a substrate. Resonant X-ray Emission Spectroscopy (RXES) probes the occupied molecular orbitals. It is elemental and site specific so can therefore determine the electronic properties of molecules. Near Edge X-ray Absorption Fine Structure (NEXAFS) Spectroscopy is also element specific and relies on measuring the amount of absorption of X-rays incident on the molecule.

2.2 PTCDA

3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) is one such organic molecule mentioned above for use in semi conductors. This project focused exclusively on the simulation of this particular molecule. PTCDA is composed of 24 Carbons, 6 Oxygens and 8 Hydrogen atoms. This planar molecule has it's Carbons arranged in benzene-like rings with the Oxygen at both ends (anhydrous carboxylic groups) of the molecule and the hydrogens filling up the remaining spaces along the side of the molecule.

PTCDA has D_{2h} symmetry, which means that it has an inversion centre and is invariant under rotation about 360/N degrees. N=2 here. There are several inequivalent sites in this molecule; 7 Carbons, 2 Oxygens and 2 Hydrogens. This means that the molecule can be constructed by replication of these inequivalent sites by rotation. These sites were named C1-C7 and O1-O2 as follows in fig. 1 on the following page. Hydrogen is excluded from this diagram due to it's lack of interesting properties for soft X-ray spectroscopies.

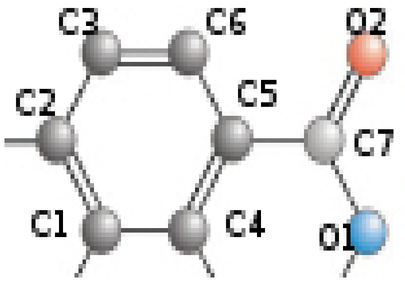


Figure 1. PTCDA inequivalent atomic sites

3. Introduction

3.1 PTCDA Crystal Structure

PTCDA has been studied and analysed by many researchers using methods such as electron spectroscopy and electron diffraction[1]. Most of the analysis done has been of multilayer films on different substrates like Ag or CuPc. Organic thin films, however, frequently grow with different crystal structures and orientations, or polymorphs, than would be observed in bulk material samples. Knowledge of the crystal structure of organic materials is important for X-ray spectroscopies because orientation of a molecule and direction of incoming X-ray photons will determine which spectra are observed.

In the case of PTCDA, there are two notable polymorphs that have been noted and characterised by T. Ogawa et al.[1] . These have been dubbed the α and β modifications. Both modifications lie on the (102) lattice plane and differ by slight angular inclinations caused by steric effects (i.e. overlapping electron orbitals effecting conformation), as can be seen in fig. 2, and both crystal modifications are composed of layers of the same sheet with some shifting.

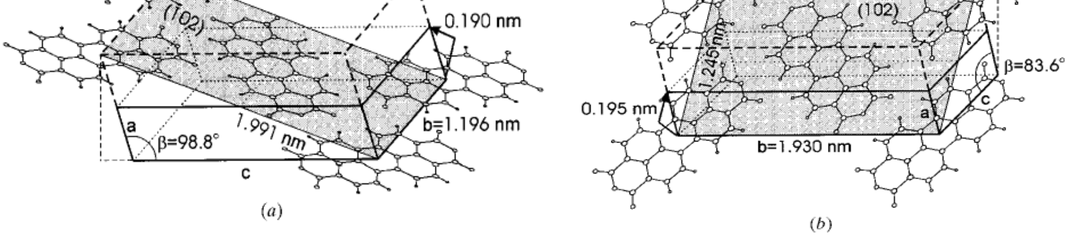


Figure 2. Lattice packing for (a) α modification and (b) β modification. Image from Ogawa et al. [1]

3.2 Molecular Orbitals

The usual p-orbitals associated with electronic structure can overlap in different ways to produce different molecular orbitals. Two types of particular interest in this study are pi type (π) and sigma type (σ) bonds. π bonds are created when two p-orbitals overlap along their axis of symmetry, combining two lobes, whilst σ bonds consist of two over lapping p-orbitals intersecting edge on. Obviously, due to the planar structure of PTCDA one can see that σ type bonds will occur along with sp^2 hybridisations in the plane of the molecule while only π type bonds are formed along the axis perpendicular to the plane of the molecule. This is an important point for considering spectra obtained from simulations where photons excite the molecule along particular directions. From here on the plane of the PTCDA molecule will be referred to as the yz-plane, with the x-axis being the axis perpendicular.

The unoccupied orbitals in the molecule, where electrons can be promoted to should they be excited by an energetic X-ray photon, are called "starred" states. Thus when an electron is excited up to an unoccupied π orbital it is in a π* state. Two other important naming conventions are the that of "Highest Occupied Molecular Orbital" (HOMO) and "Lowest Unoccupied Molecular Orbital" (LUMO). The HOMO is the molecular orbital of highest energy occupied by an electron, while the LUMO is the orbital of next highest energy, obviously not occupied in the ground state.

3.3 StoBe-deMon Software

The program used in this project to simulate X-ray spectroscopies of PTCDA is called StoBe. This program is Fortran based and uses a system of keywords as input code, designed to select options the user may desire to implement such as selecting an energy convergence parameter or specifying which type of X-ray spectroscopy to simulate. StoBe uses Gaussian type molecular orbitals as a solution to the Kohn-Sham equations of DFT.

3.4 Density Functional Theory Basics

Density Functional Theory (DFT) is based on quantum mechanical theories by Hohenberg and Kohn stating that given a system of electrons, the external potential is uniquely and exactly determined by the electron density. These theorems establish a variational approach for calculation of the energy, which is given in DFT by a functional of the density. This functional is composed of several terms and contains an exchange-correlation functional and DFT relies upon a good approximation for this functional as it is rarely known.

The Kohn-Sham (KS) equations introduce the concept of KS orbitals which are mathematical objects used to calculate the kinetic energy term of the DFT functional. These equations are used to make DFT computationally practical and are used by the StoBe software for calculations. The KS equations need to be solved iteratively and treat the system as non-interacting electrons moving in a potential. The following are the KS equations, discussed in more detail in B. Brena's thesis[2];

$$V_{\mathrm{eff}} = v(\vec{r}) + \int \frac{\rho \vec{r}\prime}{|\vec{r} - \vec{r}\prime|} \mathrm{d}\bar{\bar{\mathrm{r}}}\prime + v_{\mathrm{xc}}(\vec{r}) \quad (3.4.1)$$

$$[-1/2\nabla + V_{\mathrm{eff}}]\psi_i = \varepsilon_i \psi_i \quad (3.4.2)$$

$$\rho(\vec{r}) = \sum_{i}^{\mathrm{occ}} \sum_{s}^{\mathrm{spin}} |\Psi(\vec{r}, s)|^2 \quad (3.4.3)$$

Here is the external potential from electron-nuclei interactions, is the electron density, $v_{\mathrm{xc}}(\vec{r})$ is the exchange-correlation potential and the term in the integrand in eqn(3.4.1) is the electrostatic potential from distribution of the system of electrons.

3.5 Project Outline

This investigation into the simulation of PTCDA X-ray spectroscopies can be divided into three different sections, two of which are covered in this report.

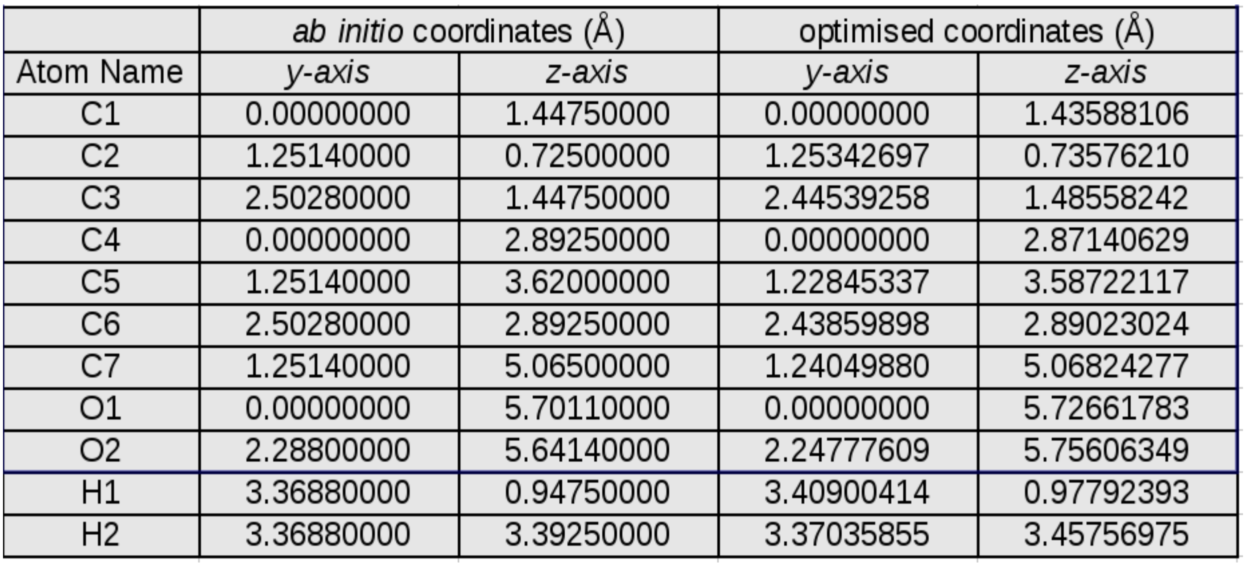
- **DFT Calculations:** A necessary precursor to any simulation of X-ray emission or absorption spectroscopy. Optimised geometry of the PTCDA molecule was to be completed and a determination of of all densities of states, occupied and unoccupied. The orbital KS energies of the core molecular orbitals for the Carbon and Oxygen sites were also to be noted. These calculations were to be done taking symmetry into account.
- **NEXAFS:** Using the optimised geometry obtained earlier, the transition state method of determining NEXAFS transition moments was to be used to obtain spectra of each Carbon and Oxygen site in different measurement geometries. These were then to be summed.
- **RXES:** XES spectra were to be produced by simulating a hole on each of the core atomic site molecular orbitals and these were to be summed to obtain total spectra.
  N.B. RXES is covered in E. McClean's report and is not discussed here.

4. Computational Details and Results

4.1 Geometry Optimisation

To perform any X-ray spectroscopy simulations such as RXES or NEXAFS, a knowledge of the occupied molecular orbitals were required. Firstly, an estimate of the Cartesian coordinates was sought. Recording an electron diffraction pattern on an imaging plate detector, T. Ogawa et al.[1] determined the average bond length between the different atoms in a molecule of PTCDA. Using these experimentally dervied distances along with simple geometry, a set of Cartesian coordinates in Angstroms were determined.

The geometry of the simulation was set up such that the z-axis lay along the spine of the molecule. The reason for this was that if the atoms were specified other than on this axis, StoBe would have constructed the molecule using symmetry by reflecting the given coordinates through the z and y axes and concluded a different number of atoms in the molecule than in reality. Using parameters such as atomic number the program simulated a set of new optimised coordinates. The original ab initio and optimised coordinates can be seen below in table (4.1.1).



	ab initio coordinates (Å)		optimised coordinates (Å)	
Atom Name	*y-axis*	*z-axis*	*y-axis*	*z-axis*
C1	0.00000000	1.44750000	0.00000000	1.43588106
C2	1.25140000	0.72500000	1.25342697	0.73576210
C3	2.50280000	1.44750000	2.44539258	1.48558242
C4	0.00000000	2.89250000	0.00000000	2.87140629
C5	1.25140000	3.62000000	1.22845337	3.58722117
C6	2.50280000	2.89250000	2.43859898	2.89023024
C7	1.25140000	5.06500000	1.24049880	5.06824277
O1	0.00000000	5.70110000	0.00000000	5.72661783
O2	2.28800000	5.64140000	2.24777609	5.75606349
H1	3.36880000	0.94750000	3.40900414	0.97792393
H2	3.36880000	3.39250000	3.37035855	3.45756975

Table (4.1.1) ab initio and StoBe optimised coordinated for PTCDA molecule simulation

Please note that the coordinates of the equivalent atomic sites for atoms reflected through the y and z axes have the same absolute value and differ only in sign due to the D_{2h} symmetry of PTCDA. These coordinates were then used to determine PTCDA's densities of states.

4.2 Densities of States (DOS)

The partial densities of states (PDOS) was obtained by use of the optimised coordinates previously determined by StoBe and a helper program used to generate arrays of PDOS for graphical output. The occupied PDOS for each inequivalent Carbon and Oxygen atom were simulated and then summed to produce a graph of the total occupied DOS. The graphs (4.2.1-4) below show the occupied PDOS for a selection of inequivalent atoms (excluding Hydrogen). The remainder are in **Appendix I**. Should it be required a breakdown of the density of states into p_x, p_y and p_z could be obtained. For an example of the breakdown, the PDOS graph of C1 includes this.

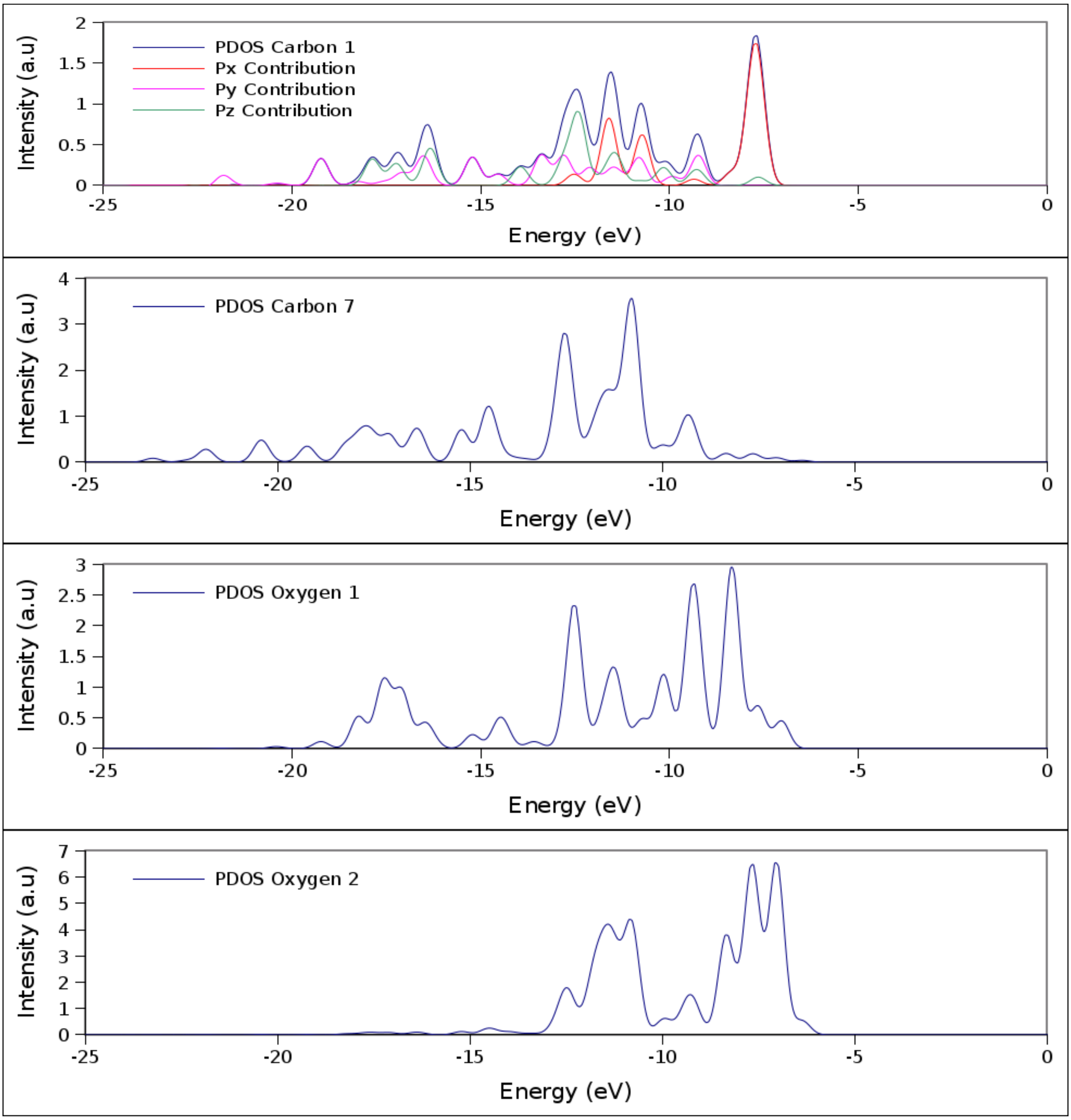


Fig (4.2.1-4) Partial Densities of States of C1, C7, O1 & O2 respectively

Should the unoccupied densities of states for any atom be required the keyword, "virtual", was inserted into the input StoBe file and an output of predicted unoccupied PDOS was generated.However the total density of states (TDOS), both unoccupied and occupied can be compared with other computational work and experimental photoemission spectra and so the total recorded DOS is included below in Fig (4.1.5)

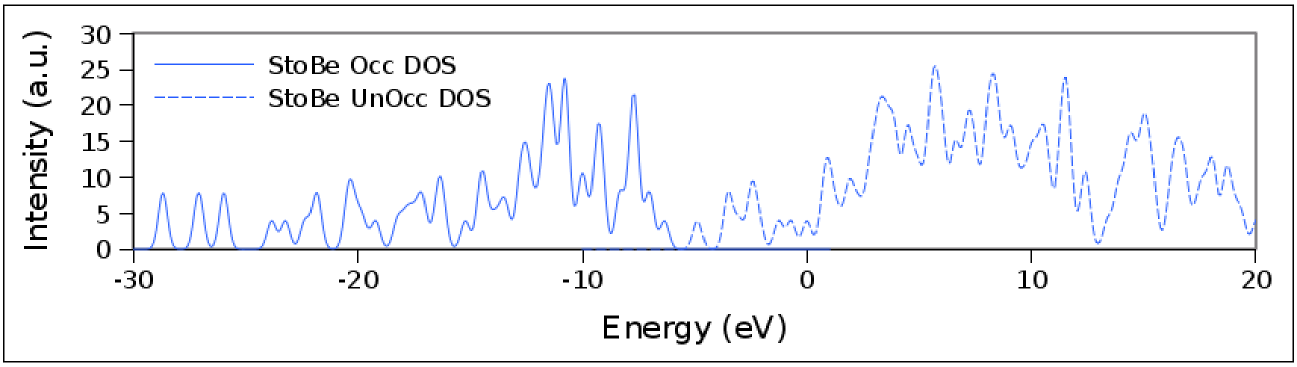


Fig (4.2.5) Total Densities of States. The solid line is Occupied DOS and dashed line is Unoccupied DOS

The LUMO and HOMO are represented in this graph. The HOMO is in the region of -6.4eV and the LUMO at about -4.9eV according to the StoBe calculations. The occupied and unoccupied TDOS simulations can be compared against previously computed DFT and semi-empirical Hartree-Fock method calculations to determine their accuracy. Below is a plot of the StoBe calculation for the TDOS compared to simulations run by H. Vázquez et al.[3] (DFT) and separately by I. Hill et al. [4] (Hartree-Fock) in the -10eV to 10eV range.

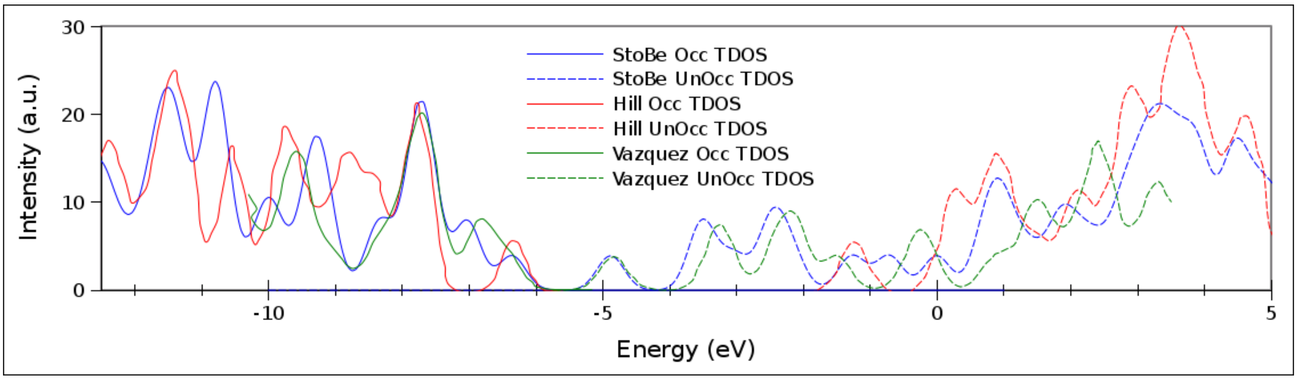


Fig (4.2.6) Plot of StoBe TDOS vs. Hill et al. and Vazquez et al. computational simulations

It must be noted that the intention of the Hill et al. simulations was to simulate Ultra-violet Photoemission Spectroscopy (UPS) and Inverse Photoemission Spectrocopy (IPES) and not to generate molecular orbitals. Due to the ability of experimental UPS and IPES to determine TDOS, a simulation of these be comparable to the StoBe calculation. The overall shape of the simulated TDOS compares well with the two computational plots. However a shift in the location, and hence energy, of the LUMO and HOMO appears when the StoBe calculation compares with the plot Vazquez et al. and that data is thus shifted by -2.3eV to match the StoBe computation. See [5] for more on UPS and IPES.

Also, although the Hill et al. calculation appears to agree when compared with the StoBe occupied DOS, it differs significantly when compared with the unoccupied DOS, probably meaning the UPS calculation was more similar to the StoBe DOS simulation than the Hill et al. IPES simulation. Though the Vazquez et al. computation is shifted in energy to the StoBe simulation, the shape is quite similar and both include unoccupied orbitals around the -5eV to -2eV range that the Hill et al. graph appears to be missing. This may be in part due to a computational approximation made by Hill et al., called Intermediate Neglect of Differential Overlap (INDO) or an inherent aspect of simulating and measuring IPES.

The TDOS simulation can also be compared with experiment, although with less success than when compared to other computational simulations. Hill et al. compare their simulations to experimental UPS and IPES spectra measured from a thin film of PTCDA. Note that the UPS spectra is used to compare the occupied bands while the IPES is compared to the unoccupied TDOS. Some lack of correspondence can be explained by solid state polarisation effects in the experimental spectra as discussed in [4].

Below is the comparison of StoBe TDOS with the experimental UPS and IPES spectra of [4]. It can be seen that the simulation of the occupied TDOS agrees well with the UPS spectra while the unoccupied TDOS is similar to the IPES experimental spectra, as would be expected. It is also worth noting the absence of the unoccupied molecular orbitals in the -5eV to -2eV range, just as in the Hill et al. simulation.

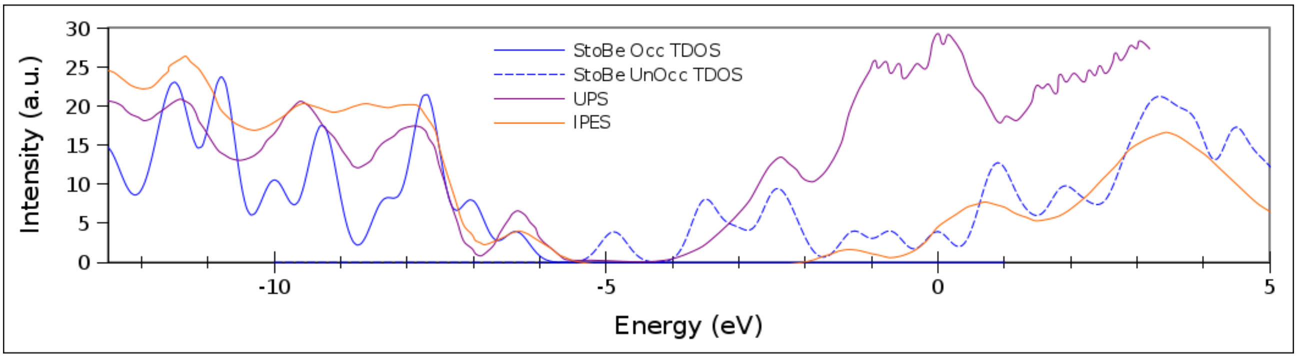
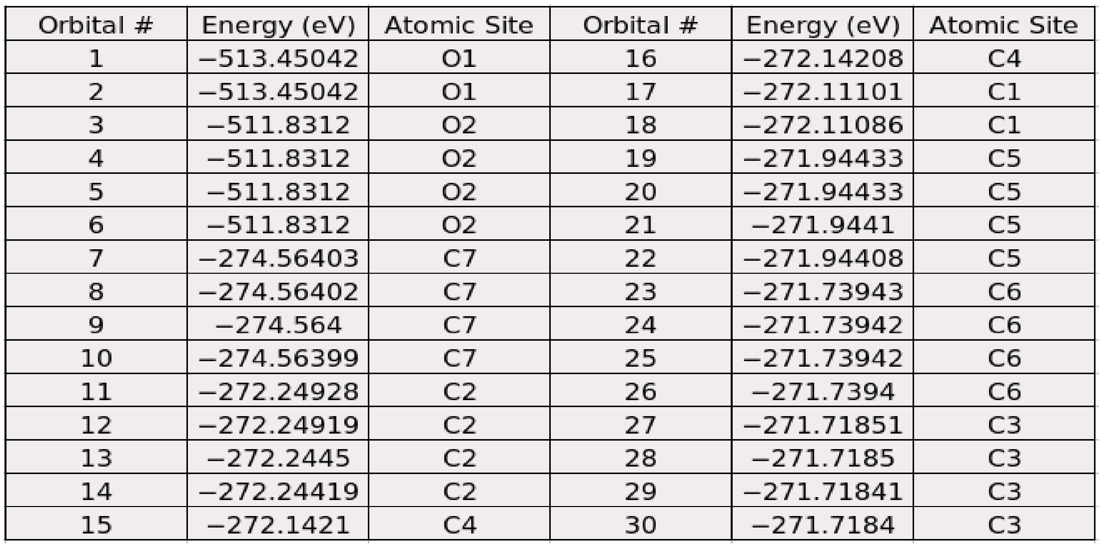


Fig (4.2.7) StoBe TDOS simulation compared with UPS and IPES experimental spectra

4.3 Core Binding Energies

From the output of StoBe calculations it was possible to determine which atomic site different binding energies were associated with. Using the eigenvector matrices StoBe output it was found which core levels were based on which atomic sites. The first 30 binding energies, in decreasing order, were tabulated along with their corresponding atomic site. These orbitals were arranged first by symmetry and then by energy by the StoBe program. This data is shown on the following page in Table (4.3.1). Please note that all binding energies refer to the 1s orbital of the mentioned atoms.



Orbital #	Energy (eV)	Atomic Site	Orbital #	Energy (eV)	Atomic Site
1	−513.45042	O1	16	−272.14208	C4
2	−513.45042	O1	17	−272.11101	C1
3	−511.8312	O2	18	−272.11086	C1
4	−511.8312	O2	19	−271.94433	C5
5	−511.8312	O2	20	−271.94433	C5
6	−511.8312	O2	21	−271.9441	C5
7	−274.56403	C7	22	−271.94408	C5
8	−274.56402	C7	23	−271.73943	C6
9	−274.564	C7	24	−271.73942	C6
10	−274.56399	C7	25	−271.73942	C6
11	−272.24928	C2	26	−271.7394	C6
12	−272.24919	C2	27	−271.71851	C3
13	−272.2445	C2	28	−271.7185	C3
14	−272.24419	C2	29	−271.71841	C3
15	−272.1421	C4	30	−271.7184	C3

Table (4.3.1) First 30 core binding energies and corresponding atomic site.

To determine whether the computed binding energies were accurate a comparison with J. Gustaffson et al.[6] was performed for the binding energies of both Carbon and Oxygen. Though, roughly, the plots of the binding energies and their relative frequencies were similar in line shape they differed significantly in position. The Oxygen binding energy plot of [6] had to be shifted by -20.3eV, while the Carbon binding energy plot was shifted by -18.7eV.

A cursory comparison with an Oxygen 1s binding energy given by E. Clementi et al.[7] shows that the StoBe calculation has this binding energy with a +40eV shift and a +20eV shift from results given in [6]. The reason for such a large discrepancy is unknown to us at this point. Please see below in Fig (4.3.1) for plots of the StoBe binding energy with comparison to binding energies given in [6].

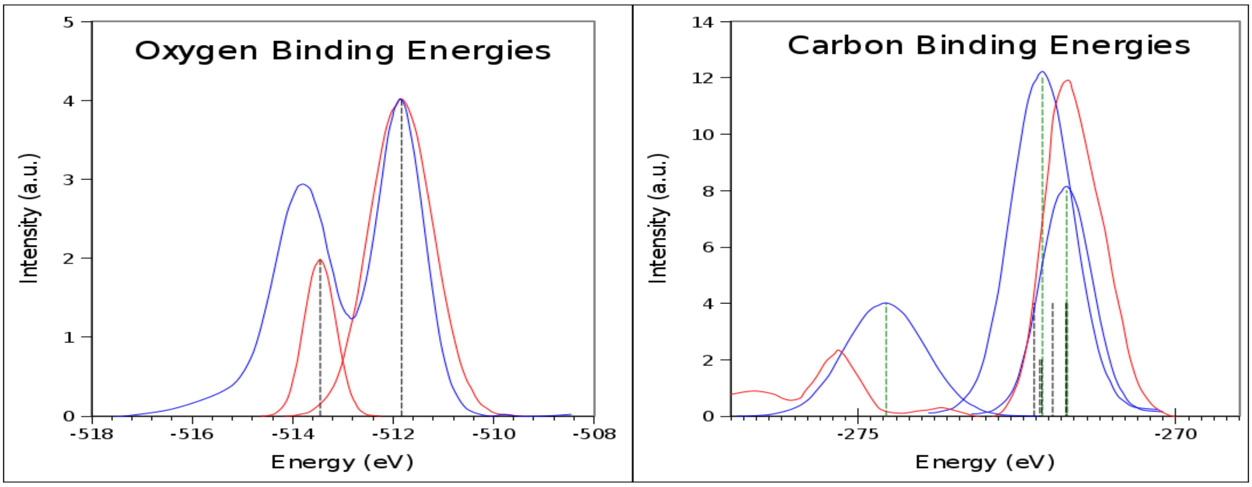


Fig (4.3.1) Plot of StoBe calculated binding energy (Gaussian functions fitted) vs. binding energy plots from H. Gustaffson et al.[6].. The red lines are the StoBe calculation, the blue lines are experimental plots from [6]. Note also that the dotted black/green lines are the positions of the binding energies with a length dependent on the frequency of this binding energy. A legend was not included for technical reasons.

4.4 NEXAFS

In XAS, a core electron is excited into an unoccupied molecular orbital above the Fermi level. The total intensity of the spectra produced in XAS is determined by the quantity of unoccupied states in the initial state. Because a created core hole is centred on a specific atomic site, the unoccupied states are projected onto this site as the ionised atom is in a highly excited state. This core hole decays by XES or by non-radiant Auger processes. See A. Nilsson's[8] descriptions of these processes for more detail. As in PTCDA, if there are many ineqivalent atoms of the same element, the spectra may have overlapping features and thus cannot be decomposed into specific atomic features experimentally. However, computational simulations of these spectroscopies can determine each atomic site's contribution to the overall spectra.

To simulate these processes, a computational method known as the "transition state method" was implemented as a code using StoBe. The simulation requires a half-occupied core orbital to be placed at the site of the ionisation. The other atoms of the same element as that of the site of the "half-filled" atom were all described by effective core potentials. These potential eliminates the 1s level of each site and thus makes the description of the core hole state much simpler by reducing effects that would be unhelpful to the final spectrum.

Also, a special (triple zeta) new basis state is centred on the ionisation site which is essentially a linear combination of diffuse functions used to describe the new state. The reason this method is employed is to avoid using the final state molecular orbitals to describe the molecule at the beginning of the computation as the final state of such a X-ray excitiation scenario would differ from the initial state. The presence of the core hole, would in effect, change the description of the initial molecular orbitals. Thus the "middle" or transition state is described. For a more detailed explanation of the computational details please see **Section III** of [9].

NEXAFS spectroscopies are sensitive to polarisation and spectra differ when X-rays of different polarisations are used (of course, depending on the structure of the molecule). When polarised in the plane of the PTCDA molecule we refer to the X-rays as p-polarised and s-polarised when the X-rays are polarised perpendicular to the plane of the molecule. To simulate the s-polarisation spectroscopy the polarisation was simply inputted into the StoBe code. However to simulate the p-polarised spectroscopy, the polarisation would need to be simulated with different rotations of the polarised X-ray included, and an average of the calculations taken. A simplification was to simulate the X-ray as unpolarised and have these photons impinge at a 90° angle to the plane of the molecule.

A NEXAFS simulation was run for all inequivalent atoms, also in each case simulating the p and s-polarisations. These spectra were summed, taking into account of multiplicity of each inequivalent atom, to determine an overall s and p-polarised NEXAFS spectra for Carbon and Oxygen. These spectra were then compared against experimentally derived results and spectra. Some Spectra were provided by Dr. Cormac McGuinness' research group of Trinity College Dublin. Spectra for C K edge NEXAFS were also taken from Y. Zou et al.[10] and from J. Gufstafsson et al.[11] and data for the O K edge NEXAFS from S. Park et al.[12]. First to be displayed is a comparison between our StoBe NEXAFS simulations and experimental spectra from both Y. Zou et al.[10] and J. Gufstafsson et al.[11] for the Carbon K edge, for both s and p-polarisations, which can seen on the next page in Fig (4.4.1). The plots match in the overall line shape and peaks in the p-polarisation match quite well to [10]'s data.

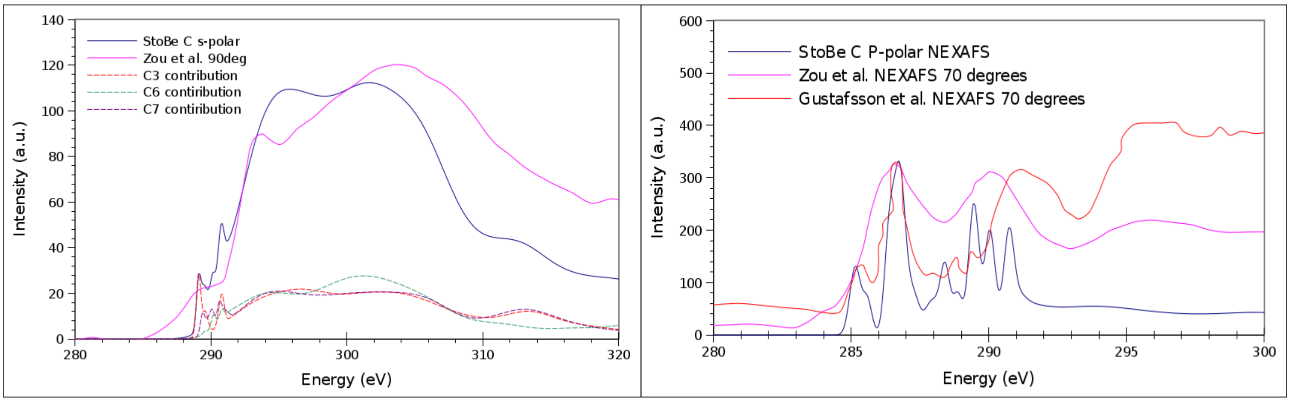


Fig (4.4.1) StoBe C K-edge NEXAFS s & p-polarisations compared with experimental data.

The lack of defined peaks in the experimental plots is most likely due to resolution issues. The peaks did not exactly match up upon plotting and so the plots needed to be shifted to match. For the p-polarised Y. Zou et al. plot, a shift of +1eV was required and the J. Gustafsson et al. plot was also shifted by 1.5 eV. No shift was required for the s-polarised comparison. These are quite small shifts and are most likely due to errors imported from extracting the experimental data from imprecise graphs and are thus unimportant. In the s-polarised StoBe plot the C3, C6 & C7 contributions are included to show where these peaks arise, which seems to be from atomic sites on the edge of the molecule. Again, these peaks do not appear in the experimental plot most likely due to "smoothing out" effects.

Below are plots of the StoBe Oxygen s polarised and p polarised NEXAFS output plots (Fig. (4.4.2)) compared with corresponding experimental plots by S. Park et al.[12] and by Y. Zou at al. Again, a clear match is seen between the shape of the plots and the location of peaks are approximately in the same location. This implies the StoBe computation is accurately simulating the NEXAFS spectroscopies of PTCDA.

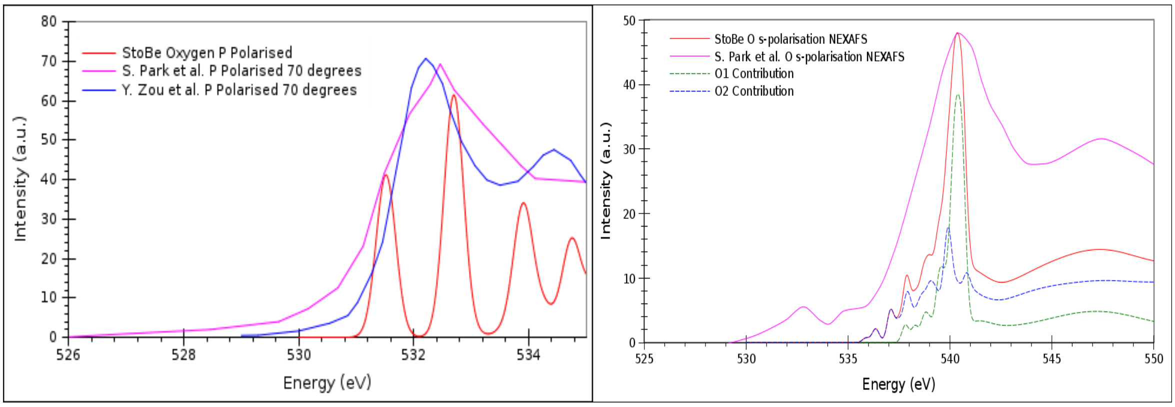


Fig (4.4.2) StoBe O K-edge NEXAFS s & p-polarisations compared with experimental data.

As there are only two contributions to the NAXAFS Oxygen simulations they are included in the s-polarised plot as an example of how the full plot can be decomposed into contributing atomic sites before summation. Please note weightings are included for each contribution depending on the number of equvalent atoms in the molecule (eg. 2 O1s and 4O2s). Another point to note is that both p-polarised experimental plots needed to be shifted by +1eV to match the StoBe plot and +1.3eV in the s-polarised plot. Either errors in extracting graphs from publications or the StoBe simulation being off by ~1eV were the likely causes.

As a final comparison for the StoBe NEXAFS simulations is a comparison of experimental data from Dr. Cormac McGuinness' research group of Trinity College Dublin. The data obtained from this group had a mixing of s and p polarisations in the plots of their O and C NEXAFS data.

Using the StoBe simulations of p and s polarisations of both Carbon and Oxygen, the ratio of p polarised contributions to s polarised contributions in the experimental NEXAFS plots was determined to be 4:11 for the C K-edge NEXAFS and 1:2 for the O K-edge NEXAFS. Roughly, the ratio is on average, 4:10, according to the StoBe simulations. Plots of this experimental data and the weighted contributions of StoBe simulated s and p polarisation NEXAFS are shown below in Fig (4.4.3). Note, no shift in energy was required for either of these comparisons.

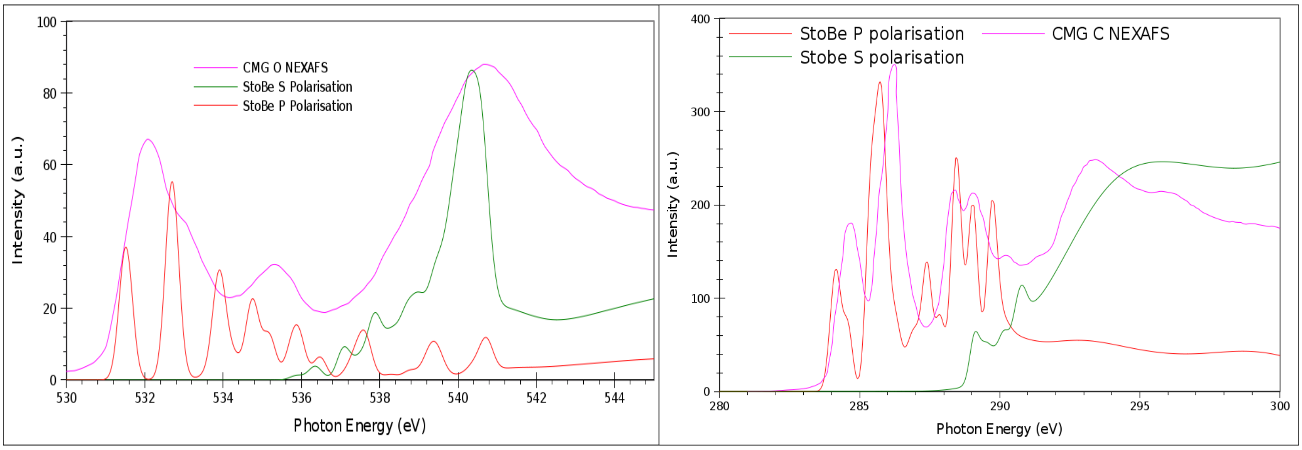


Fig (4.4.3) McGuinness' research group O & C NEXAFS with overlayed StoBe simulated s and p polarised contributions with relative weightings.

5. Conclusions

5.1 DOS Discussion

Using the StoBe simulations the HOMO was determined to be in the region of -6.4eV and the LUMO at about -4.9eV. This values differ from other computational determinations by ~2eV. Most errors in comparison in this report are likely due to the method employed (using Linux program g3data) in extracting data and graphs from scientific publications included in section. 6, references.

The TDOS simulations compared against the UPS and IPES experimental data matched up in line shape and occurrence of some peaks. However, it must be noted that some peaks occurred in the experimental plots that did not appear in the StoBe simulations and vice versa.

5.2 Binding Energies

The binding energies of the 1s levels for the atomic sites in PTCDA matched well with data from [6] concerning spread of values and frequency of particular energies but differed significantly in the exact energy value assigned to each atomic site by ~20eV. The reason for this large shift is unknown. However wrong the binding energy simulations by StoBe may have been, this did not seem to effect the simulations of NEXAFS or RXES spectroscopies of PTCDA.

5.3 NEXAFS Conclusions

The StoBe produced simulations of C and O K-edge NEXAFS spectroscopies of PTCDA were successful and seemed to accurately match results by several different research groups. The line shape and peak occurrence matched well and plots only had to be shifted by ~1eV to precisely match up in energy value. Considering the some what imprecise method of comparing plots due to graph extraction, it may be that the simulations and the experimental plots may match up even more exactly should a more should a more accurate comparison be made. Finally, the determined ratio of p to s polarisations in the McGuinnes seems reasonable. One would assume accuracy here, especially as that the plots lined up without any need to shift the energy of either plot to align peaks and line shape.

6. References

[1] T. Ogawa et al. / Acta Cryst. (1999). **B55**, 123 - 130

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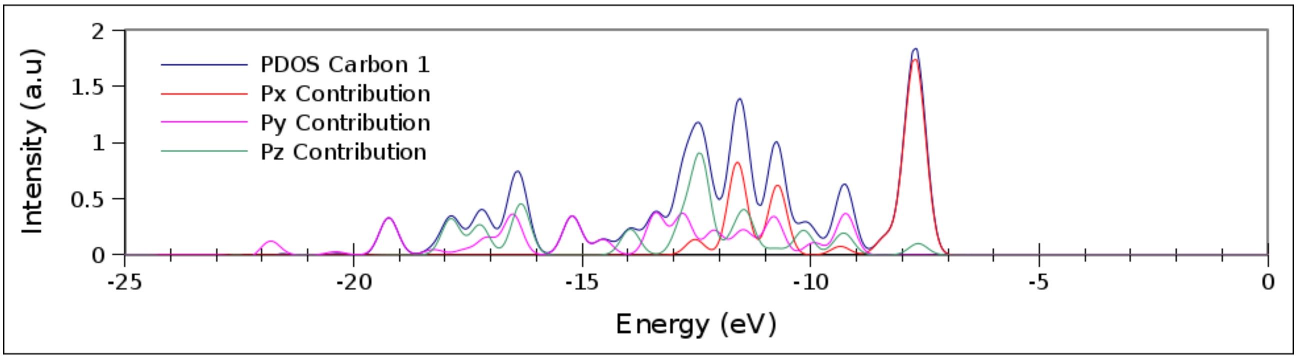
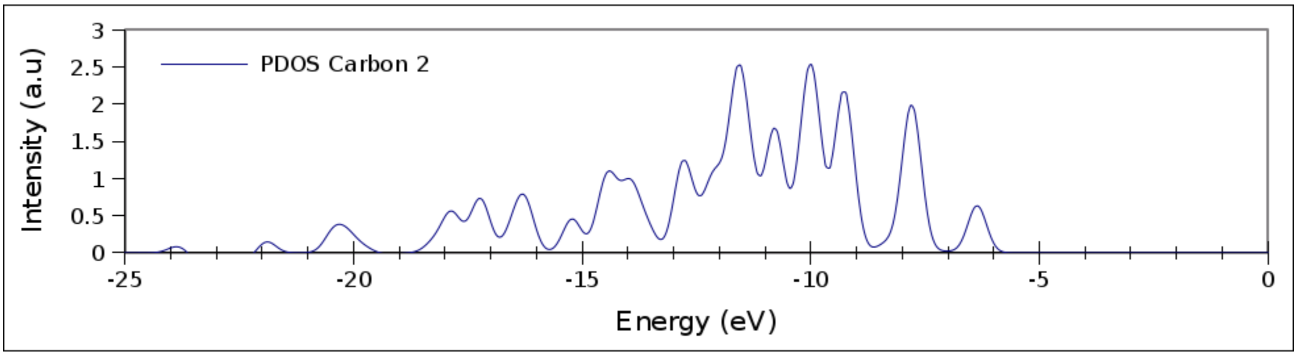
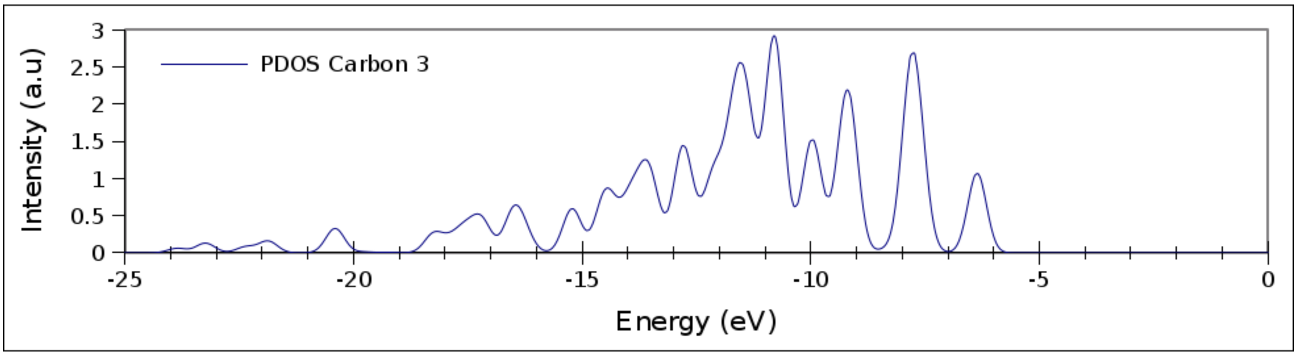
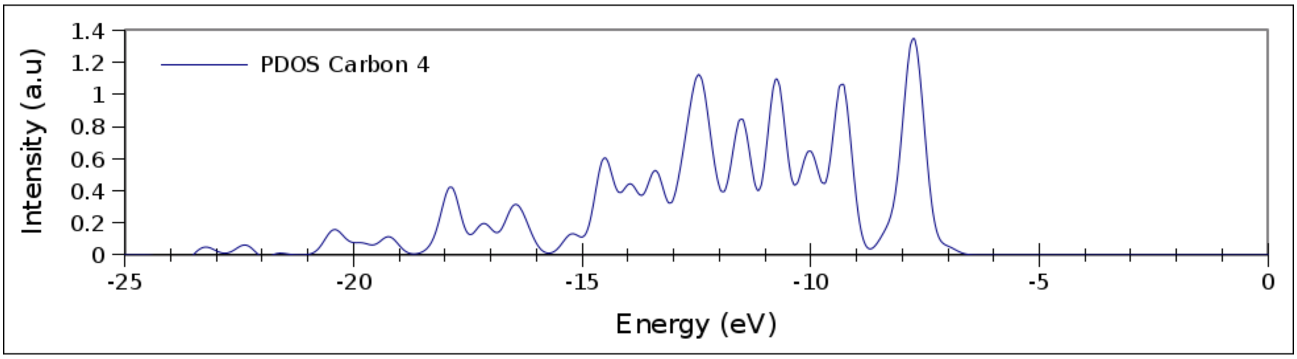
Appendix I

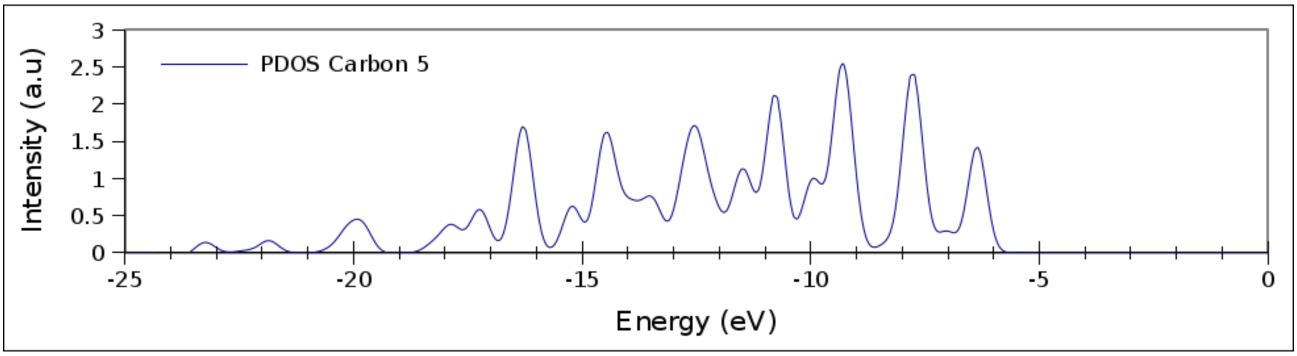
Below are plots of the occupied DOS for each inequivalent Carbon and Oxygen atom. They are in increasing numerical order, C1-7 and then O1-2.

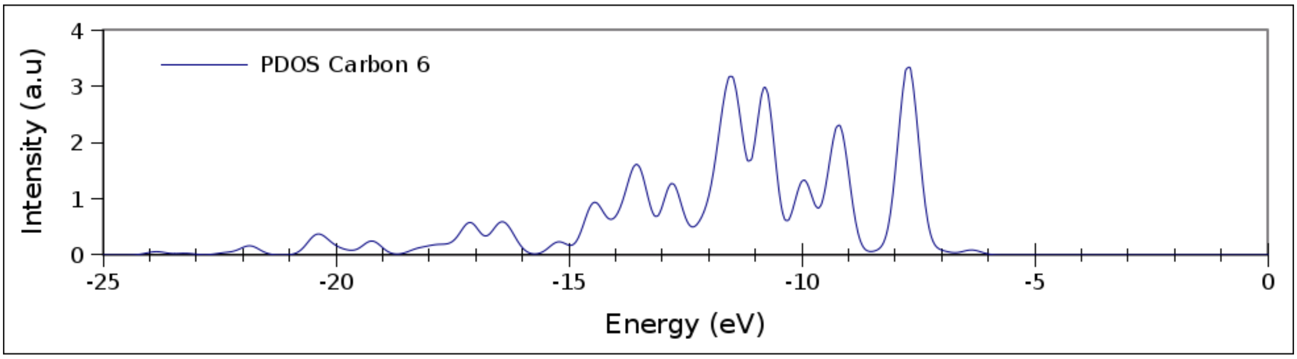




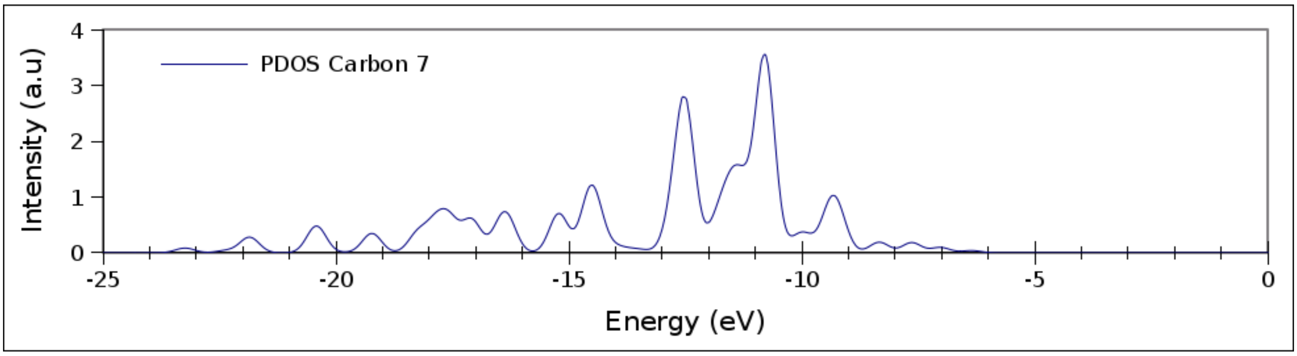


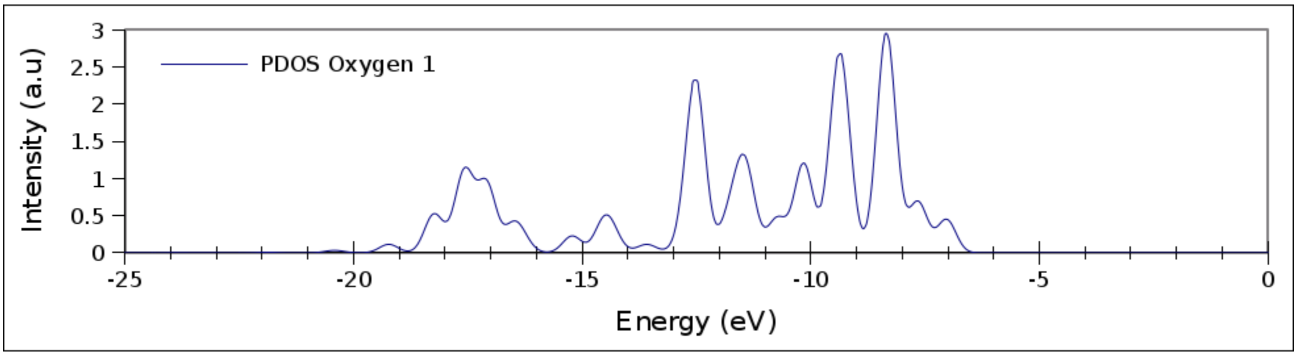

PDOS Carbon 4
Intensity (a.u)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-25
-20
-15
-10
-5
0
Energy (eV)


PDOS Carbon 5
Intensity (a.u)
3
2.5
2
1.5
1
0.5
0
-25
-20
-15
-10
-5
0
Energy (eV)

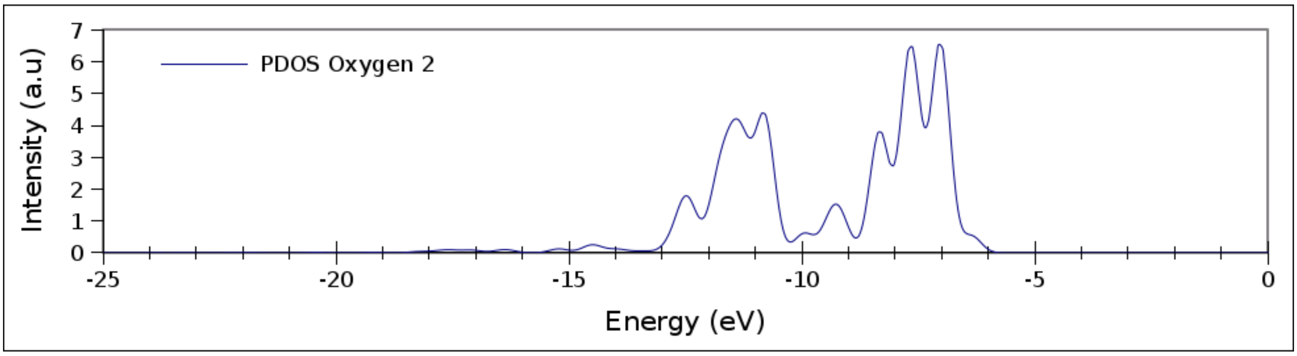

PDOS Carbon 6
Intensity (a.u)
4
3
2
1
0
-25
-20
-15
-10
-5
0
Energy (eV)

.


PDOS Carbon 7
Intensity (a.u)
0
1
2
3
4
-25
-20
-15
-10
-5
0
Energy (eV)


PDOS Oxygen 1
Intensity (a.u)
0
0.5
1
1.5
2
2.5
3
-25
-20
-15
-10
-5
0
Energy (eV)

.


PDOS Oxygen 2
Intensity (a.u)
0
1
2
3
4
5
6
7
-25
-20
-15
-10
-5
0
Energy (eV)