Avogadro with YAeHMOP Manual

Patrick Avery

Department of Chemistry
University at Buffalo
Buffalo, NY 14260-3000, USA
May 5, 2017

Contents

1 Installation

1.1 Windows

The Windows binary may be dowloaded from the following location:

`https://avogadro-yaehmop.github.io/`

You need to unzip the file. You may use whichever unzipping software that you would like. 7-Zip [1] is a good option if you do not have any unzipping software. After you have unzipped it, double click on the executable that is inside, and proceed through the security warning. Go through the install process using all the default options (you may want check the box to "Create Avogadro Desktop Item", though). Once the installation finishes, you should be able to open it with the desktop icon or through the start menu. If you wish to uninstall it, you may do so either through "Add or remove programs" or through the uninstaller that is located in your install location (most likely "C:\Program Files (x86)\Avogadro").

1.2 Mac

The Mac binary may be downloaded from the following location:

`https://avogadro-yaehmop.github.io/`

If the file does not unzip automatically, you need to unzip it. Once it has been unzipped, you will find the AVOGADRO application inside. Double clicking may not open the file for security reasons. You may need to right click the application, click "Open", and then accept it despite the warning. You may also add it to your applications by copying and pasting it into your /Applications directory. If you wish to uninstall it, you may do so by simply deleting the application file.

1.3 Linux

The Linux binary may be downloaded from the following location:

`https://avogadro-yaehmop.github.io/`

You may unzip this zipped file through the GUI or the terminal. If you choose to use the terminal, the following command will do: "tar -xzvf linux-avogadro-yaehmop.tgz". In the unzipped and untarred directory, the AVOGADRO executable is "avogadro-yaehmop/bin/avogadro". You may move the "avogadro-yaehmop" directory around, but do not move or change the files that are inside. You may uninstall the program by simply deleting the directory.

2 Preparation for DOS or Band Structure

This section includes the general setup that is needed for a DOS or band structure calculation. We will use diamond, a known insulator, as an example.

1. First, we need to start AVOGADRO and open a diamond file.

   After AVOGADRO has been opened, click "Open" in the top right corner, and navigate through the file dialog to the "crystals" directory that comes with it. Diamond is located in "elements" and it is named "C-Diamond.cif". Open this file. Note that if the file is grayed out and you cannot open it, you may need to change the file types at the bottom of the file dialog to "All files" (on Mac, you need to click the "Options" button first).

   Once you have opened up the file, diamond should appear on your screen as it does in Fig. 1. Note that this is a conventional cell, not a primitive cell.

2. Next, we need to reduce diamond to its primitive cell and make sure it is in its standard orientation.

   Although band structures and density of states calculations can be performed with non-primitive cells, they will typically give us extra information that we do not need. Thus, it is common practice to reduce a cell to its primitive form before performing the calculations. As for the orientation, it is important to note that the three-dimensional points in reciprocal space depend upon the orientation of the cell in real space. For
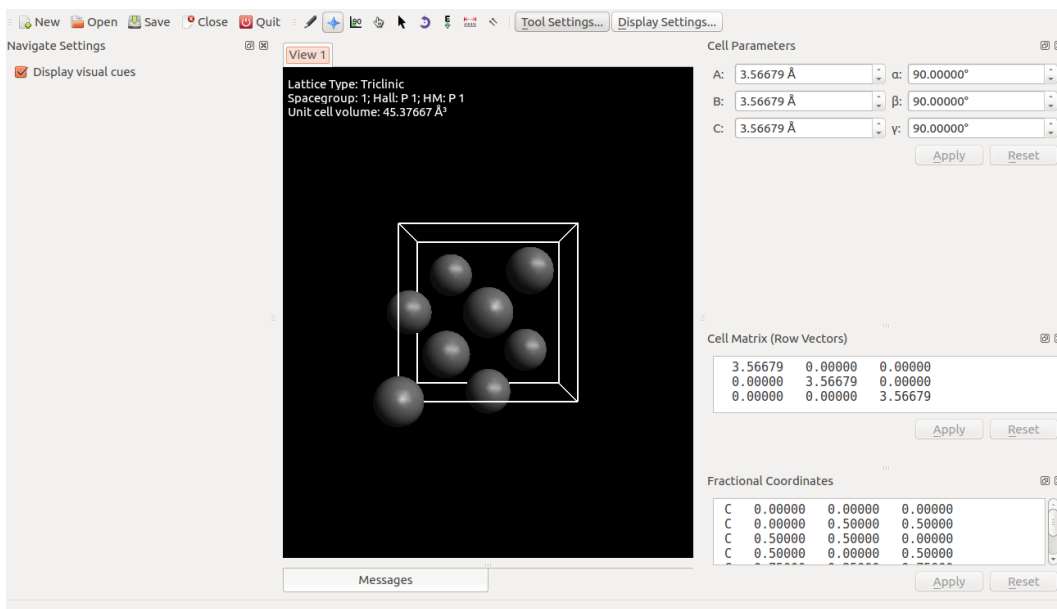
Figure 1: Diamond in its Conventional Cell

band structures, it is necessary to make sure, then, that the orientation is standardized so that the band structure may be compared to other band structure calculations. The proper orientation depends on the type of Bravais lattice that the cell has. Note that the orientation may matter for density of states as well, but because the user will usually use a mesh, orientation may not make a difference.

Both of these operations (primitive reductions and cell standardization) can be done in one operation in AVOGADRO. First, the space group tolerance needs to be set to a reasonable value. Click "Crystallography"->"Settings"->"Tolerance for symmetry operations...". Change the tolerance to be 0.0001 and press "OK". Next, click "Crystallography"->"Reduce"->"Reduce Cell (Primitive and Standardize)".

Once you have done this, diamond should look like that in Fig. 2. In addition to there only being two atoms in the unit cell now, the actual shape of the cell will have changed as well. The top left corner should now display the lattice type and space group ($Fd3m$) correctly.

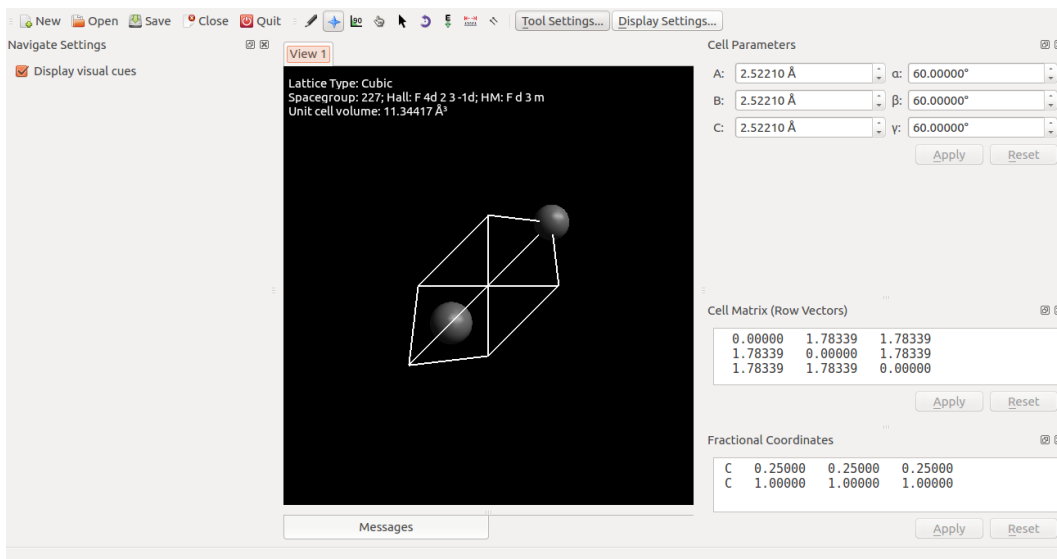Figure 2: Diamond in its Primitive Cell

3 Density of States Calculation

Density of states calculations calculations can be used to determine the energies of the electron states, and it can be used to determine the Fermi level (thus, density of states calculations should usually be performed before a band structure calculation).

First, we are going to select the options for the density of states calculation.

Click "Extensions"->"Yaehmop"->"Calculate Density of States". The dialog box in Fig. 3 should appear.

The "Number of valence electrons" will automatically be generated using the atoms in the unit cell. This number may be adjusted (one reason for changning it would be if an atom were charged, for example). For our purposes, the guess of "8" electrons is fine.

The "k points" box is where the user may select the k points to be used. Most of the time, the user will probably just use a mesh (such as "15x15x15"). The larger the numbers in this mesh, the more points will be sampled and the more accurate the calculation will be. However, be aware that if you use too many points for a system with too many atoms, your operating system may shut down YAEHMOP while it is running (and AVOGADRO will continue as if you did not ask it to calculate anything). You may also add in k points as
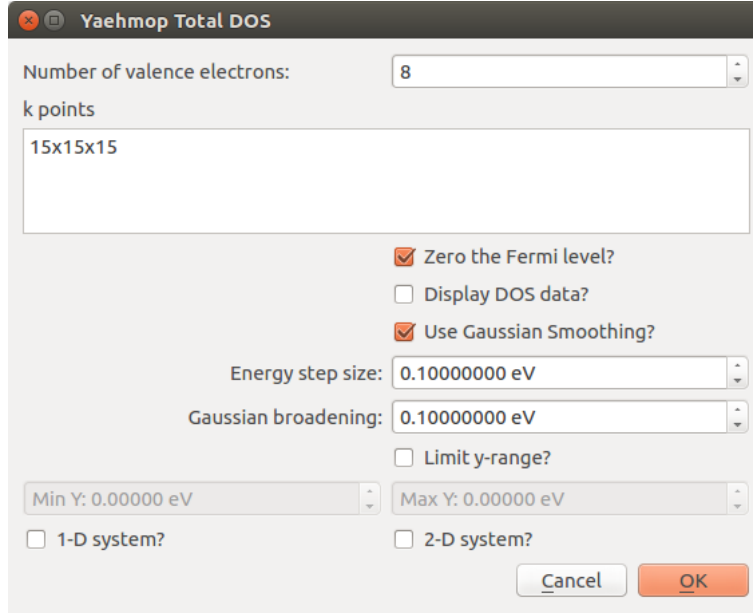
Figure 3: Density of States Dialog

<x> <y> <z> <weight> where the weight is how many times it will be counted. This can be useful if you used other software to generate k points based upon the symmetry (which can reduce computation time). "15x15x15" will be fine for our case.

The Fermi level is always calculated in these density of states calculations. Thus, we are able to check "Zero the Fermi level?", and the points will automatically be adjusted based upon discovered Fermi level (note that the Fermi level depends upon the number of valence electrons). For our case, please check "Zero the Fermi level?"

"Display DOS data?" will display the data so that it may be copied and pasted into a file. Then, the data may be examined using graphing software. The unadjusted Fermi level is printed first in the displayed data. Then, the density of states values are displayed. Finally, if Gaussian smoothing was used, integration data is printed as well. We do not need to display the density of states data here, so leave it unchecked.

"Use Gaussian Smoothing?" fits the data to Gaussian functions to make it look significantly smoother. It also enables the calculation of the integration. It is recommended to use Gaussian smoothing most of the time. For our case, please be sure that "Use Gaussian Smoothing?" is checked.

6

"Energy step size" may only be used if "Use Gaussian Smoothing?" is checked. The smaller this number is, the higher the number of points that will be created during smoothing. Thus, a smaller energy step size results in a more resolved graph. For most cases (including this one), "0.1" eV will be just fine.

"Gaussian broadening" may also only be used if "Use Gaussian Smoothing?" is checked. This number represents σ in the Gaussian distribution. The larger this number is, the smoother the graph will look. Note that higher values of Gaussian smoothing may make the density of states appear to cross the Fermi level. Note that this may sometimes be an artifact of smoothing, and you may want to decrease the Gaussian smoothing to check and be sure that the density of states crosses the Fermi level. The same is true for semi-metals. For our case (and most cases), "0.1" eV is fine.

If the "Limit y-range?" checkbox is checked, the y-range of the displayed graph will be limited to be between "Min y" and "Max y". We can leave "Limit y-range?" unchecked in our exercise. Note that if you set these values in the density of states dialog, the saved values will be changed in the band structure dialog to match them.

Since we are performing the calculation on a 3-dimensional sytem, we will not check "1-D system?" or "2-D system?". Note that if you ever wish to use these, a 1-dimensional system has periodicity along the A lattice vector, and a 2-dimensional system has periodicity along the A and B lattice vectors.

When your selected options match that of Fig. 3, you may begin your density of states calculation. Press the "OK" button. After a few seconds of calculating (AVOGADRO will gray out while YAEHMOP is running... if it does not, then something is wrong with the installation), Fig. 4 should appear.

The Fermi level is plotted as a dashed line. Note in this plot that there is a band gap of about 5 eV. This is a reasonable band gap for diamond, and it accurately portrays that diamond is an insulator. If smoothing is used, the integration will be plotted as a blue line (and the axis for the blue line is at the top of the graph). The blue line crosses the Fermi level
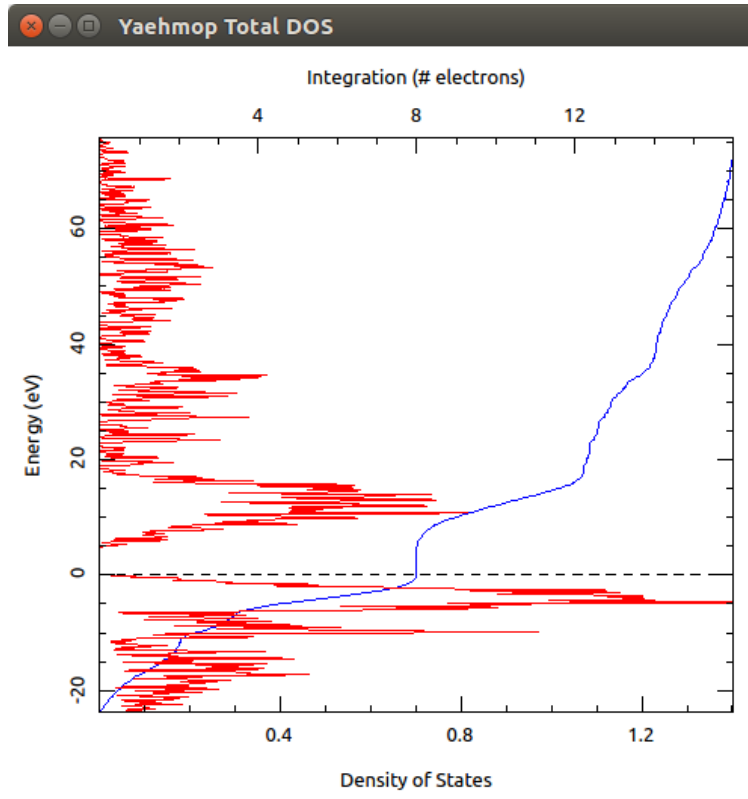
Figure 4: Density of States for Diamond

at the number of valence electrons, and it reaches double the number of valence electrons at the top of the graph.

The user may zoom in on the graph. The user may also translate the graph by holding right-click and dragging. If the user double-clicks the graph, it will return to its default axes.

That concludes the density of states exercise. Calculating the density of states of other materials can be done in the same way. It is preferable to calculate the density of states before the band structure in order to obtain an accurate Fermi level for the band structure calculation.

4   Band Structure Calculation

Band structure calculations can also be very useful for obtaining information about molecular orbitals in a solid. If the Fermi level is known, they can be used to determine whether the

solid is a metal or not. Note that the user may want to perform a density of states calculation first in order to obtain the correct Fermi level (demonstrated in Section 3) if they have not done so. Please have your cell reduced to its primitive form and in its proper orientation (see Section 2) before performing the band structure calculation.

First, we are going to select the options for the band structure calculation.

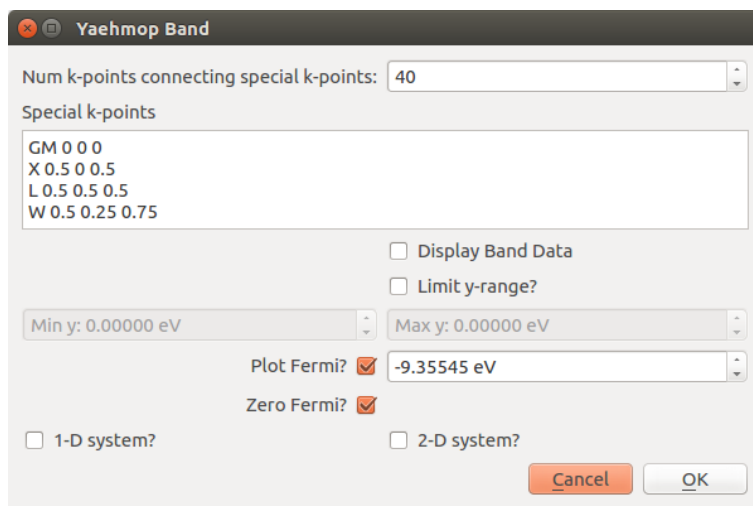Click "Extensions"->"Yaehmop"->"Calculate Band Structure". The dialog box in Fig. 5 should appear.

Figure 5: Band Structure Dialog

The "Number of k-points connecting special k-points" is the number of k-points to be sampled between each special k-point. Increasing this number will increase the resolution of the plot, but it will also make the calculation slower. For our purposes, 40 will suffice.

In the "Special k-points" section, special k-points will automatically be generated if the space group was correctly detected. The space group of the crystal can be seen in the top left corner of the view (as can be seen in Fig. 2). The user may detect the symmetry by reducing the cell to its primitve form or using the "Perceive Spacegroup" feature under "Crystallography->Spacegroup". If the space group is *P1* or undetected, only the Gamma point will be present. The special k-points that are automatically generated are the special k-points that contain no variables. The list of these special k-points can be found for each

space group on the Bilbao website [2]. In the "Special k-points" box, special k-points may be added, removed, or changed to vary the points and pathways that are explored in reciprocal space. In our example, the default special k-points will be fine.

If the "Display Band Data" checkbox is checked, then the data will be printed to a dialog that will be displayed ater the calculation is complete. The user may copy and paste the data elsewhere to plot it with other plotting software. We can leave this unchecked in this exercise.

If the "Limit y-range?" checkbox is checked, the y-range of the displayed graph will be limited to be between "Min y" and "Max y". We can leave "Limit y-range?" unchecked in our exercise. Note that if you change these values in the band structure dialog, the density of states dialog values will be changed to match them.

If the "Plot Fermi?" checkbox is checked, the Fermi level will be plotted as a dashed line, and the correct Fermi level needs to be given in the spinbox on the right. Note that Fermi levels are calculated by performing density of states calculations. Because of this, the Fermi level spinbox will automatically be set to be the value of the most recent density of states calculation. If you just performed a density of states calculation on diamond, this value will be set to -9.35547 eV. Fill in the box with the correct Fermi level (-9.35547 eV) if it is not set. For this exercise, please check "Plot Fermi?" and be sure the correct Fermi level is set.

If the "Zero Fermi?" checkbox is checked, all of the data will be adjusted so that the Fermi level is at zero. This cannot be set if "Plot Fermi?" is not checked because the Fermi level cannot be zeroed if we do not know what it is. For this exercise, please check "Zero Fermi?"

Since we are performing the calculation on a 3-dimensional sytem, we will not check "1-D system?" or "2-D system?". Note that if you ever wish to use these, a 1-dimensional system has periodicity along the A lattice vector, and a 2-dimensional system has periodicity along the A and B lattice vectors.

Once all the options are set, the final step is to plot and examine the band structure.

Once you have set all of the options given in Fig. 5, press the "Ok" button. After a very short time, the band structure plot should appear, and it should look like Fig. 6.
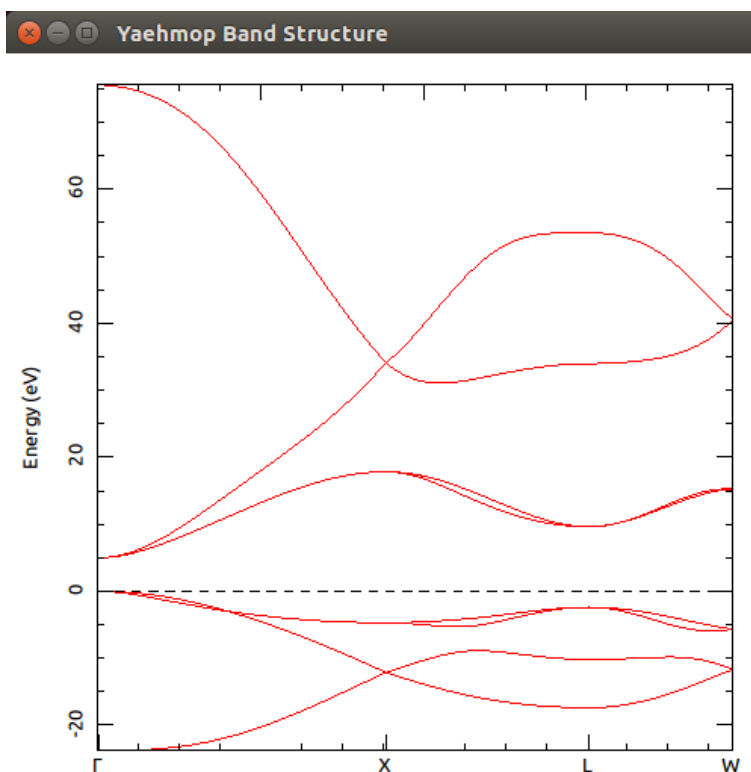

Figure 6: Band Structure for Diamond

The Fermi level is plotted as a dashed line. Note in this plot that there is a band gap of about 5 eV at the Gamma point. This is a reasonable band gap for diamond, and it accurately portrays that diamond is an insulator.

Note that the special k-points on the x-axis are spaced out according to their distance in reciprocal space. Also note that the user may zoom in on the graph and right click it to translate it (although the x-axis labels may not remain true). The user may double click to return to the original orientation.

That concludes the diamond band structure exercise. Calculating the band structure of other materials can be done the same way. Be sure to perform a density of states calculation first to get an accurate Fermi level.

5 Projected Density of States Calculation

Performing a projected density of states calculation can be very helpful for identifying components in a total density of states plot. In this tutorial, we will perform an example with graphite.

First, open up the C-Graphite.cif file located in the "crystals"->"elements" directory that comes with AVOGADRO, and then perform a "Reduce Cell (Primitive Reduce and Standardize)". If you do not know how to do this, see the beginning of Section 2.

Once you have performed the primitive reduction and standardized the cell, your graphite crystal should look like that in Fig. 7.
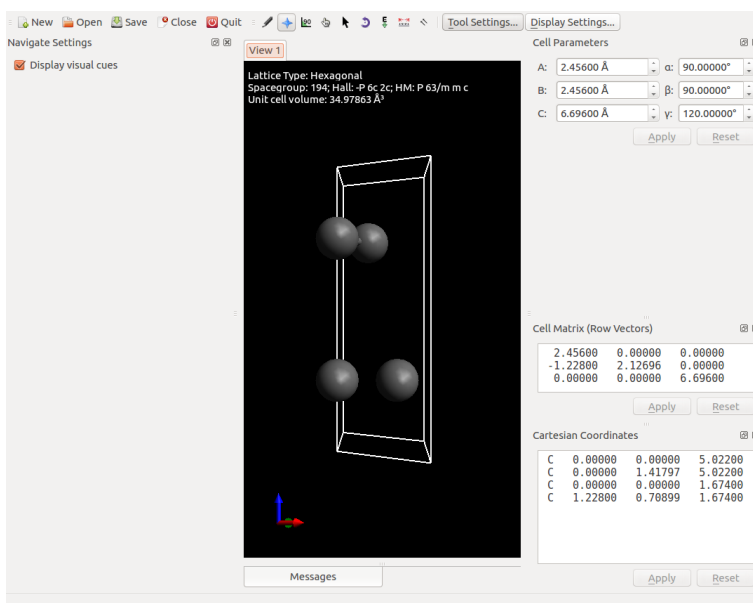

Figure 7: Standardized Graphite Crystal

Next, we are going to fill in the settings for our projected DOS calculation. Click "Extensions"->"Yaehmop"->"Calculate Projected Density of States...", and fill in the dialog box as shown in Fig. 8. If you wish to copy and paste the "Projections" text, it is as follows:

C s
orbital 1 1.0, 5 1.0, 9 1.0, 13 1.0
C px & py

orbital 2 1.0, 3 1.0, 6 1.0, 7 1.0, 10 1.0, 11 1.0, 14 1.0, 15 1.0

C pz

orbital 4 1.0, 8 1.0, 12 1.0, 16 1.0

Figure 8: Projected DOS Dialog for Graphite

Other than the "Projections" option, the "Integrate PDOS?" option, and the "Display Total DOS?" option, if you do not know what any of the options are, refer to Section 3 since the majority of the options are identical to the Total DOS options.

In the "Projections" box, the user specifies the projections that they want to see. Each projection line is divided up as follows:

<type> <contrib1> <weight1>, <contrib2> <weight2>...

<type> can be either "atom" or "orbital", <contrib> is the atom's (or orbital's) number, and <weight> is the weight of that contributor.

By default, the set of projections is generated for different atom types. Atoms are numbered with the same ordering as can be seen in the bottom right of Fig. 7. The numbering for orbitals is a little bit more difficult to determine since different atom types have different numbers of orbitals.

To assist with obtaining the correct numbers of orbitals, the "Display Orbital Projections" and "Display Detailed Orbital Projections" buttons were added. When these buttons are pressed, the text in "Projections" will be replaced with a set of projections with the orbital numbers identified. "Display Orbital Projections" groups orbitals of the same type and from the same type of atom together. "Display Detailed Orbital Projections" only groups orbitals of the same type for each individual atom together.
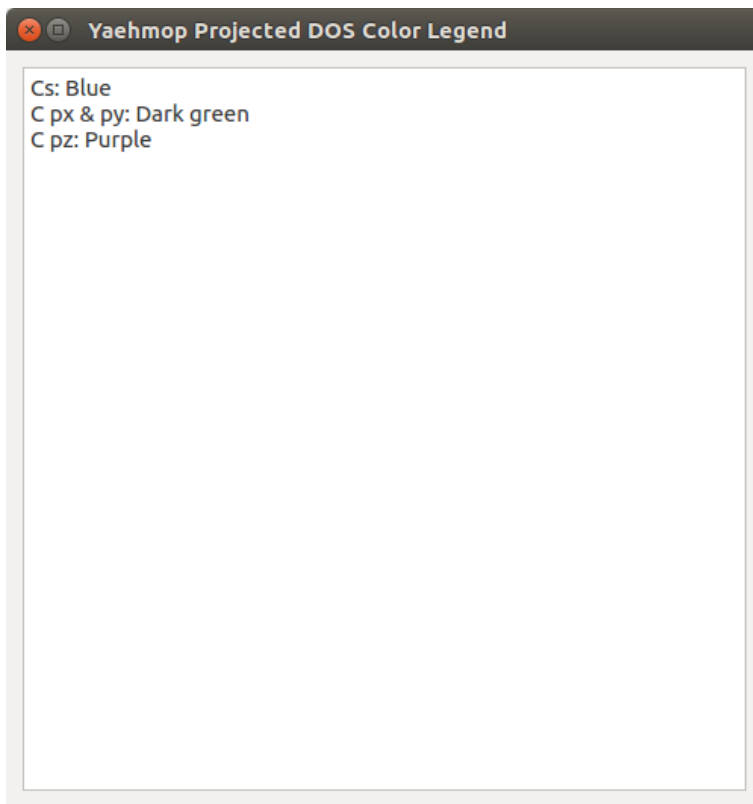

Figure 9: Color Legend for Graphite Projected DOS

In addition, to assist with identifying the different curves in the plot, if a projection has a line immediately above it that begins with a "#", that line will be used for the title in the legend.

14

The projections in Fig. 8 correctly separate the projections into s, (px,py), and pz orbitals (px and py are identical).

When "Integrate PDOS?" is checked, the projected DOS curves are integrated and plotted as well. The projected DOS integrations have the same color as their corresponding projected DOS curve, but they are thinner.

"Display Total DOS?" plots the total DOS along with the projected DOS. We do not need it checked for this exercise.

Once all of the settings are correct, click "Ok" to begin the calculation. It may take a few seconds to complete (if you have a slower computer, you can reduce the k points to 10x10x10). Once the calculation finishes, the plot and a color legend will appear. The color legend will appear as Fig. 9.

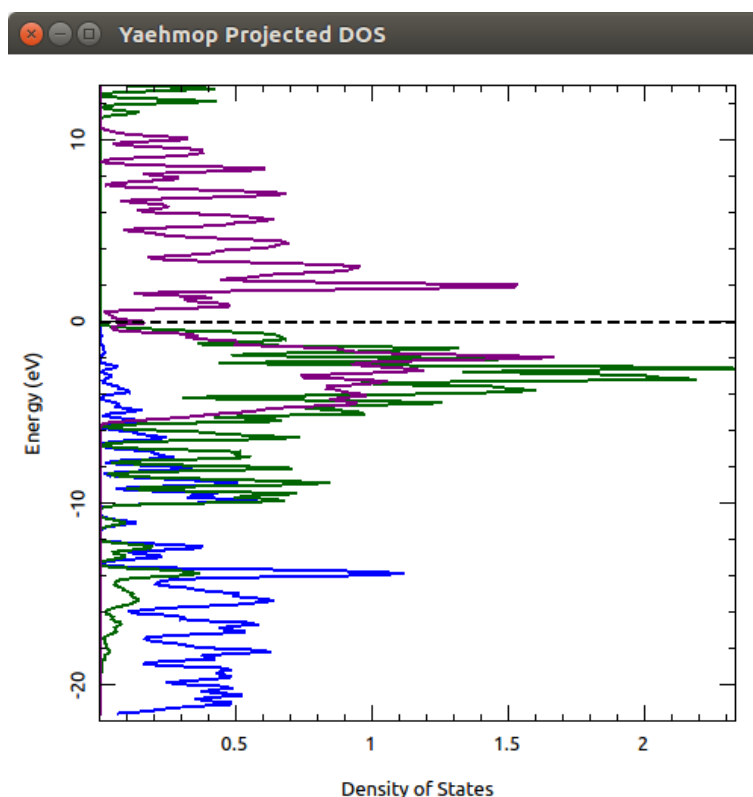In addition, the plot should appear as Fig. 10.

Figure 10: Projected DOS for Graphite. Blue: s orbitals. Dark green: px and py orbitals. Purple: pz orbitals.

As the color legend states, the s orbitals are blue, the px and py orbitals are green, and the pz orbitals are purple. Because the pz orbitals do not hybridize with the s orbitals, they remain higher in energy. The px and py orbitals, on the other hand, do hybridize with the s orbitals, and thus they extend down into the region below the pz orbitals. Note that there is perhaps a little too much mixing between the px,py orbitals and the s orbitals since there is usually a larger gap between the fermi level and the px,py projected DOS.

The mixing between the px,py orbitals and the s orbitals can be illustrated even further by performing another projected DOS calculation such as that in Fig. 8 except with the "Display DOS data?" and the "Integrate PDOS?" boxes checked. The resulting graph is given in Fig. 11. As the color legend indicates, the integration lines are the same color as the corresponding PDOS curves, but they are thinner. Upon examining the data in the "Yaehmop Projected DOS Results" dialog box that appears, one can see that at the Fermi level, the s orbitals integrate to about 4.53 electrons, the px,py orbitals integrate to about 7.46 electrons, and the pz orbitals integrate to about 4.01 electrons. If there were no hybridization, we would expct the s orbitals to integrate to about 8 electrons and the p orbitals to integrate to about 8 electrons in total. However, since there is hybridization between the s and px,py orbitals, these numbers are different. Instead, we cay say there are about 12 sp^2 electrons (the s electrons plus the px,py electrons) and 4 pz electrons.

On a final note, Fig. 12 demonstrates that graphing a projected DOS alongside a band structure plot can greatly assist in identifying the different bands.

That concludes the PDOS section. Be sure to use "Display Orbital Projections" and "Display Detailed Orbital Projections" buttons to assist with numbering the orbitals correctly!

6 Crystal Orbital Overlap Population Calculation

Crystal Orbital Overlap Population (COOP) allows us to see bonding and anti-bonding interactions between two atoms or orbitals. As an example, we are going to perform a
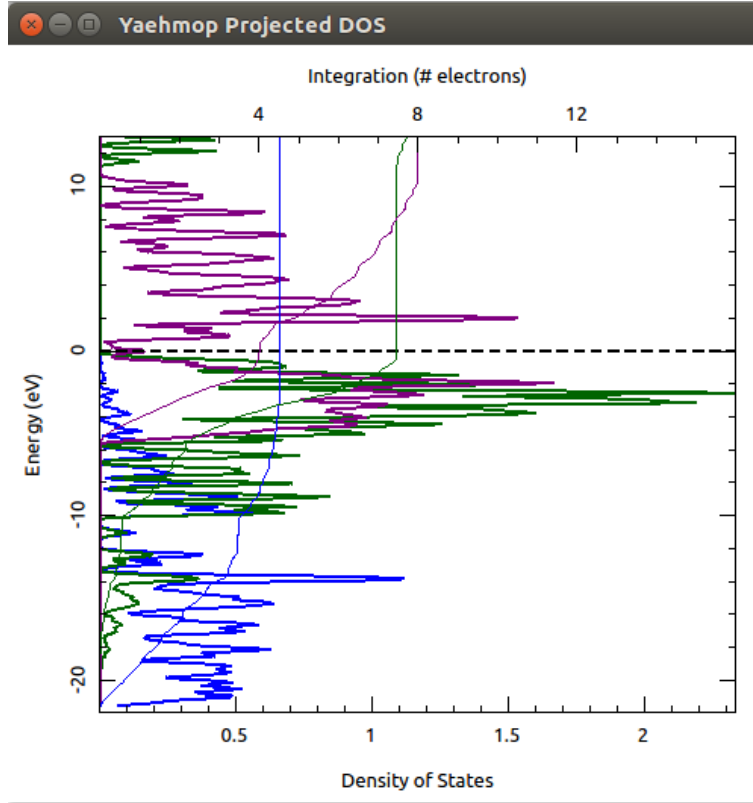
Figure 11: Example of Projected Density of States Integration with Graphite
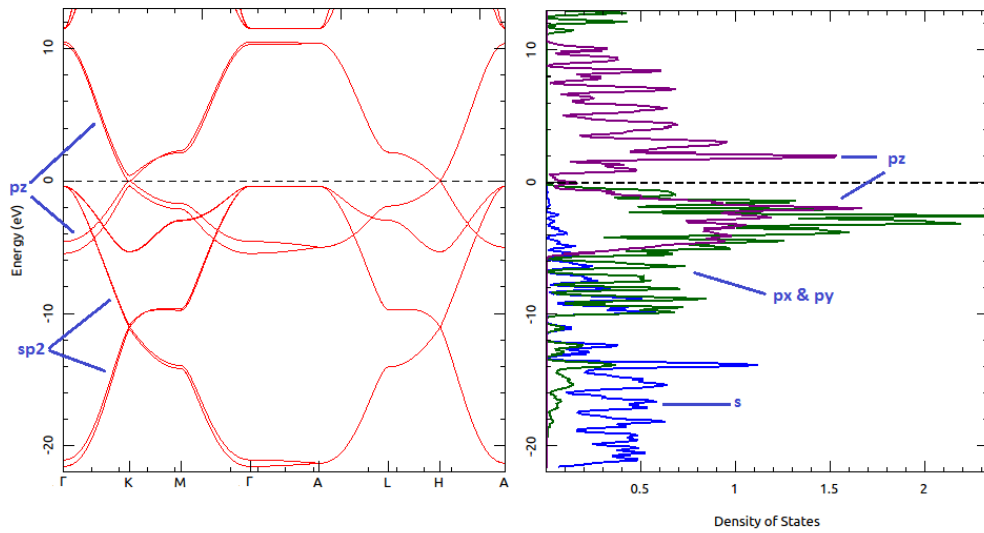

Figure 12: Comparison of Band Structure and PDOS for Graphite. Both were calculated with YAᴇHMOP

calculation on a linear hydrogen atom chain as was done by Roald Hoffmann in *Solids and Surfaces* [3]. This example will also demonstrate the use of a one-dimensional system.

Our linear hydrogen atom chain that we will be creating will have the atoms spaced 1 Å apart. Building this in AVOGADRO is simple. First, open AVOGADRO and click "Crystallography"->"Add Unit Cell". In the cell editor that appears on the right-hand side, set A, B, and C to all be 1, and set α, β, and γ to all be 90.0. Then, click in the coordinates section on the bottom right (it does not matter if it is Cartesian or if it is Fractional), type "H 0 0 0", then click "Apply". Your periodic hydrogen atom should look like that in Fig. 13.
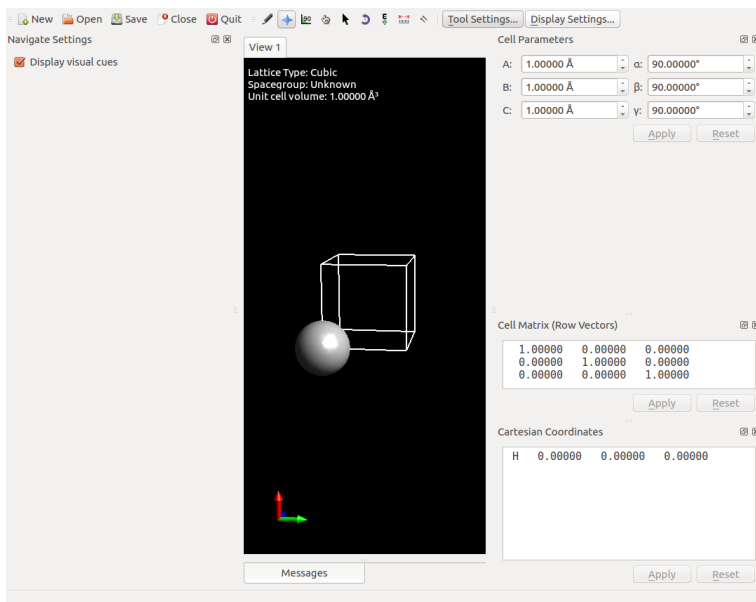
Figure 13: Periodic Hydrogen Atom

Note that as it is drawn, this hydrogen crystal is technically periodic in all directions. When choose to use a one dimensional system in the COOP dialog, however, it will only treat one direction (the A lattice vector) as being periodic. This means that it technically does not matter what the B and C lattice vectors are. We only set them to 1 Å for consistency.

Now that we have built the hydrogen atom system that we will use for our hydrogen atom chain, we can proceed to choose the settings for the COOP calculation. Click "Extensions"->"Yaehmop"->"Calculate Crystal COOP...", and fill in the dialog box as shown in Fig. 14.

"Number of valence elections" only adjusts the Fermi level. It should automatically have been set to "1" because there is only one hydrogen in the system. For systems that are ionic, this can be changed. We should leave it as "1" here.

Figure 14: Crystal Orbital Overlap Population (COOP) Dialog

"k points" is similar to that in the total DOS and partial DOS calculations. You can use any mesh that you would like, and higher numbers typically mean that more points will be calculated (although it will take longer). Since we are only using a one-dimensional system along the A vector, the k points in the directions of the B and C vectors do not make a difference. That is why we set the k points to be "300x1x1".

The "COOPs" section is where we (not surprisingly) describe the COOPs. Each line in the COOPs section is as follows:

<type> <coopNum> <contrib1> <contrib2> <a> <b> <c>

where <type> should either be "atom" or "orbital", depending on whether we are calculating a COOP between atoms or between orbitals (note that it may also be "h-atom" or "h-orbital" if you wish to perform a Hamiltonian COOP calculation - also known as COHP [4]), <coopNum> is a specifier where all COOPs the same <coopNum> will be averaged together to produce a single line, <contrib1> is either <atom1> or <orbital1> depending

on the type, <contrib2> is either <atom2> or <orbital2> depending on the type, and <a> <b> <c> specify the cell that <contrib2> is to be in. So, for example, if <a> <b> <c> is "0 0 0", <contrib2> is in the unit cell. If <a> <b> <c> is "1 0 0", <contrib2> is in the cell neighboring the unit cell in the A direction.

In our case, we are performing a COOP between two hydrogen atoms in neighboring unit cells. Thus, <type> is "atom", the <coopNum> is 1 (it does not matter since we only have one COOP anyways), <contrib1> is atom number 1 (hydrogen), and <contrib2> is atom number 1 (hydrogen again) in the cell neighboring the unit cell in the A direction ("1 0 0" for <a> <b> <c>). Thus, we are performing the COOP between two hydrogen atoms that are adjacent to each other in our linear hydrogen chain.

"View Atom Numbers..." displays a dialog that shows the user the atom numbers. This can be particularly helpful for larger systems. For our system, it isn't all that helpful since it is easy to figure out that our single atom would be atom number "1".

"View Orbital Numbers..." displays a dialog that shows the user the orbital numbers. This can also be particularly helpful for larger systems since the orbital numbers are not always easy to count out. For our system, it isn't all that helpful either since there is only one orbital: the hydrogen s orbital.

If the "Zero Fermi?" checkbox is checked, all of the data will be adjusted so that the Fermi level is at zero. This can be very helpful to see which states are occupied and which are not, so we check this box here.

"Display COOP data?" will display the data so that it may be copied and pasted into a file. Then, the data may be examined using graphing software. The unadjusted Fermi level is printed first in the displayed data. Then, the COOP values are displayed. We do not need to display the COOP data here, so leave it unchecked.

"Use Gaussian Smoothing?" fits the data to Gaussian functions to make it look significantly smoother. This can be very helpful in many situations. However, we will miss significant details in this calculation if we perform smoothing, so we leave this unchecked.

"Energy step size" may only be used if "Use Gaussian Smoothing?" is checked. The smaller this number is, the higher the number of points that will be created during smoothing. Thus, a smaller energy step size results in a more resolved graph. For most cases "0.1" eV will be just fine. We are not performing smoothing here, so this option does not matter right now.

"Gaussian broadening" may also only be used if "Use Gaussian Smoothing?" is checked. This number represents σ in the Gaussian distribution. The larger this number is, the smoother the graph will look. Since we are not using smoothing here, we leave this unchecked.

If the "Limit y-range?" checkbox is checked, the y-range of the displayed graph will be limited to be between "Min y" and "Max y". To help us see features of the graph, we check "Limit y-range?" here and set "Min y" to be -9.0 and "Max y" to be 31.0.

In order to make our hydrogen chain linear instead of 3-dimensional, we need to check "1-D system?" at the bottom. This makes the system periodic along the A lattice vector. In the case "2-D system?" being checked, the system would be periodic along the A and B lattice vectors.

Once you have set all of the options to match that in Fig. 14, click "Ok". It should not take very long for the calculation to finish and the results (Fig. 15) to appear.

Note that a color legend should also appear as a separate dialog box. The legend prints out the title for each COOP (as they appear in the yaehmop output) and a color. The default is blue, so that is what we have here.

Positive values in the COOP indicate bonding overlap, and negative values in the COOP indicate anti-bonding overlap. Note also that there is a black vertical line at COOP == 0 to help in visualizing whether the COOP is negative or not. In our case, the lowest energy section corresponds to all the hydrogen atoms being in phase with each other, so the lowest energy section is certainly bonding. As the energy of the system increases, more and more atoms become out of phase with their adjacent atoms, so the interaction becomes more and more anti-bonding. Fig. 17 from Hoffmann's book [3] can help us visualize this phenomenon
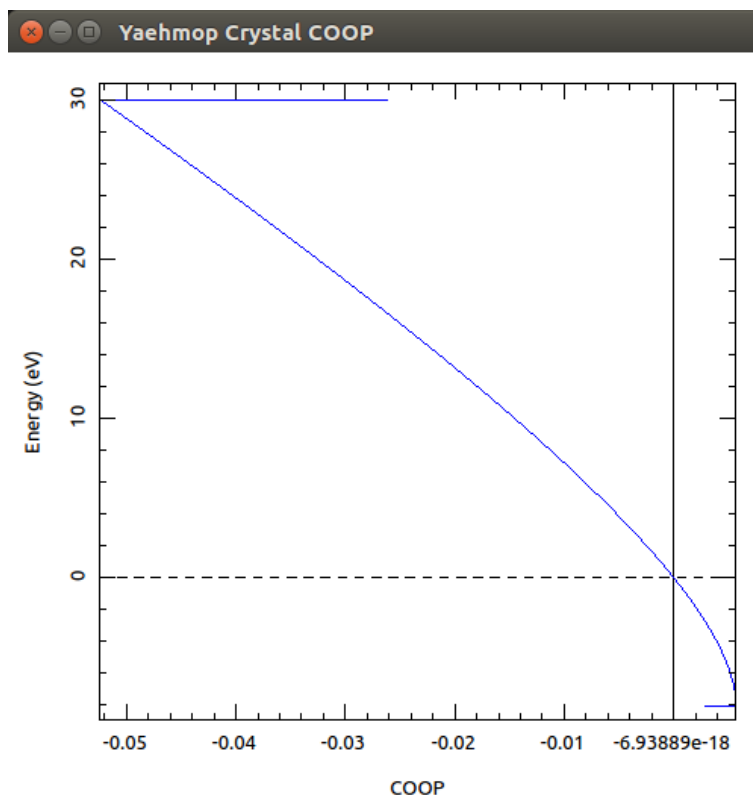
Figure 15: H Chain 1-2 COOP

better.

In 17, note the band structure on the left side. As the k-vector increases, more and more atoms become out of phase with their adjacent atoms, and this results in the increase in energy. We performed a COOP calculation with two adjacent hydrogen atoms, so our plot matches the "1,2" plot in the far right figure. The differences between our plot and Fig. 17 arise from the fact that Fig. 17 was generated using Hückel theory, yet we are using extended Hückel theory with YAEHMOP. Standard Hückel theory does not calculate overlap integrals, and it is thus a little bit less accurate. Regardless, our trends are the same: interactions between adjacent hydrogen atoms begin as bonding, and as energy increases, the interactions become anti-bonding (because the phase between adjacent atoms is changing).

We can also perform the "1,3" COOP calculation that he has displayed in his figure. We do so with the following options in the dialog:

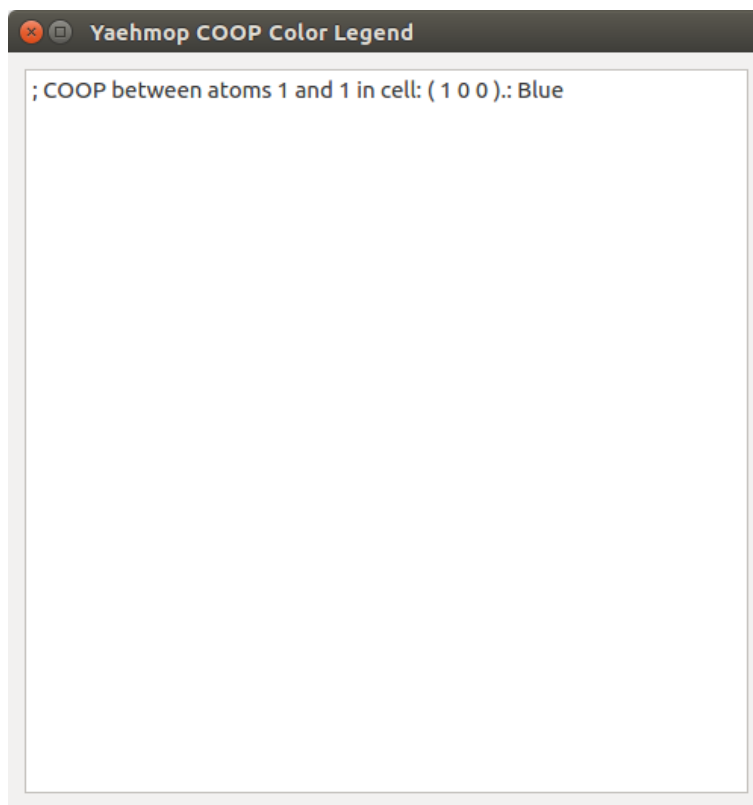Note that the only change is that <a> <b> <c> is now "2 0 0". This means that the

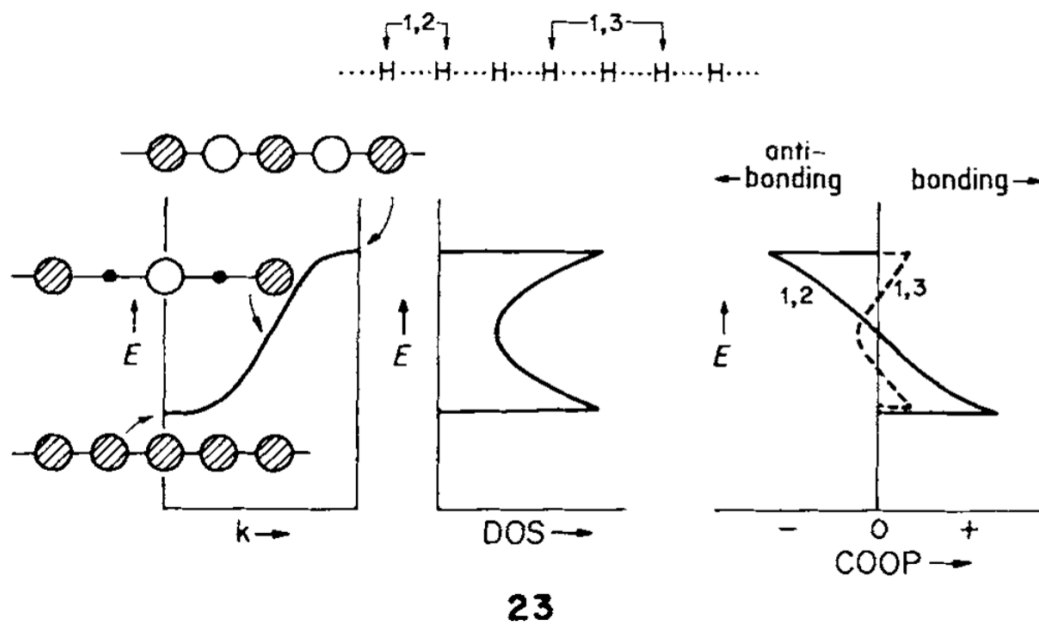Figure 16: H Chain COOP Legend

23

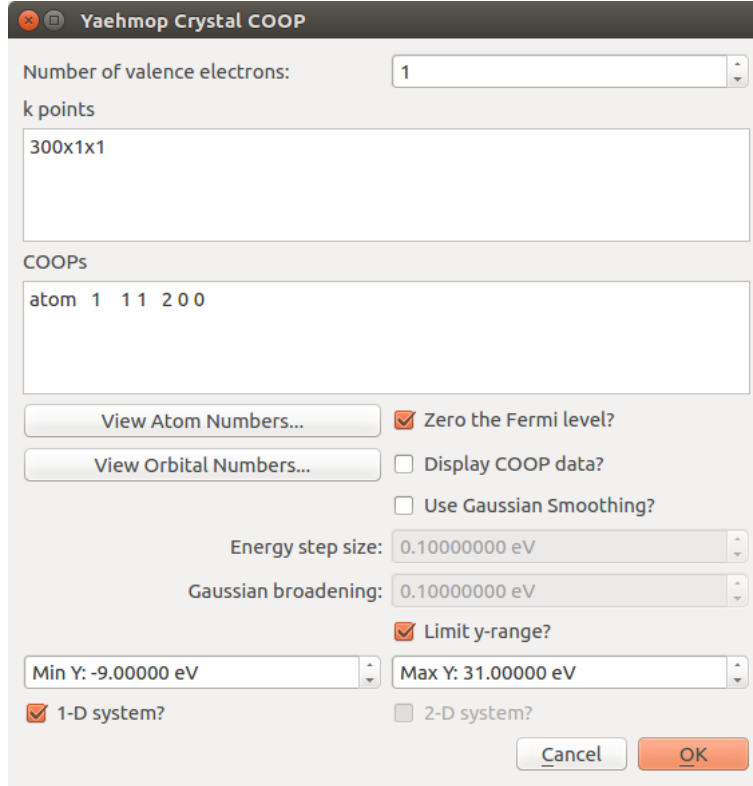Figure 17: COOP from *Solids and Surfaces*[3] of a linear H chain calculated with Hückel theory

Figure 18: COOP dialog for 1-3 H interaction

second hydrogen atom is two cells away from the unit cell in the A vector direction. When we perform this calculation, we obtain Fig. 19.

In our linear hydrogen chain, the atoms are still all bonding at the minimum energy. As we increase the energy, more of the 1,3 hydrogen pairs become out of phase with each other, so anti-bonding interactions dominate. Once we approach the highest energy, however, every neighboring atom has a different phase, and this results in the 1,3 pairs all being in phase with each other. Thus, the interaction between 1,3 pairs becomes bonding again at higher energies.

This concludes the COOP section. Other COOPs can be performed in a similar way. Be sure to use the "View Atom Numbers..." and "View Orbital Numbers..." buttons to see what the atom and orbital numbers are!
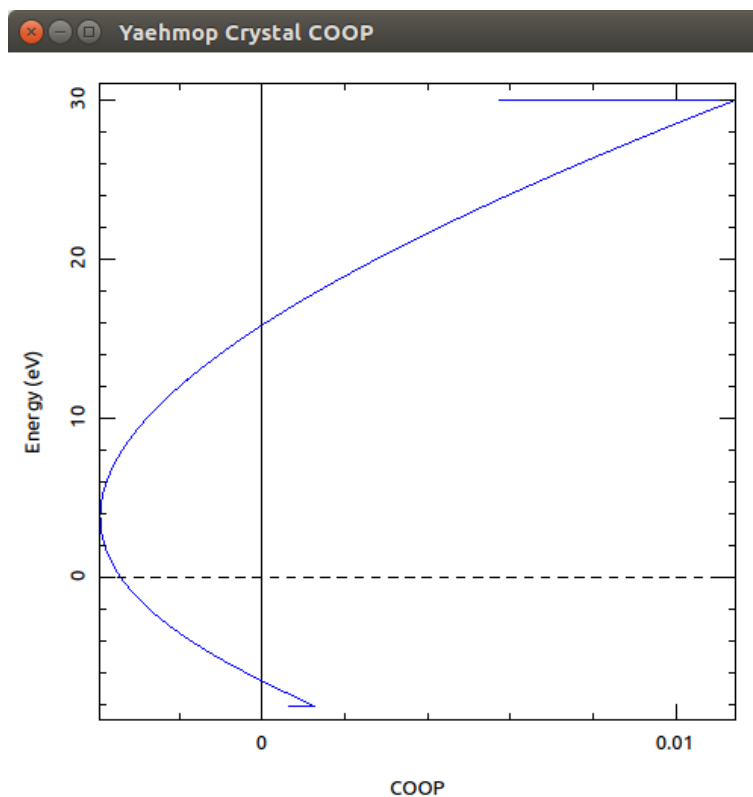
Figure 19: H Chain 1-3 COOP

7 Acknowledgements

This program would of course not be possible without the use of AVOGADRO. The main webpage for AVOGADRO and the first paper are cited in the bibliography [5, 6]. The program would not be possible without the use of YAEHMOP (developed by Dr. Greg Landrum) either [7]. The author thanks Dr. Eva Zurek and Dr. Jochen Autschbach at the University at Buffalo for their discussion as well.

References

[1] https://sourceforge.net/projects/sevenzip/.

[2] http://www.cryst.ehu.es/cryst/get_kvec.html.

[3] R. Hoffmann, *Solids and surfaces: a chemist's view of bonding in extended structures.* VCH Publishers, 1988.

[4] R. Dronskowski and P. E. Bloechl, "Crystal orbital hamilton populations (cohp): energy-resolved visualization of chemical bonding in solids based on density-functional calculations," *J. Phys. Chem.*, vol. 97, pp. 8617–8624, 1993.

[5] http://avogadro.cc/wiki/Main_Page.

[6] M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeersch, E. Zurek, and G. R. Hutchison, "Avogadro: an advanced semantic chemical editor, visualization, and analysis platform," *J. Cheminform.*, vol. 4, p. 17, 2012.

[7] http://yaehmop.sourceforge.net/.