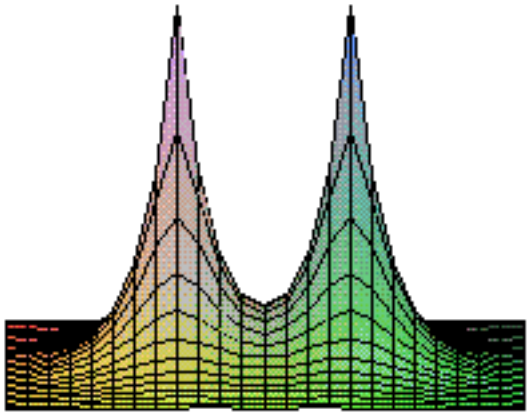
Maple Lab



Websites www.maplesoft.com, www.maple4students.com

start xmaple

xmaple &

Inside the main Maple window there are two smaller windows; a (green) Help window and a blank (white) worksheet where you can enter Maple commands. Minimize the Help window for now. Note the help-menu on the right. You can get *context-sensitive help* by highlighting a single word and clicking on help.

Examples of the maple syntax

$f := x \rightarrow x;$

$g := x \rightarrow x - x^3/3!;$

smartplot(sin(x),f(x),g(x));

Right-click on the plot to alter the range of the X and Y axes.

Legends Select "Display Legend" under the Options pull-down menu.

Save your work often (.mws format). xmaple tends to crash!

1-D Atomic Orbital plots

$f1s := r \rightarrow exp(-r);$

$1s$ atomic orbital

$f2s := r \rightarrow (2 - r) * exp(-r/2.0);$

$2s$ atomic orbital

$f3s := r \rightarrow (27 - 18 * r + 2 * r^2) * exp(-r/3.0);$

$3s$ atomic orbital

smartplot(f1s(r),f2s(r)/4.0,f3s(r)/10.0);

3-D Atomic Orbital plots

$r := (x, y) \rightarrow sqrt(x^2 + y^2);$

smartplot3d(f1s(r(x,y)));

Left-click to rotate the plot. Right-click to add axes.

smartplot3d(f3s(r(x,y))/10.0);

Zoom in on the graph of f3s to see the difference between f3s and f1s.

$f2px := (x, r) \rightarrow x * exp(-r);$

$2p_x$ atomic orbital

$f2py := (y, r) \rightarrow y * exp(-r);$

$2p_y$ atomic orbital

smartplot3d(f2px(x,r(x,y)));

smartplot3d(f2py(y,r(x,y)));

Add axes to the f2px and f2py plots to see the difference between the two functions.

Bonding and Anti-Bonding Molecular Orbitals in the Hydrogen Atom

smartplot3d(f1s(r(x,y)));
The 1s atomic orbital on one H-atom

smartplot3d(f1s(r(x-5,y)));
The 1s atomic orbital on the other H-atom. Extend the range of the plot to get the whole orbital in the picture. Add axes to the plots of the two 1s atomic orbitals so that you can see the difference between them. Rotate both plots so that the x-axis is aligned from left to right. Make sure that negative X is to the left and positive X is to the right.

smartplot3d(f1s(r(x,y))+f1s(r(x-5,y)));
The 1s σ-bonding molecular orbital. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

smartplot3d(f1s(r(x,y))-f1s(r(x-5,y)));
The 1s σ^*-anti-bonding molecular orbital. Add axes and align the X-axis . Extend the range to include the whole plot if necessary

smartplot3d(f2px(x,r(x,y))-f2px(x-5,r(x-5,y)));
The 2px σ-bonding molecular orbital. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

smartplot3d(f2px(x,r(x,y))+f2px(x-5,r(x-5,y)));
The 2px σ^*-antibonding molecular orbital. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

Π Bonding Orbitals

smartplot3d(f2py(y,r(x,y))+f2py(y,r(x-5,y)));
The 2py π-bonding molecular orbital. Add axes and align the X-axis. Extend the range to include the whole plot if necessary Include a second plot where the orbital is aligned alonged the Y-axis.

smartplot3d(f2py(y,r(x,y))-f2py(y,r(x-5,y)));
The 2py π^*-antibonding molecular orbital. Add axes and align the X-axis. Extend the range to include the whole plot if necessary Include a second plot where the orbital is aligned alonged the Y-axis.

The Electron Density in a Bonding Orbital

Comment/caveat: In this section the orbitals should be "normalised". This complicates the mathematical expressions without changing the pictures much, so normalisation will be neglected.

smartplot3d(f1s(r(x,y))^2);

The 1s atomic orbital *electron density* on one H-atom

smartplot3d(f1s(r(x-5,y))^2);

The 1s atomic orbital density on the other H-atom. Extend the range of the plot to get the whole orbital in the picture. Add axes to the plots of the two 1s atomic orbitals so that you can see the difference between them. Rotate both plots so that the x-axis is aligned from left to right. Make sure that negative X is to the left and positive X is to the right.

smartplot3d((f1s(r(x,y))+f1s(r(x-5,y)))^2);

The 1s σ-bonding molecular orbital density. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

smartplot3d((f1s(r(x,y))-f1s(r(x-5,y)))^2);

The 1s σ^*-anti-bonding molecular orbital density. Add axes and align the X-axis . Extend the range to include the whole plot if necessary

smartplot3d((f1s(r(x,y))+f1s(r(x-5,y)))^2-f1s(r(x,y))^2-f1s(r(x-5,y))^2);

The 1s σ-bonding molecular orbital: **buildup of density in the bonding region**. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

smartplot3d((f1s(r(x,y))-f1s(r(x-5,y)))^2-f1s(r(x,y))^2-f1s(r(x-5,y))^2);

The 1s σ^*-antibonding molecular orbital: **depletion of density in the bonding region**. Add axes and align the X-axis. Extend the range to include the whole plot if necessary

Lab Report Email me a single file (.mws format) containing pictures of:

1. The σ-bonding molecular orbital.
2. The σ^*-antibonding molecular orbital.
3. The buildup of density in a σ-bonding molecular orbital.
4. The depletion of density in a σ^*-antibonding molecular orbital.
5. The buildup of density in a π-bonding molecular orbital.