# Instructions for Using Spartan '14

- Log in to the computer with your Colby ID and password.
- Click on the Spartan '14 icon in the dock at the bottom of your screen.

## I. Building Molecules

Spartan has one main window where you will build structures, submit calculations, and view results. In general, it is best to only have one molecule on the screen at a time, so please save and then close each molecule before starting a new build.

To begin building a new molecule, go to File>New Build
To close a molecule when you are done, go to File>Close

Going to File>New Build will automatically bring you to the builder/edit structure menu, but you can also access this menu anytime by pressing the [icon] button. In this view, you will have the builder menu on the right side of the screen:
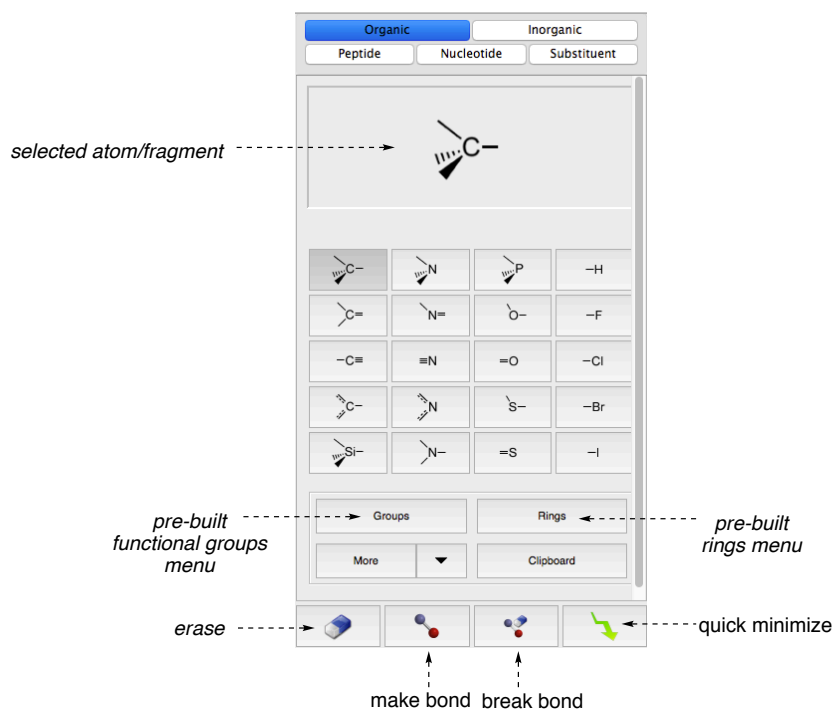


This menu will allow you to select atom types, bonding geometries, functional groups, and ring structures that can be added to your structure. Anything that is highlighted will be added to your structure if you click on the main window (in the "open valence" position that you select). For example, if you click the main window with the tetrahedral carbon selected as shown above, you will get a carbon with 4 open valences to appear (note that

the yellow lines signify open valences. Open valences will automatically turn into hydrogen atoms unless you specify otherwise):
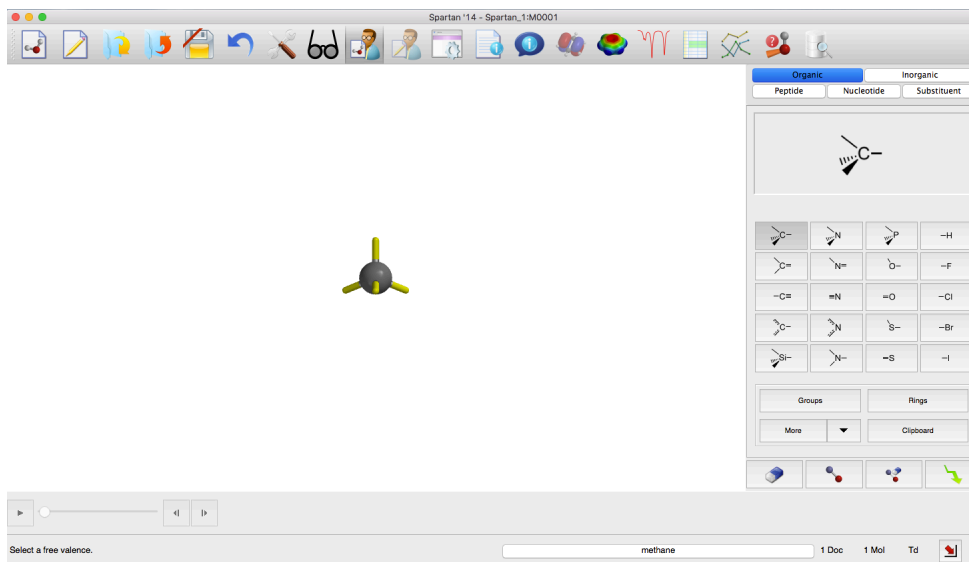


You can manipulate your structure with the mouse (rotation, zoom in/out, etc.) and continue to build by selecting atoms and groups from the builder menu and adding them to open valences on your structure. Some helpful building tips:

- You can make bonds (single, but also double or triple bonds) by using the "make bond" button and selecting any 2 open valences. This is a very easy way to add pi-bonds.
- You can double click an atom to change the atom type (for example, if you have a nitrogen atom selected in the builder, double clicking on a different atom type will change that atom to a nitrogen). This can be very handy in conjunction with the "groups" and "rings" menus.
- Once you have added a few atoms/functional groups, it helps to push the "quick minimize" button to clean up the structure (this is especially helpful for more complex structures).

## II. Setting Up and Running Calculations

When you have built your molecule, you are ready to set up a calculation. Do this by going to Setup>Calculations, which brings up the calculation window:
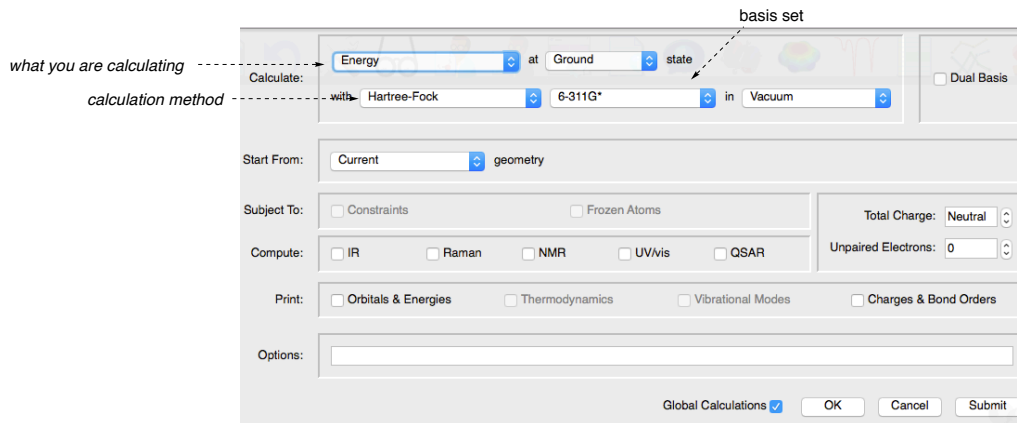


From the pull-down menus identified above, select what you want to calculate, the method you wish to use, and the accompanying basis set. This menu is also where you would identify unpaired electrons and/or charge, if applicable to your structure. Once you are done in this menu, you can press "Submit" in the lower right to begin your calculation, and save your file when prompted to do so.

### *Some information about Computational Chemistry terms and methods:*

The two simplest calculations you can perform are labeled "Energy" and "Equilibrium Geometry". In an Energy calculation (also called single point energy), the program will keep the molecule in exactly the conformation that you have drawn. In an Equilibrium Geometry calculation (also called a geometry optimization), the program will allow the bond lengths and bond angles to change, and single bonds to rotate, in order to minimize the energy of the structure.

There are many different methods for calculating molecular properties and behaviors. Hartree-Fock is a type of "ab-initio" ("from first principles") calculation that attempts to solve the wave function (electronic Schrodinger equation) for the given system. These calculations take a lot of computing power, but can be increasingly accurate depending on the basis set used. In contrast, Semi-Empirical methods use approximations based on empirical data to simplify the calculations. Therefore, these methods are much faster but do not always give as accurate results, especially for more complex systems or properties.

## III. Viewing Your Results

Once you get a message that your calculation has completed, you are ready to view your results! Most of your results can be retrieved by going to Display>Properties:



For experiments in CH241, the most important parts of the molecular properties menu are identified with red arrows, above. Note that to graphically display a dipole arrow on your structure, you can click the box in the lower left.

## IV. Measuring and Altering Distances and Angles

To measure or change bond lengths, angles, or dihedral angles, go to Geometry>Measure Distance/Angle/Dihedral and then click on the appropriate number of atoms. Note that for angles and dihedrals, the order that you click is also important (go from one end to the other, don't click on one of the "middle" atoms first). The bond length/angle/dihedral information is displayed in the bottom right of the main screen:
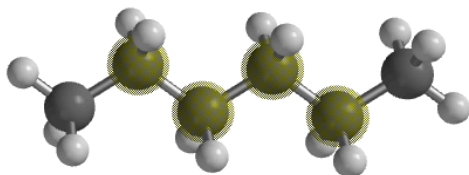
If you wish to manually change the indicated measurement, you can do so by typing directly into the box where the value is displayed, and your structure will change accordingly. For example, if you erase the 180° value shown for the dihedral angle above and change it to 0°, your structure will look like:



Dihedral(C5,C4,C3,C2) = 0.00 °    P

n-hexane          1 Doc      1 Mol      C2v
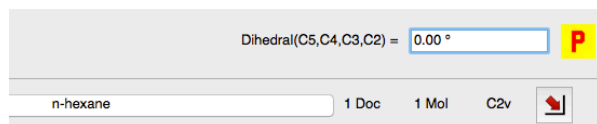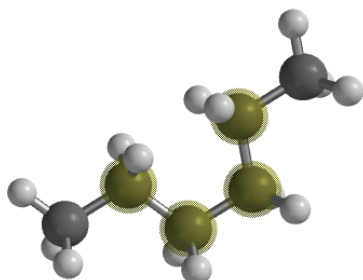
## V. Viewing Molecular Orbitals and Other Surfaces

Molecular orbitals (and other types of interesting surfaces) can be viewed by going to Display>Surfaces. This will bring up a menu that allows you to select the surfaces that you want to study:
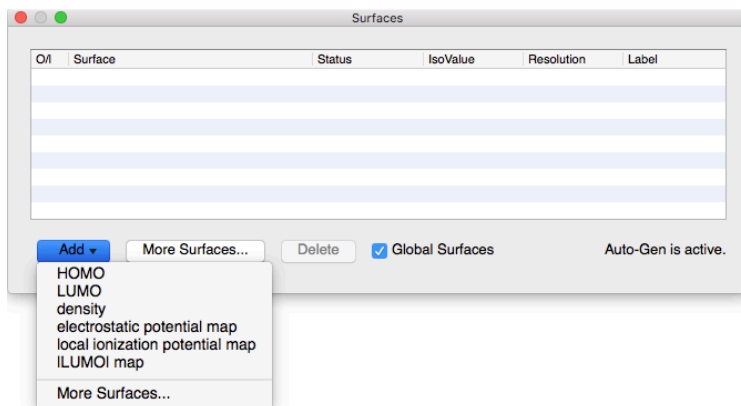


From the "Add" menu, select the surface that you want (for example, HOMO). You will have to select each surface individually (so you have to do this twice to add both the HOMO and the LUMO, for example).

Once selected, you can view the surfaces by checking the box on the left side within the surfaces menu. The surface will then be displayed on your structure. Note that for some surfaces, you may need to run an additional calculation for the computer to compute the requested surface.
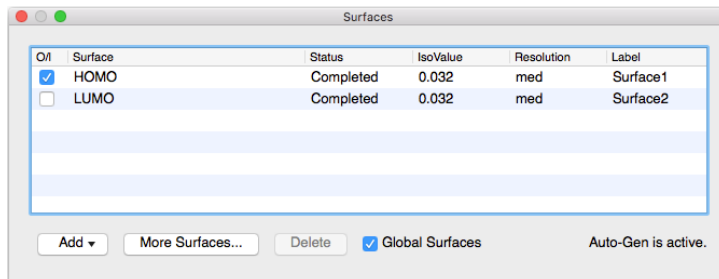


## VI. Important Notes on Units:

- Energies in atomic units (a.u.) can be converted to kJ/mol using:
  1 a.u. = 2625.5 kJ/mol
- Charges, in general, are reported in electronic charge, $e$ where 1 $e$ = 1.60 x $10^{-19}$ C