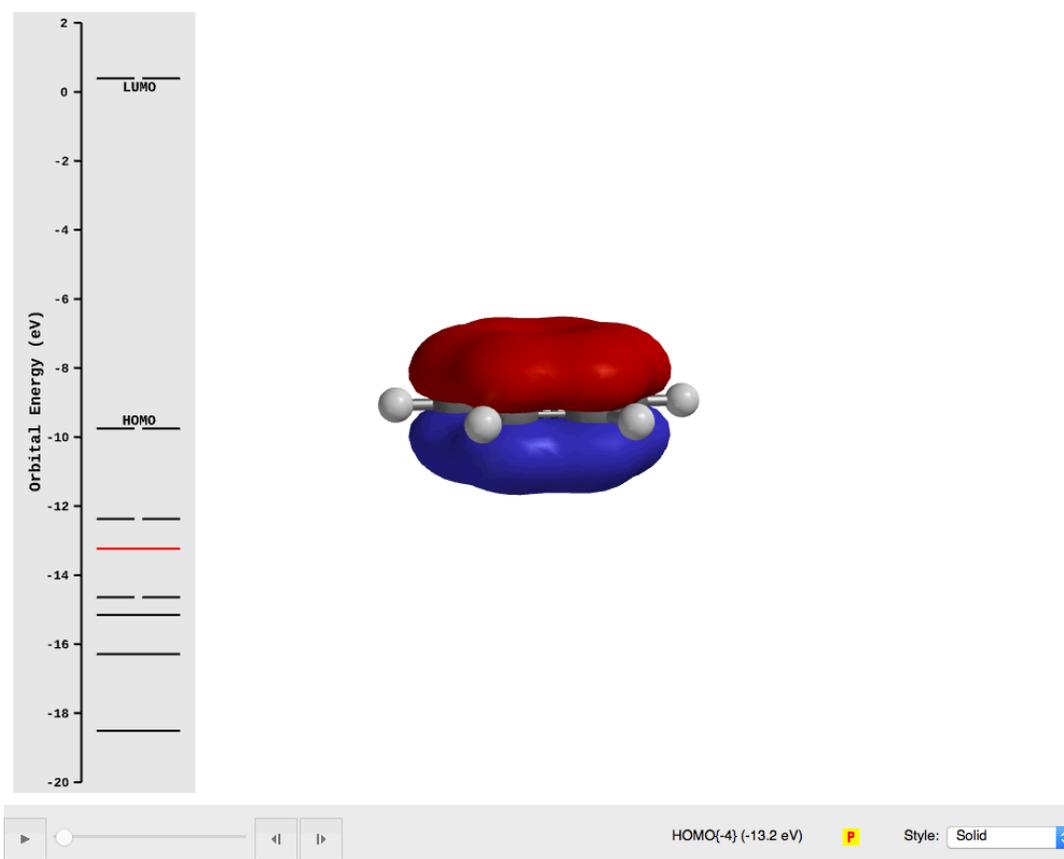


Special Instructions for Molecular Orbitals and Other Surfaces Using Spartan '14

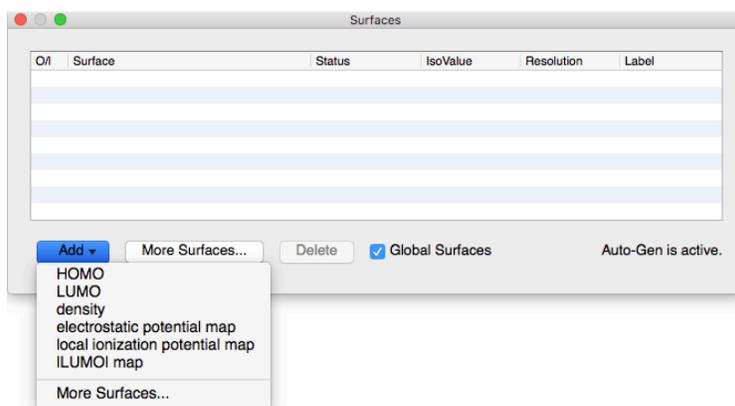
Molecular Orbitals: There are several ways to view/calculate molecular orbitals in Spartan '14. The simplest way is to select Display>Orbital Energies. This will show a series of orbitals on the left panel, along with their energies (y-axis). You can view an orbital by clicking on the "line" representing that orbital. The energy for that orbital also appears in the lower right, along with a pull-down menu that let's you change the surface appearance (solid to mesh to transparent, etc.):



Note that in this view, you cannot see the "properties" menu, but if you generate the molecular orbitals using the "surfaces" menu, then you have greater flexibility (see below).

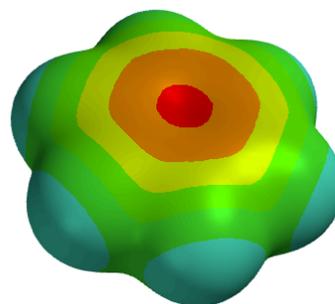
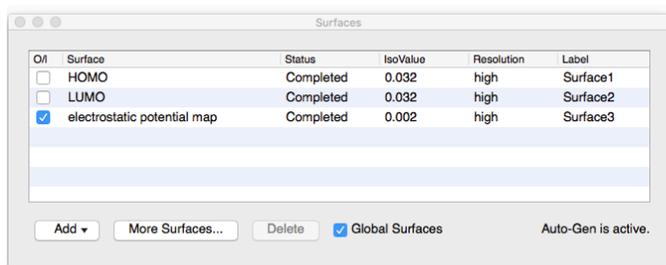
A special note on systems with unpaired electrons: When molecules have unpaired electrons, the energies of "up" spin and "down" spin electrons can be different (this is true for all the electrons in the system). Because of this, two sets of MO's will be listed – "alpha" = spin up, and "beta" = spin down. By convention, alpha orbitals are populated first, so for the purposes of General and Organic Chemistry courses, when visualizing orbitals in these systems it is simplest to look only at the alpha orbitals.

Additional Surfaces: You can also calculate and view many different types of surfaces (including molecular orbitals) by going to Display>Surfaces. This will bring up a menu that allows you to select the individual surfaces that you want to study:

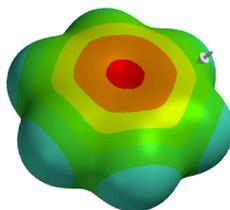
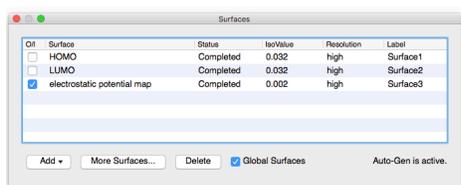


From the “Add” menu, select the surface(s) that you want (for example, HOMO). You will have to select each surface individually (so you have to do this twice to add both the HOMO and the LUMO, for example, and a third time if you also want to calculate an electrostatic potential surface).

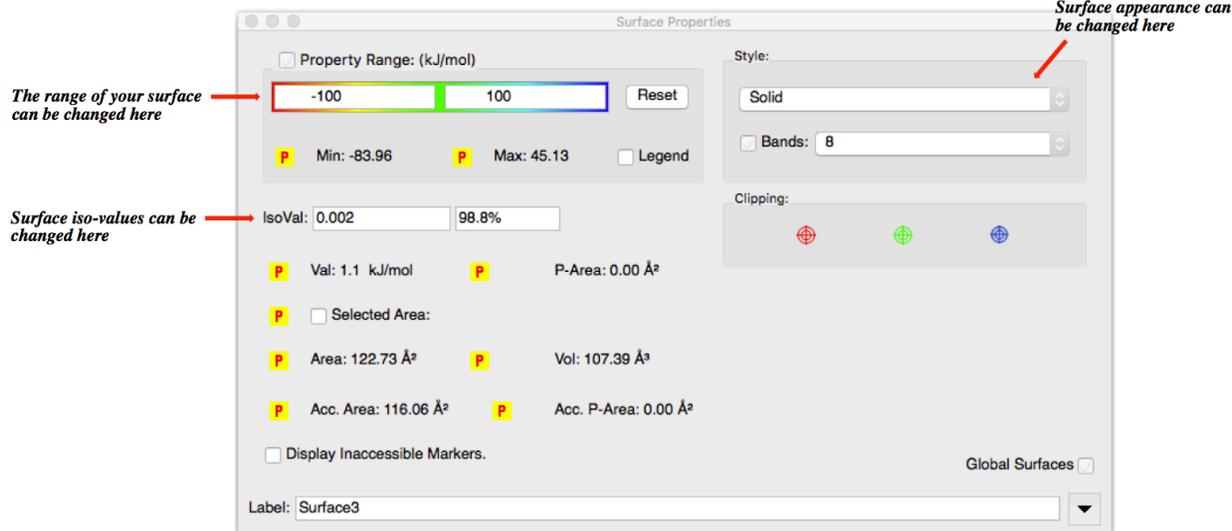
Once the surfaces are added (they will automatically be calculated as you add them), you can view the surfaces by checking the box on the left side within the surfaces menu. The surface will then be displayed on your structure. This interface also lets you overlay surfaces (by checking multiple boxes at the same time in the surfaces window). For example, shown below is the electrostatic potential surface for benzene:



While you are displaying surfaces in this way, you can also view and edit properties of that surface. First, bring up the properties window (if it isn't already open) by selecting Display>Properties. You will want to arrange your windows (both Surfaces and Properties) so you can see your molecule and also both windows. To view information about the surface in the Properties menu, click on the surface (anywhere on the surface). Once you have done all this, you should see:



The Properties menu will let you change some graphing attributes of your surface. For example, you can change the range that corresponds to the color-coding of your surface by typing directly into the “Property Range” boxes. You can also change the isovalue for the surface by typing into the IsoVal boxes (either the value box or the percent box). The surface style can also be changed.



You will get the greatest color variation for your surface (which is usually optimal) if you set your range so that it roughly matches the maximum and minimum values for your surface. For example, for the ESP surface shown above, the max and min values for the surface potentials are Min = -83.96 kJ/mol and Max = 45.13 kJ/mol. Therefore, you would get a better looking surface by setting your range to around -85 for the minimum, and +45 for the maximum.

The isovalue describes how far from the nuclei to draw the surface. In general, using default isovalues will give you the best single view of the surface property. However, by changing the isovalue you can get information on your surface property at different distances/surface volumes (smaller isovalue = farther away; larger isovalue = closer in). For electrostatic potential (that correlates well with electron density), looking at electron density farther away from the nuclei can give you a picture of what the electrons look like to other molecules, while looking closer in toward the nuclei can give you insight into the electron distribution in the bonds that hold the molecule together.