readme

November 2, 2012

Contents

1 Mini Project 1

1.1 Problem

There are many ways to visualize the electron density. One way is to plot it as a "fog" or cloud-like where the colormap represents the charge density of the electron cloud in a compound.

1.2 Method

The "fog" is plotted using in-built functions of mayavi, jasp, and some short scripts written to grab data from the OUTCAR and CHG files produced by VASP. In the attached plots, the deeper the red color, the higher is the charge density.

1.3 Files

Two scripts are written:

1. mini_v2.org

This includes the jasp commands to retrieve the VASP outputs, function calls to retrieve additional data, and the actual plotting.

The structure of this file:

a. Inputs.

b. Use of jasp to retrieve data from VASP output files.

c. Read CHG to get position of the atoms and plot them.

d. Read OUTCAR to get linkages and plot them if needed.

e. Plot simulation cell boundary if needed.

f. Plot the electron charge density.

g. Save the figure. (Default: Isometric view but other relevant views can be saved)

1.4 How to use

Steps to use this code:

a. Copy the 2 files listed above (mini_v2.org and getPosLink.py) into a new folder created in a machine that has jasp.

b. Copy the output folder containing the output files from VASP calculation into this new folder

c. In the mini_v2.org,

i. Put in the name of this output folder in variable calDir (e.g., calDir = 'h2o').

ii. Indicate if u want to plot the linkage between atoms and the simulation cell boundary.

iii. It is ready to go.

(attached in the folder is a sample output folder from VASP for h2o molecule)

1.4.1 Example of input needed (reproduced from mini_v2.org)

Inputs required from user from HERE

dirCal = 'h2o'

#1 to plot linkage between atoms (for simple molecules), 0 otherwise

plotLinks = 1

#1 to plot cell boundary, 0 otherwise

plotCell= 0
######### To HERE ####################

1.5 Limitations

No known limitation for the plotting of electron density except the need for jasp and other softwares/libraries imported in mini_v2.org and getPosLink.py. Simple molecules, periodic crystal structures, non-symmetrical and non-cubic lattices, and unit cell with a molecule that was not centered were tested.

The only limitation comes from the plotting of linkages between atoms. This is done based on the nearest neighbour list in OUTCAR. It does not know and cannot plot the presence of multiple bonds between atom pairs (e.g., double or triple bond in C2H4 and C2H2)

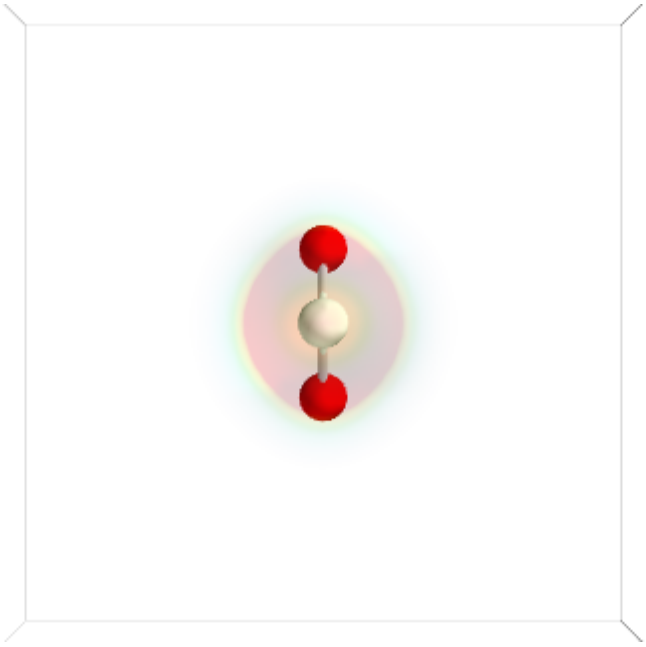
The color of each atom is arbitrary. Atoms are of the same size in the plots below but can be scaled arbitrary.

1.6 Images of electron density for several materials

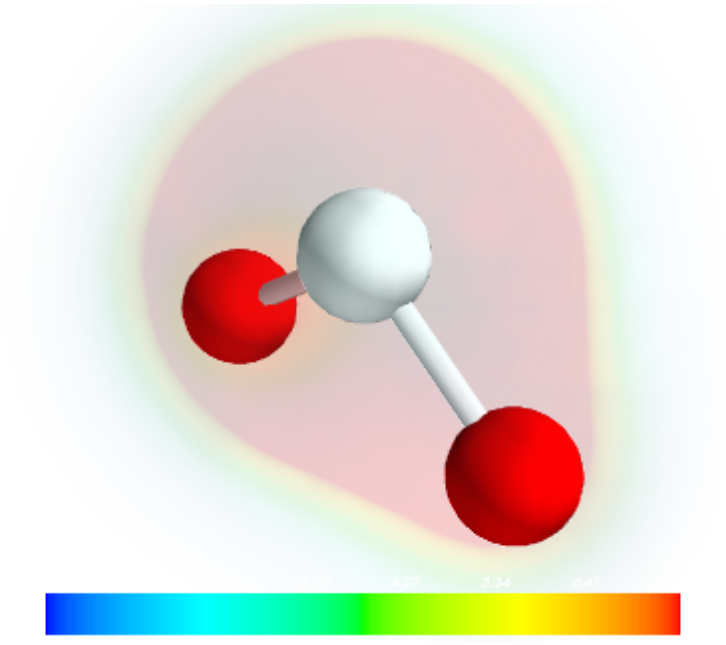
The single molecule images are generated using ENCUT = 300 except otherwise stated. The periodic structures are generated with converged ENCUT and K-PTS.

1.6.1 Single molecules

- H2O

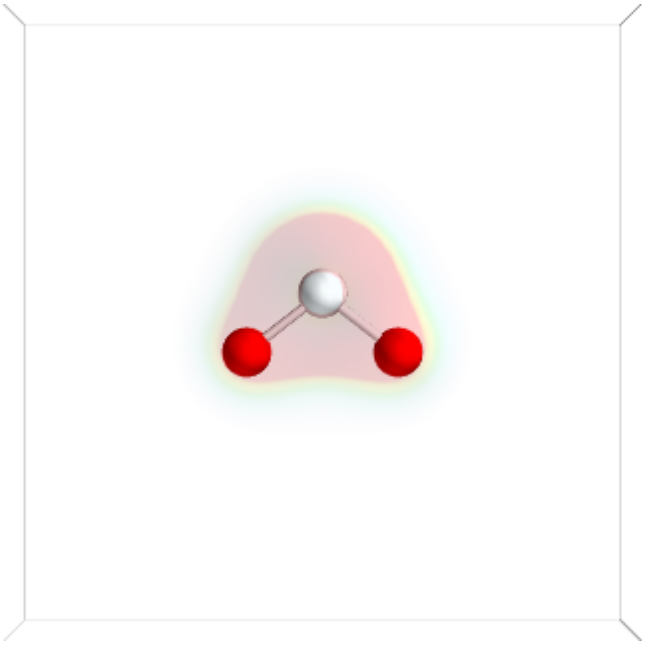


Top view

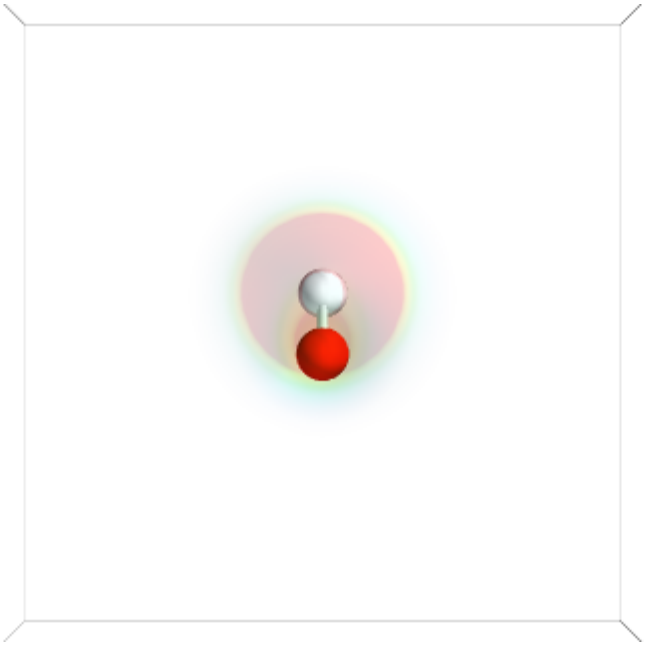


Iso view

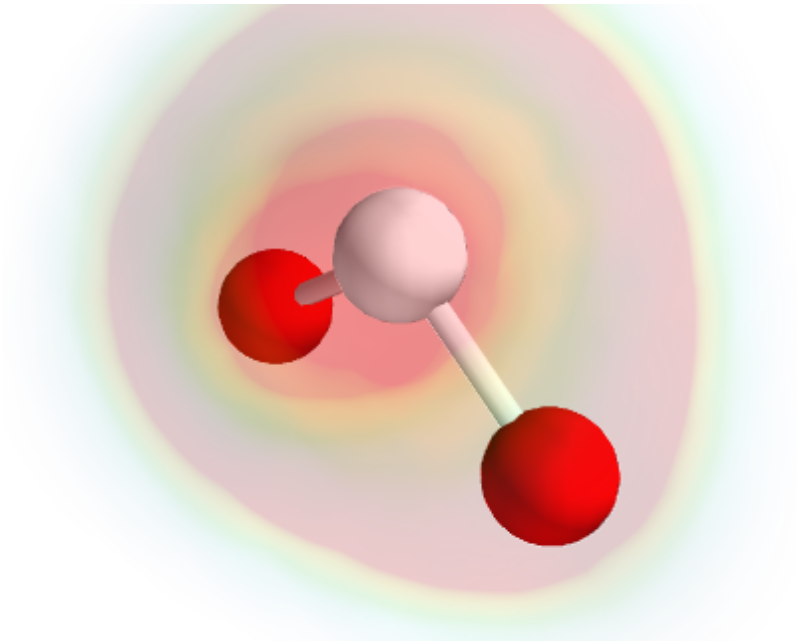
Side view



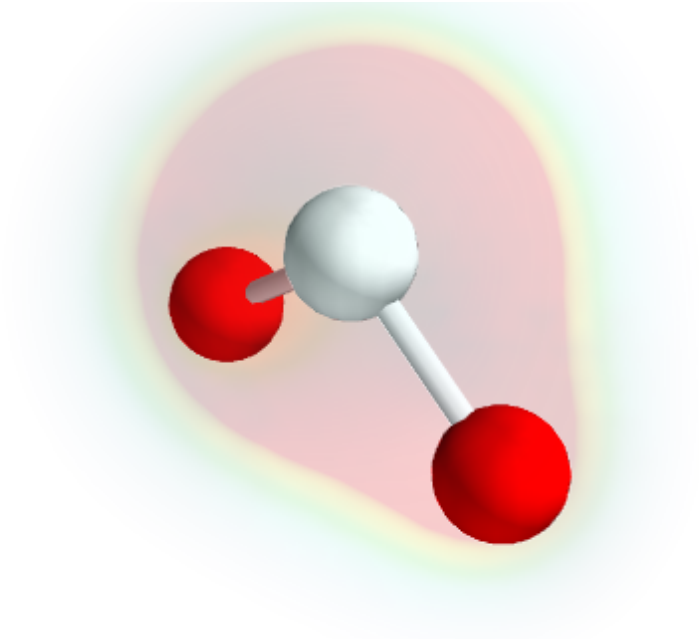
Front view



- H2O (with different ENCUT)



ENCUT = 100

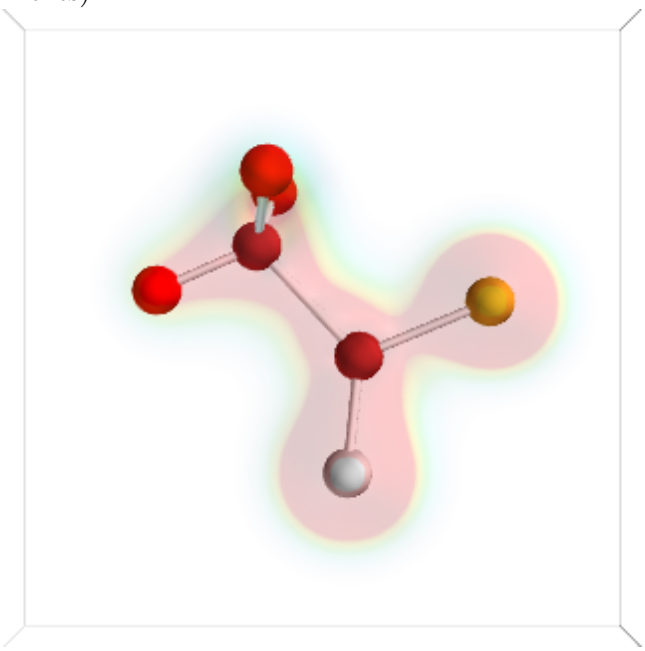


ENCUT = 400

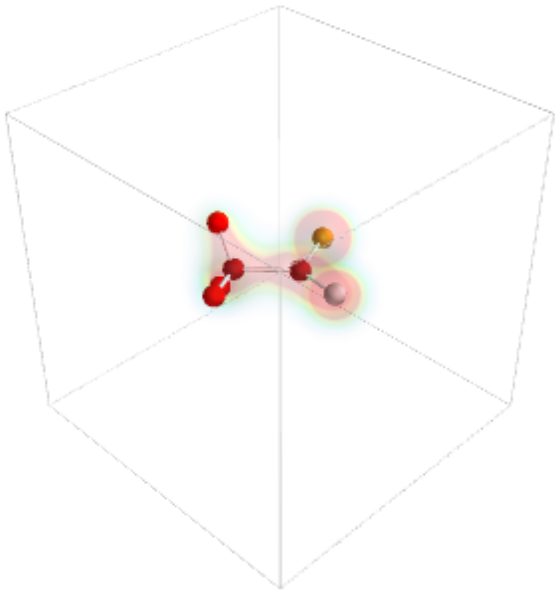
There is a difference in the electron density. The difference itself is

not shown in a single plot as the electron density grid for ENCUT = 400 is more finely divided than ENCUT = 100. This creates a need to interpolate between the points for ENCUT = 100 to get an equal sized matrix. From these two plots, the electron density spans a larger area at smaller ENCUT and has a higher density at a certain region around the molecule.

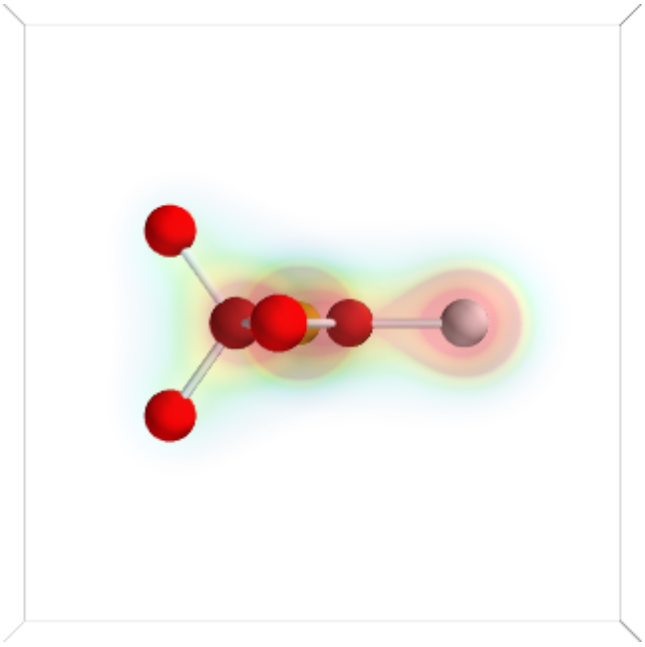
- CH3COF (4 elements)



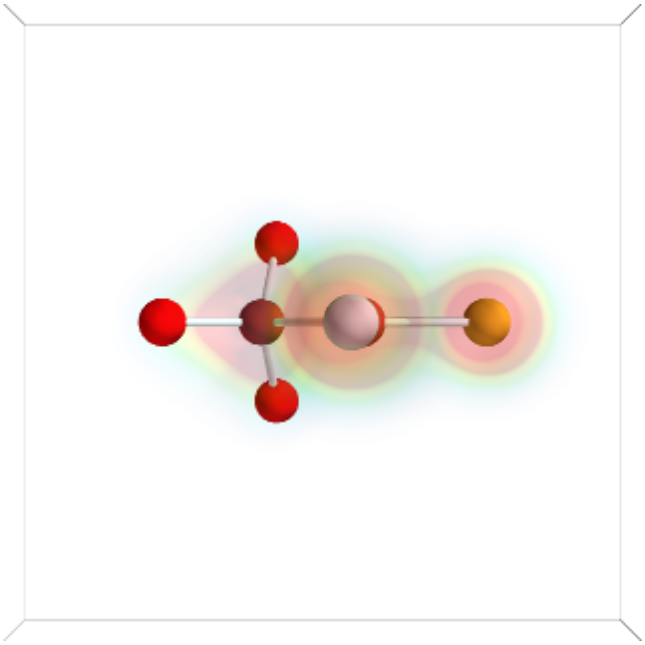
Top view



Iso view



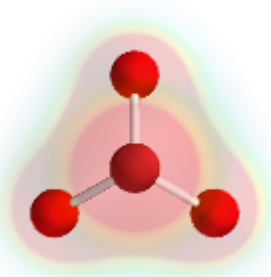
Side view



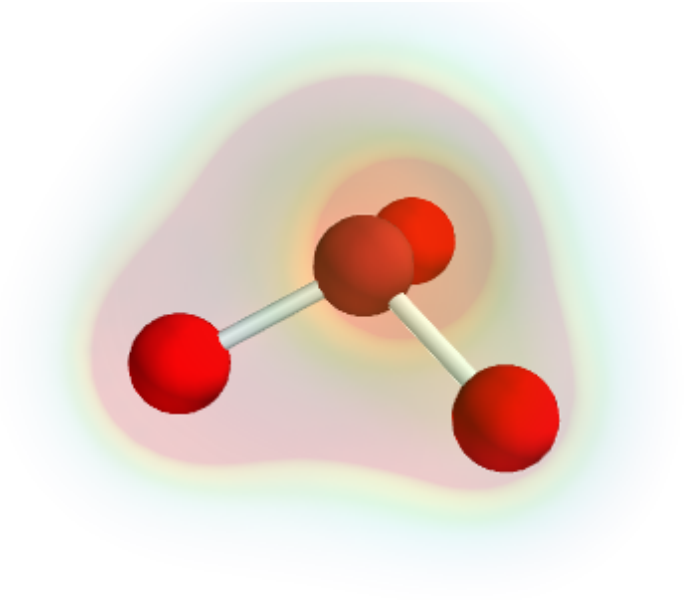
Front view

There is a localisation of the electron density around the F and O atoms (yellow and white spheres) as they are more electronegtive.

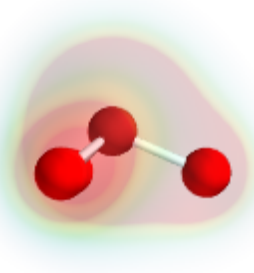
- NH3 (Lone pair of electrons)



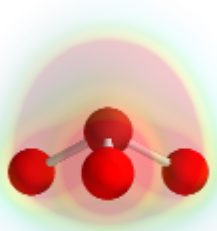
Top view



Iso view



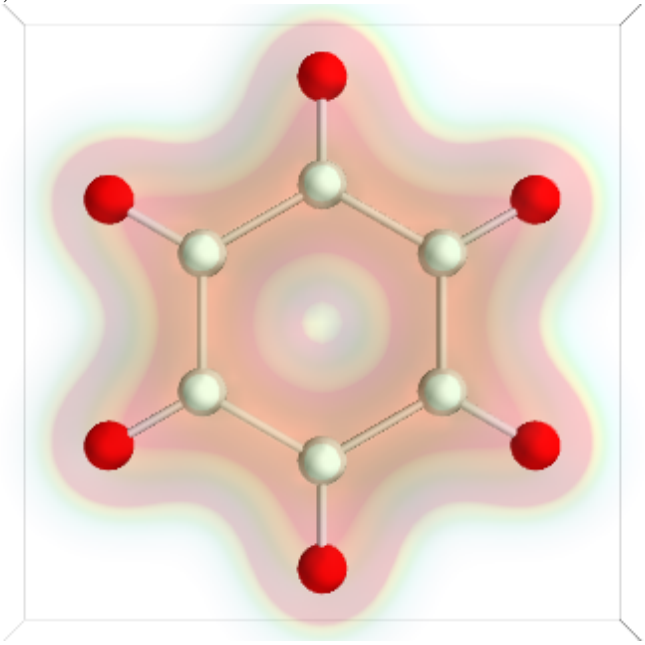
Side view



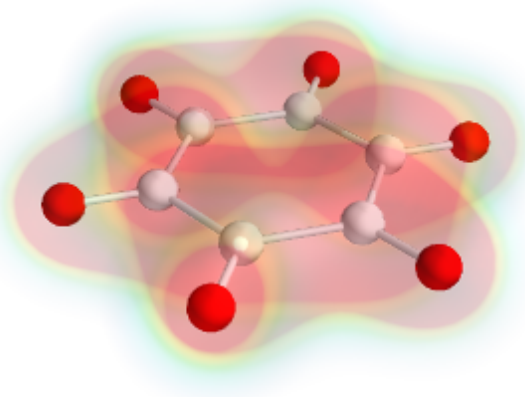
Front view

From the front view, there is a bulge in the electron density above the central N-atom (dark red) that has a lone pair of electrons.

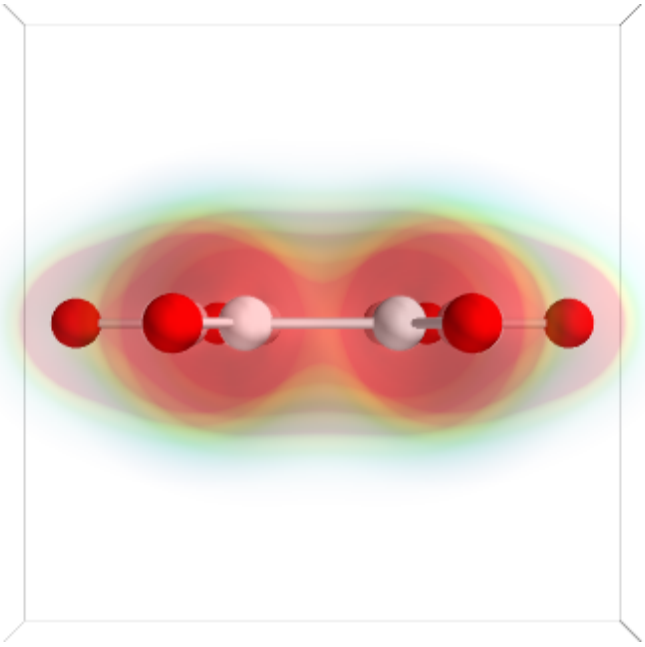
- C6H6 (Benzene)



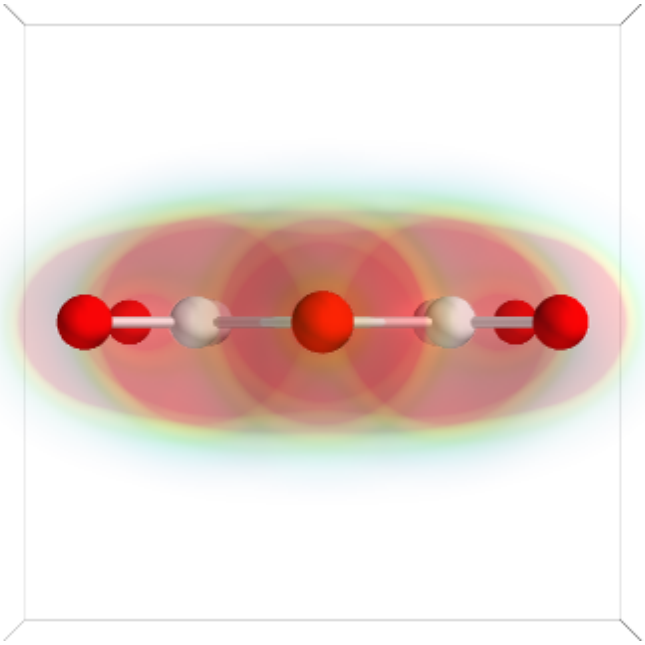
Top view



Iso view



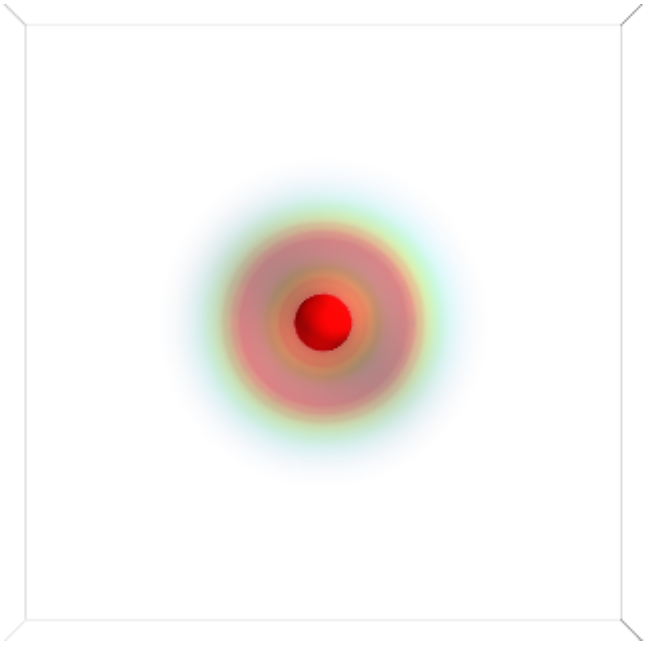
Side view



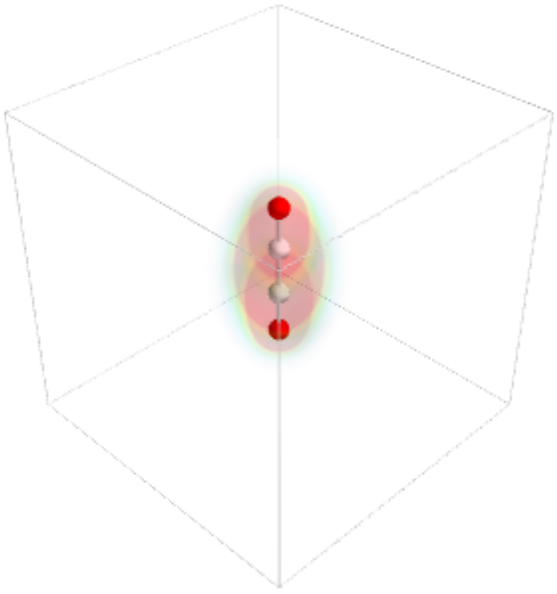
Front view

There is a concentration of electron density along the carbon backbone forming a ring. A lack of electron density in the center is observed. This mirrors the bonding nature in benzene.

- C2H2 (Triple Bond in carbon chain)

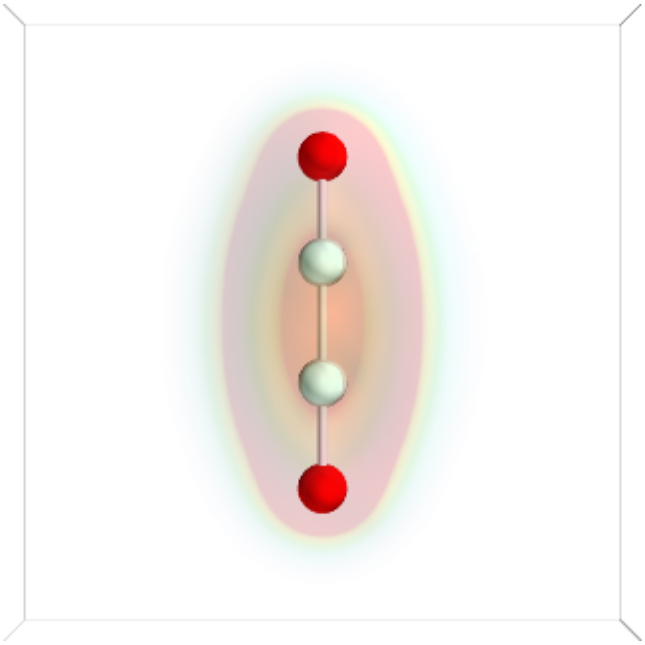


Top view

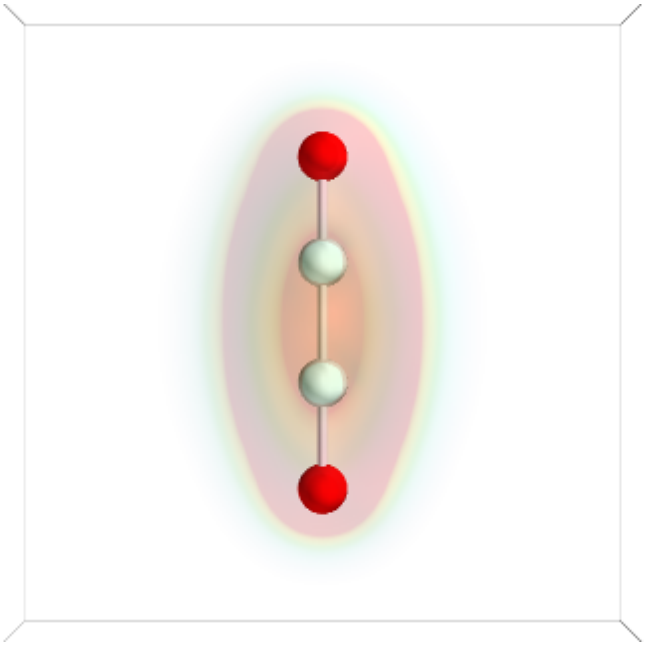


Iso view

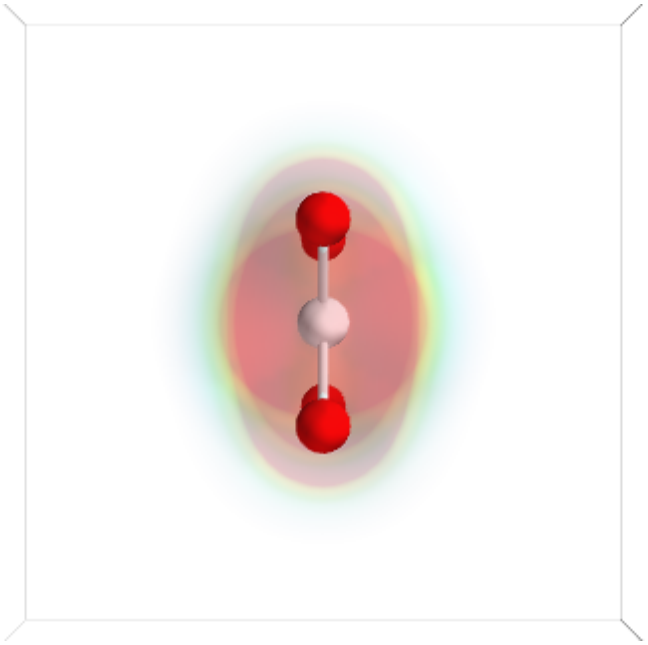
Side view



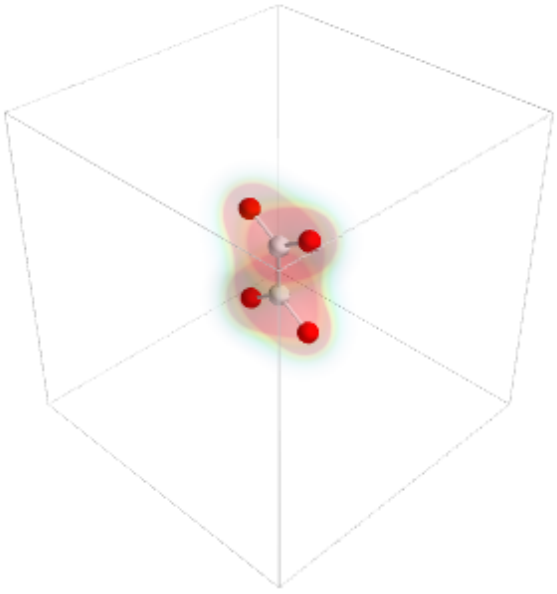
Front view



- C2H4 (Double Bond in carbon chain)

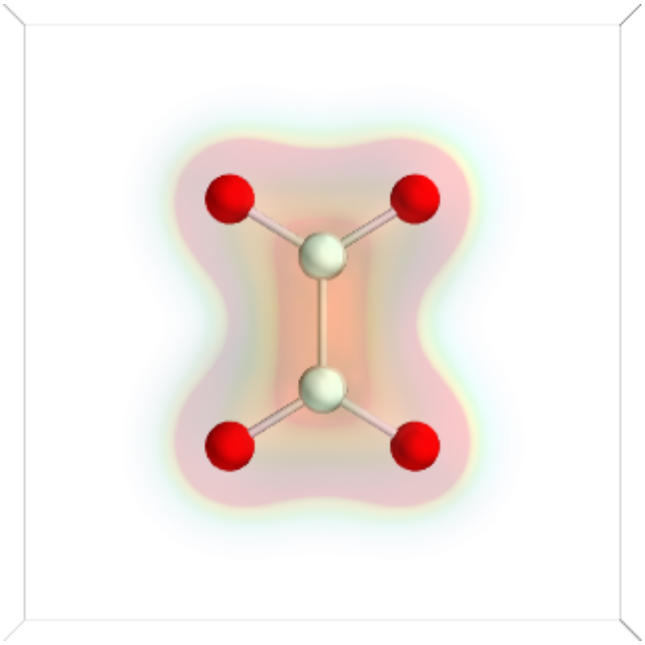


Top view

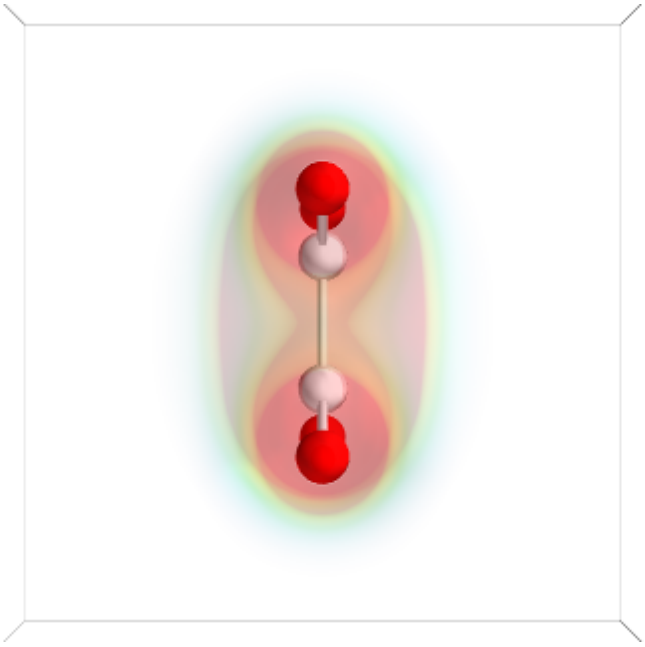


Iso view

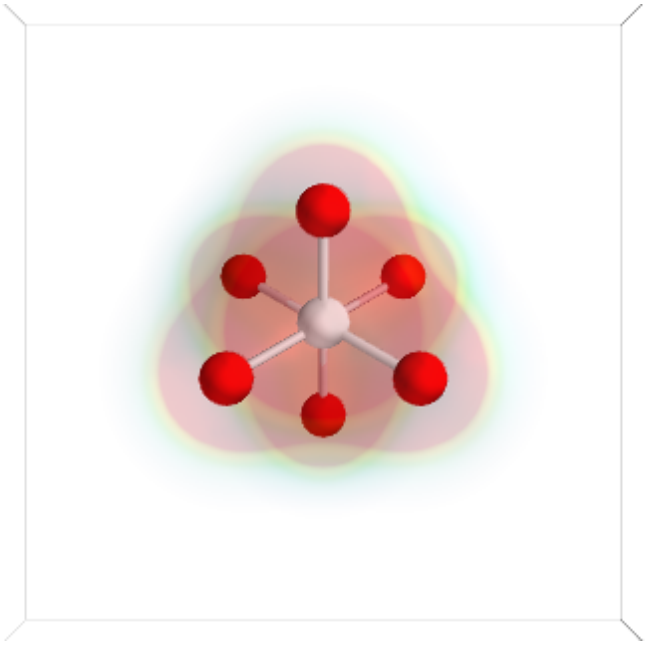
Side view



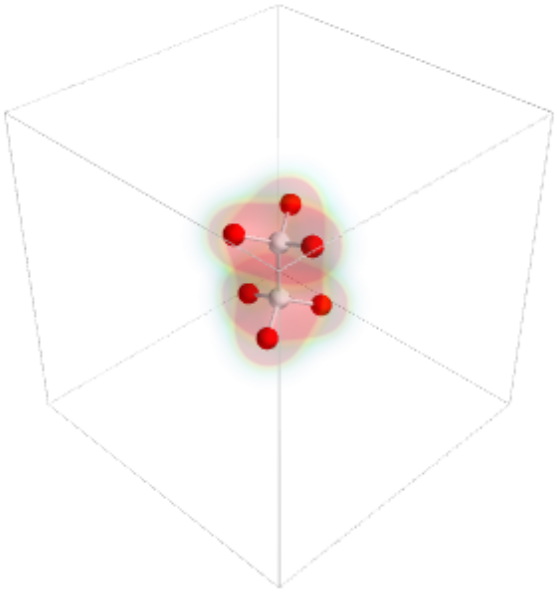
Front view



- C2H6 (Single Bond in carbon chain)

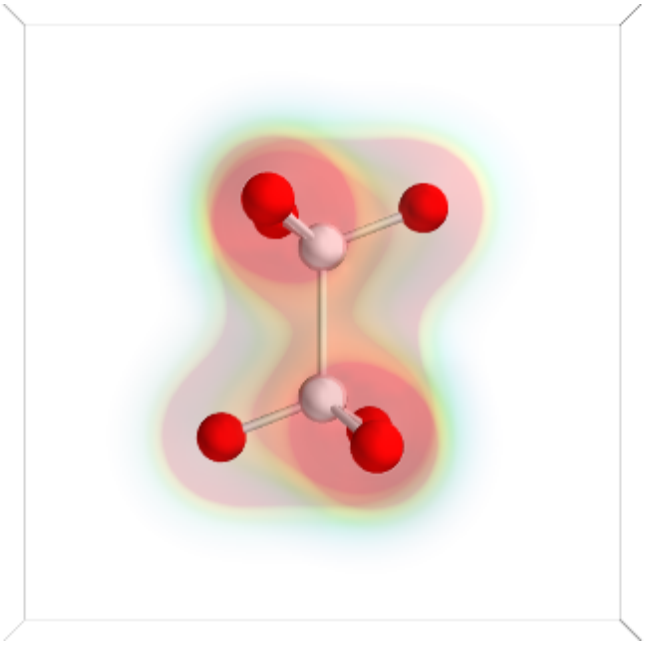


Top view

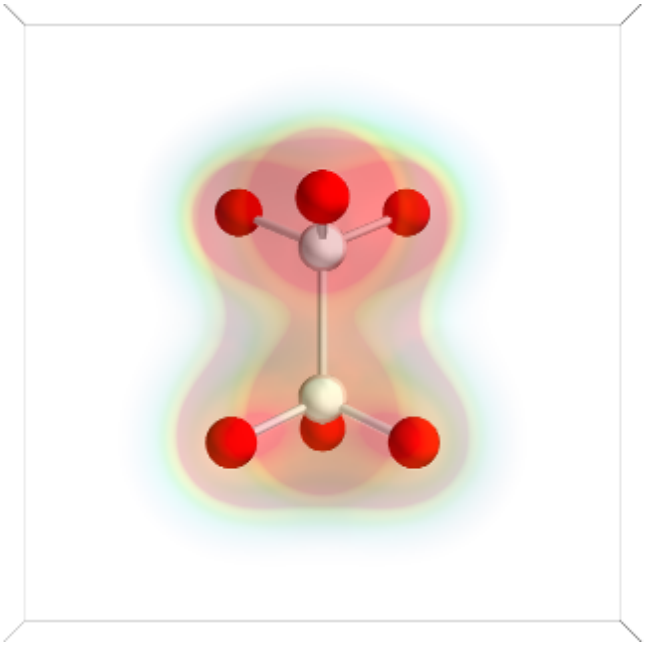


Iso view

Side view

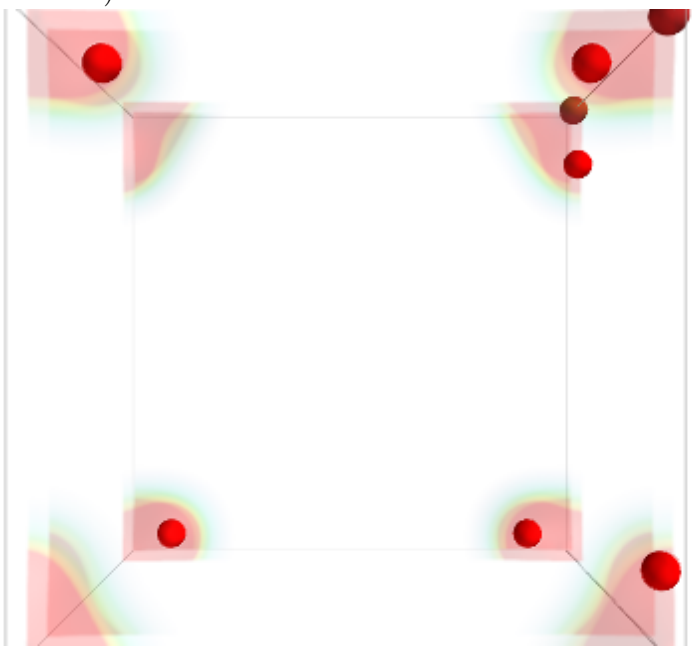


Front view

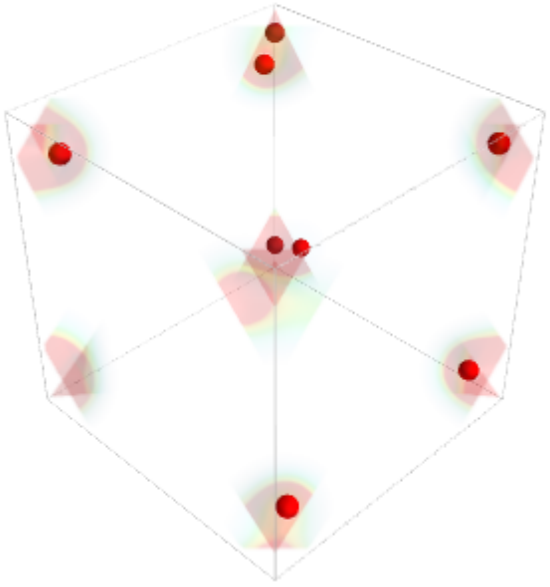


Comparison between images of C2H2, C2H4 and C2H6 shows a higher electron density between the carbon pair for C2H2 and C2H4 than for C2H6. This is due to the presence of the double and triple bond.

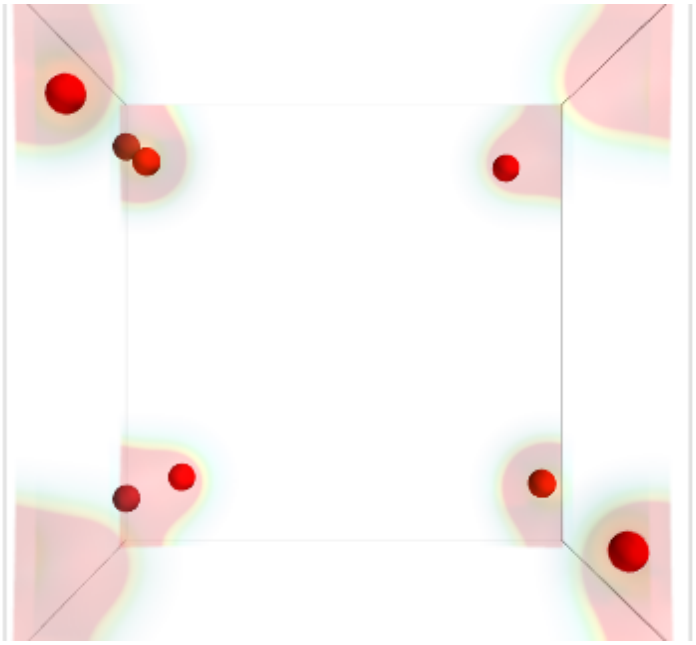
- C2H6 (Not Centered)

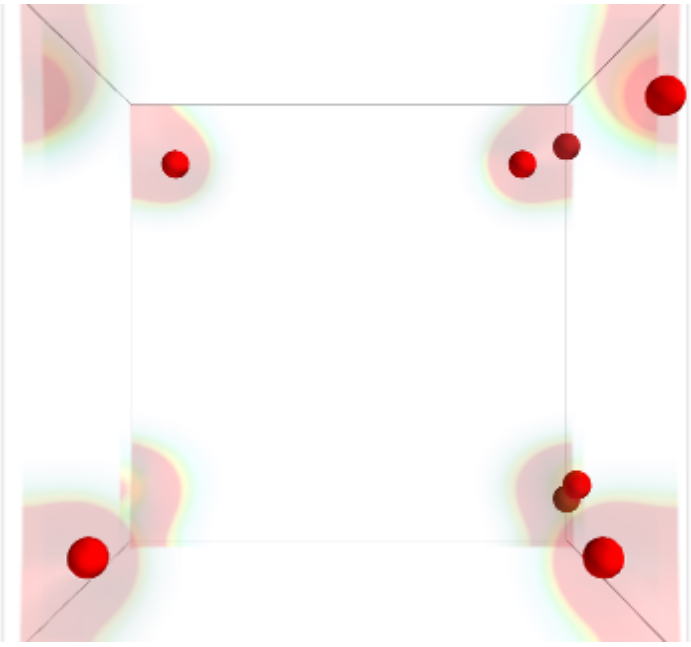


Top view



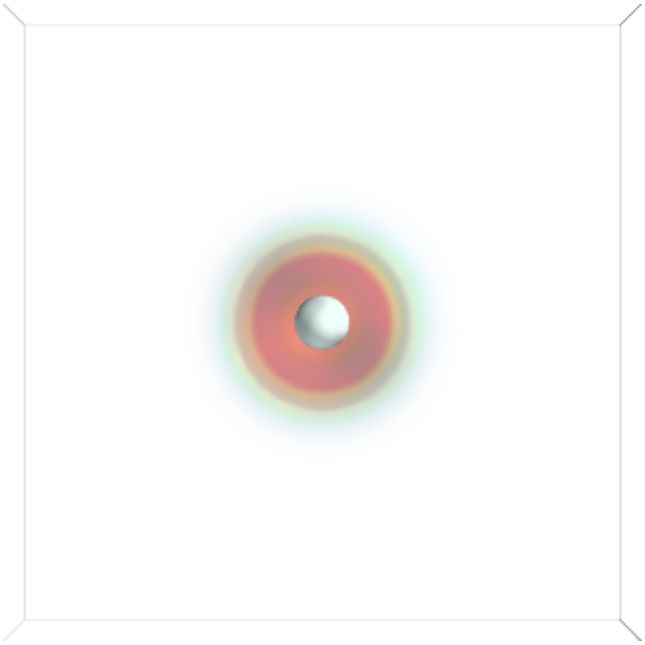
Iso view

Side view 

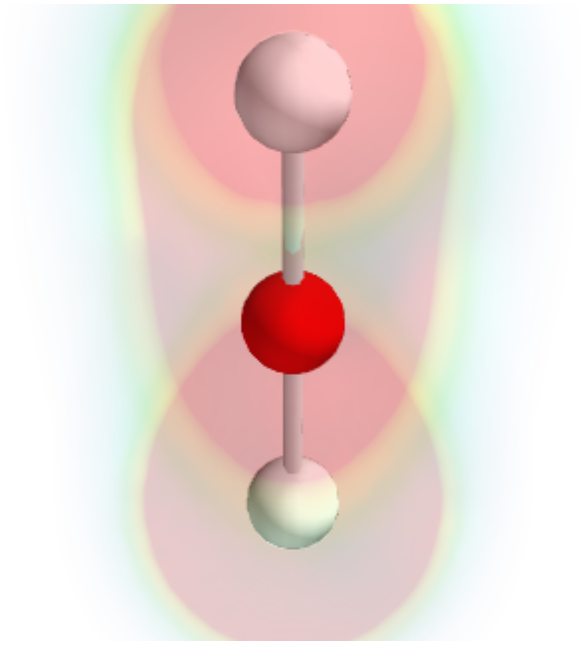
Front view 

- CO2

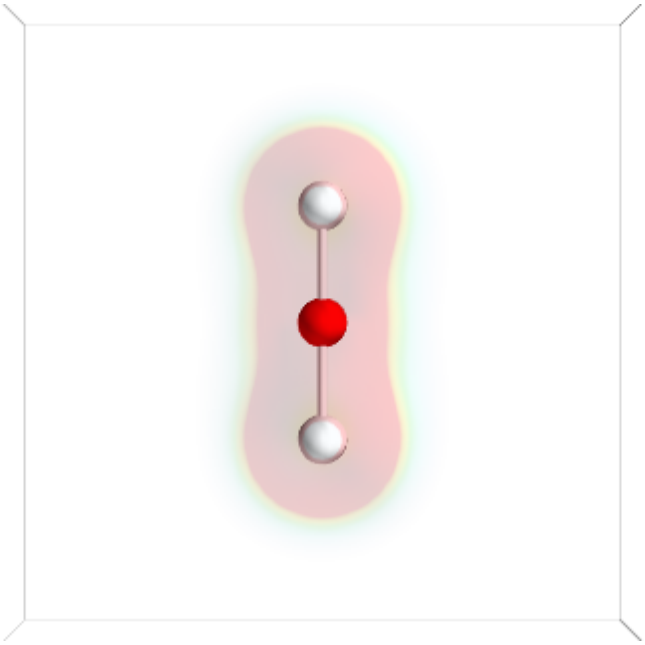
Top view



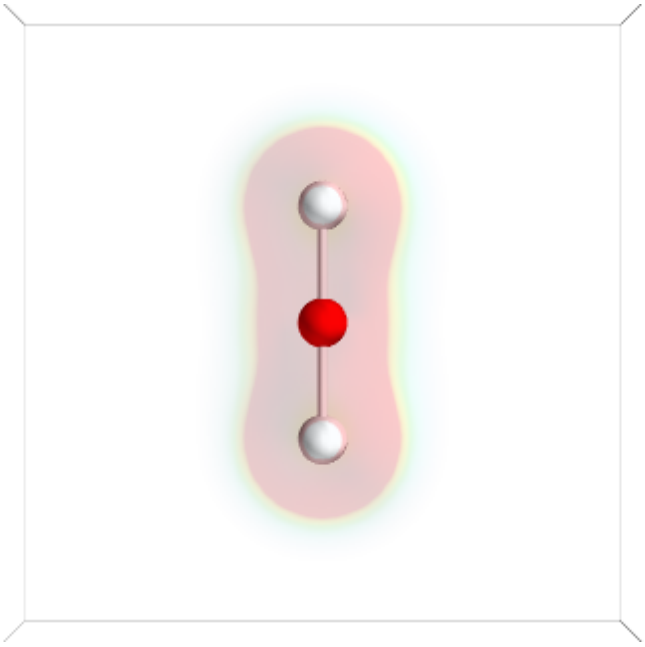
Iso view



Side view

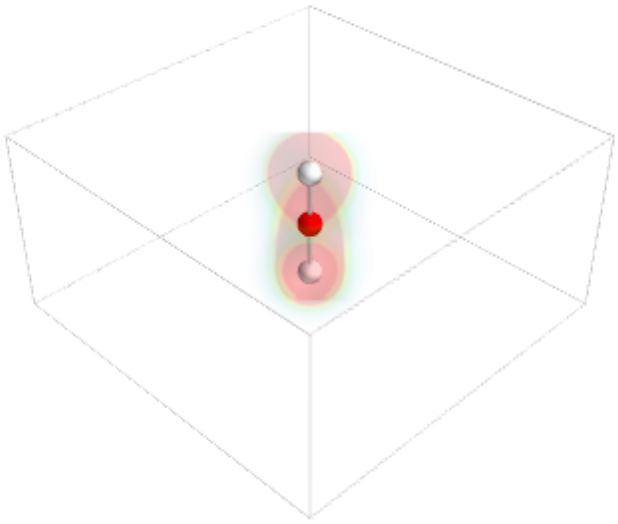


Front view

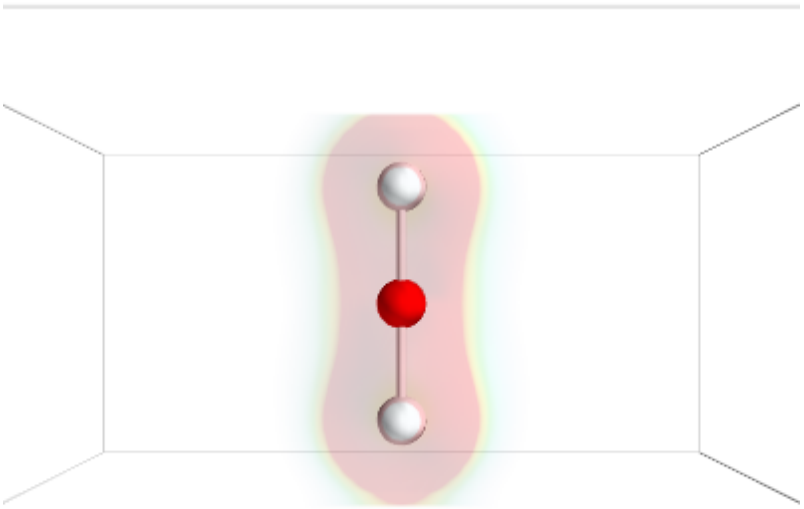


- CO2 (Non-uniform simulation cubic cell)

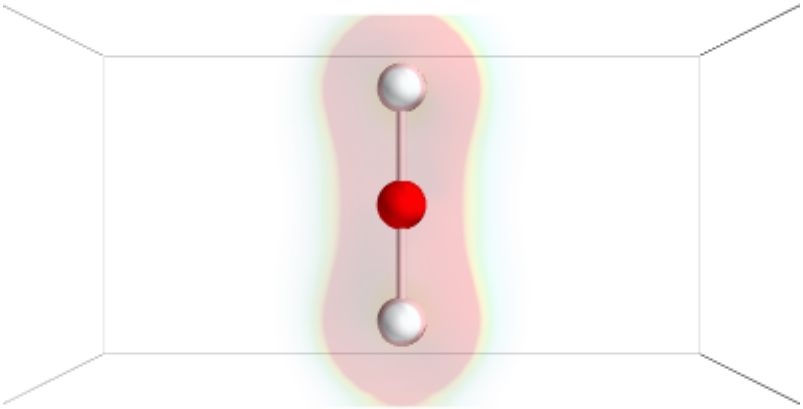
Top view



Iso view



Side view

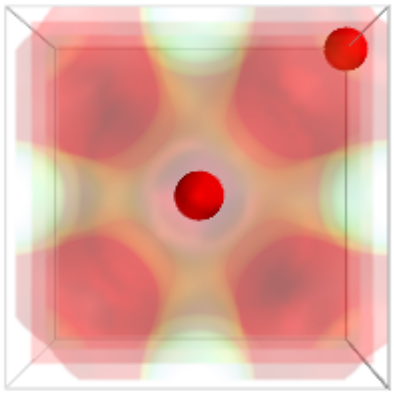


Front view

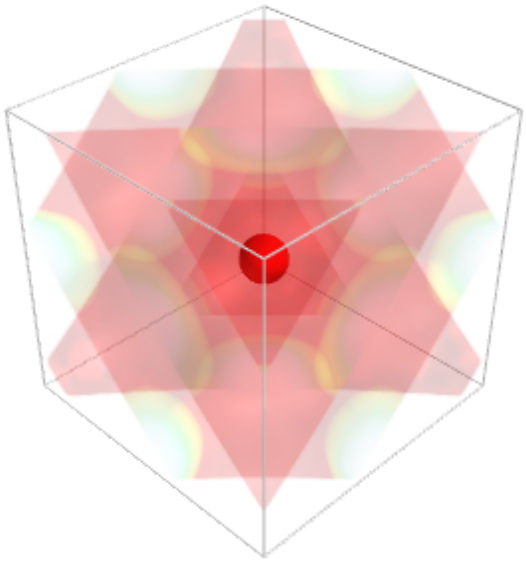
1.6.2 Periodic structures

These periodicity of these cells result in plots of electron density not being self-contained but spreads across the cell boundary.

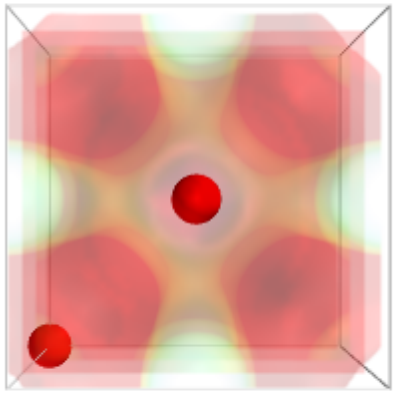
- Ta (BCC Metal)



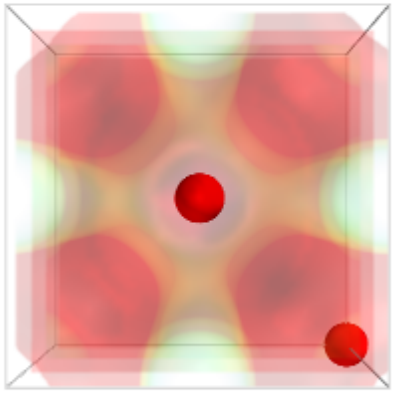
Top view



Iso view



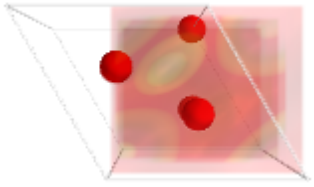
Side view



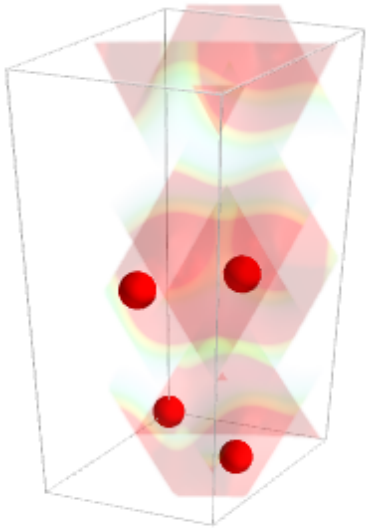
Front view

The electron cloud tends to cluster near to the center and vertices of the cell in constrast to the rock-salt structure of TaC shown below.

- Graphite (Planar hexagonal)

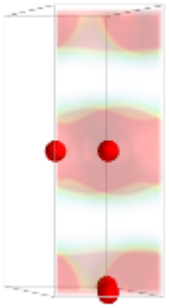


Top view



Iso view

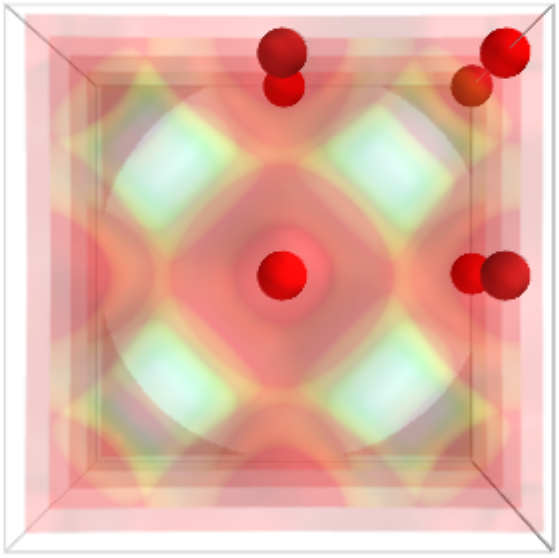
Side view



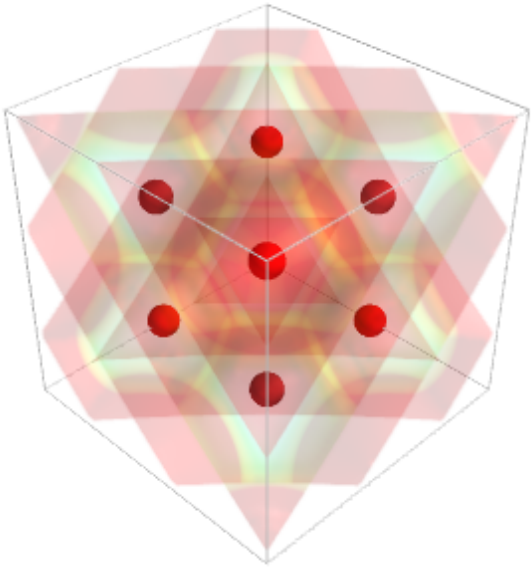
Front view

The electron density is separated into distinct layers, similar to the physical atomic arrangement in graphite.

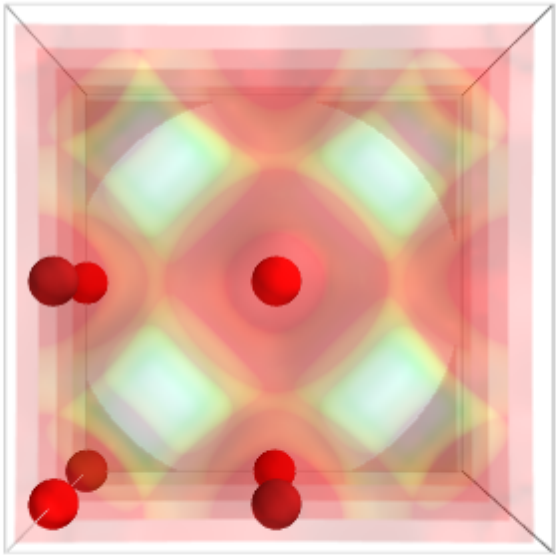
- TaC (rock-salt structure)



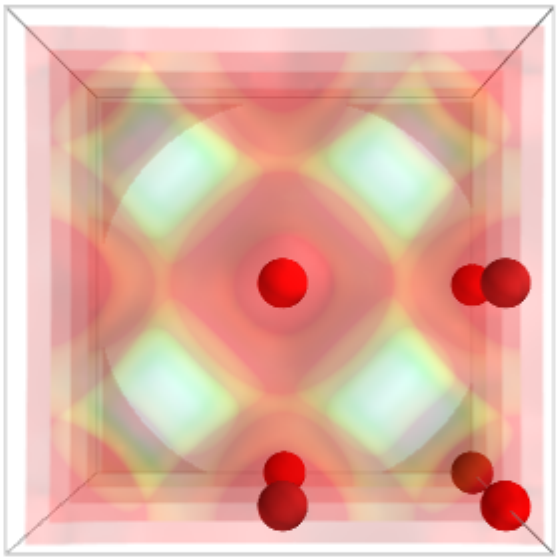
Top view



Iso view



Side view



Front view

There are more “hollow” regions enclosed within the simulation cell in this rock-salt structure as compared to the BCC Ta. The number density and arrangement of the atoms in this structure differ from BCC, pulling electrons closer around each atom.