

readme

November 2, 2012

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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 get-PosLink.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.

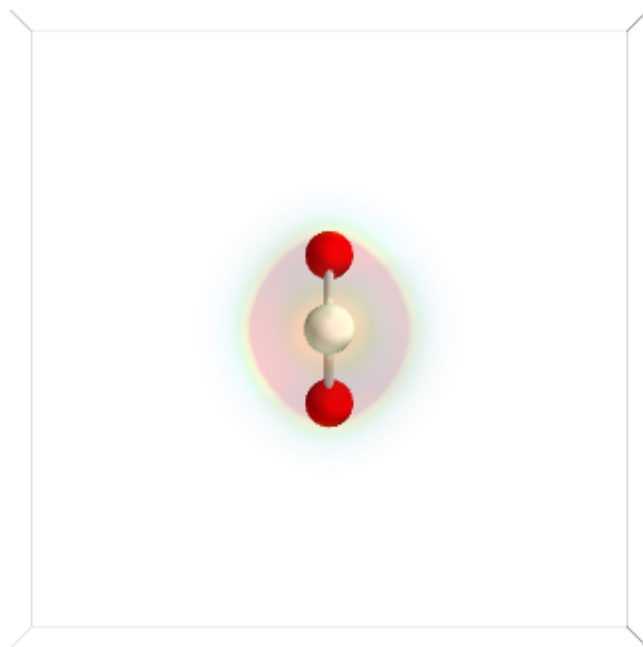
1.6 Images of electron density for several materials

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

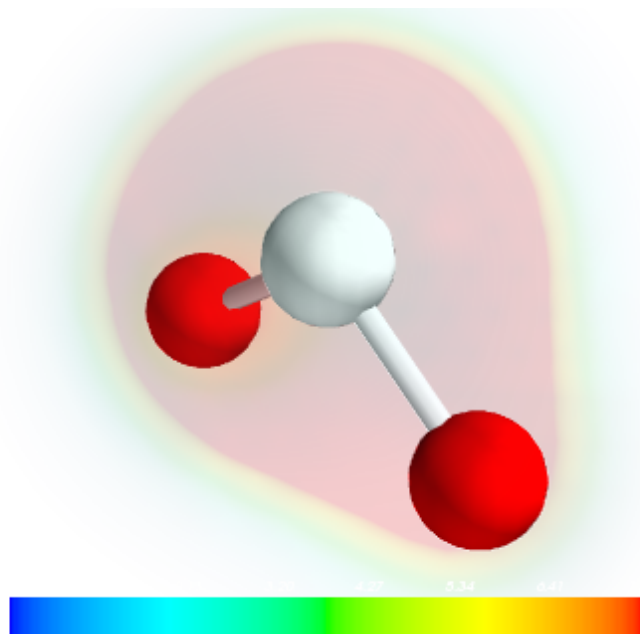
1.6.1 Single molecules

- H₂O

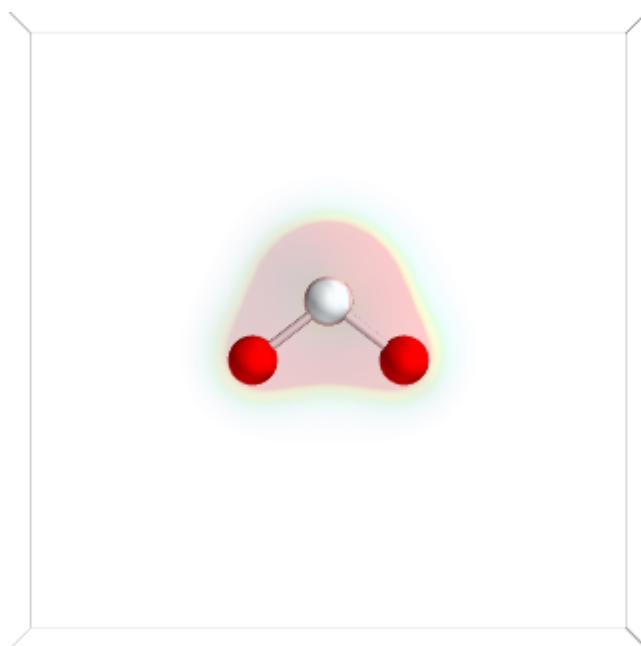
Top view



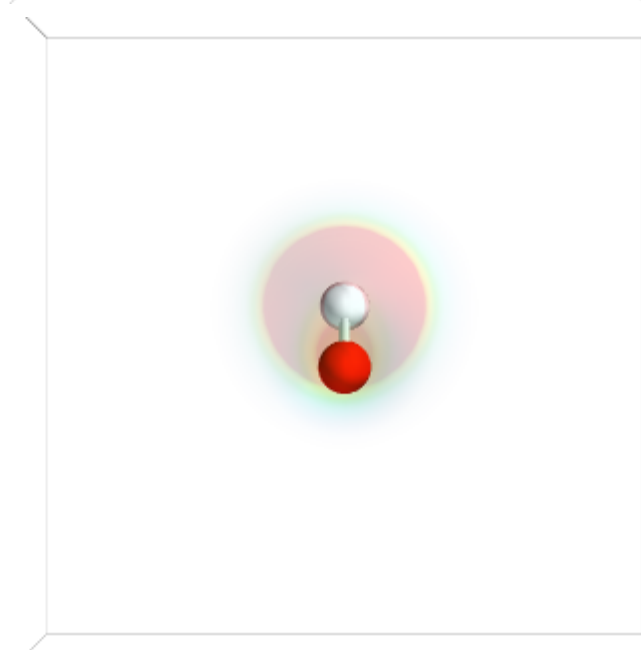
Iso view



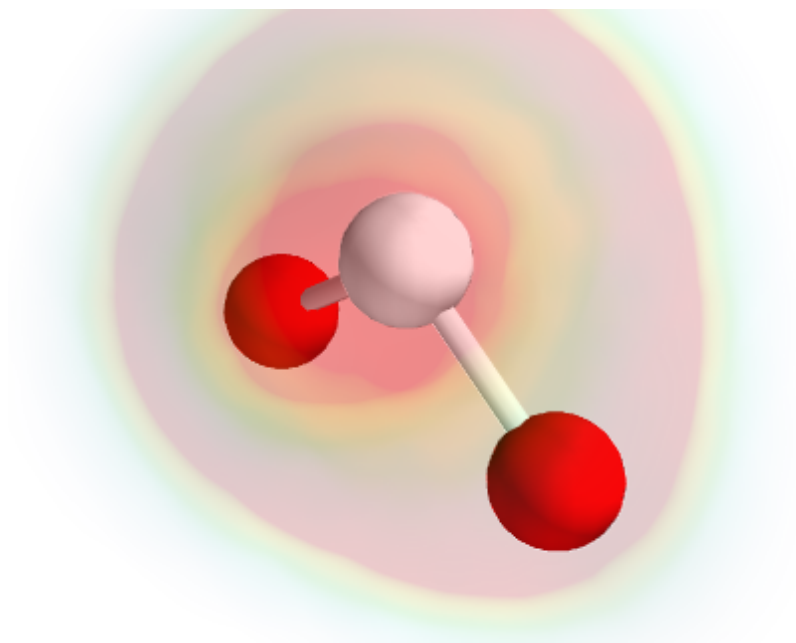
Side view



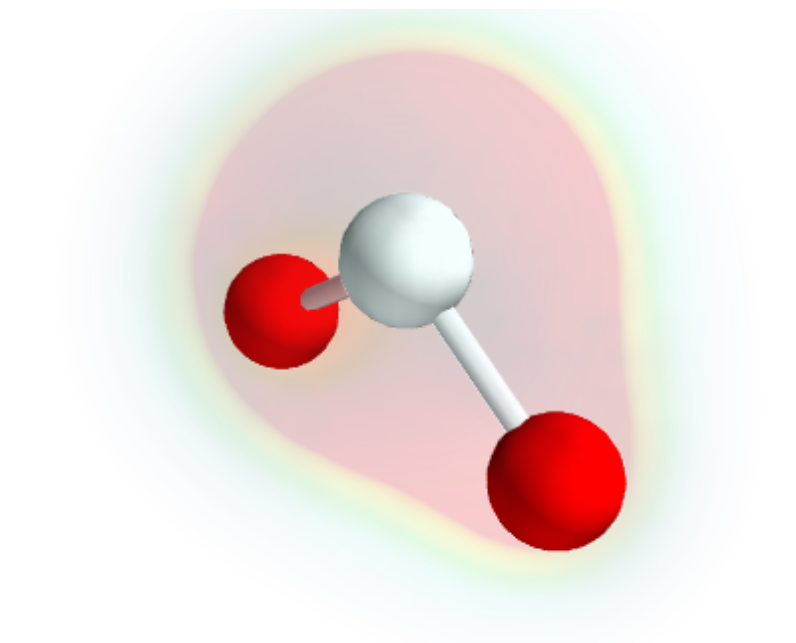
Front view



- H_2O (with different ENCUT)



ENCUT = 100



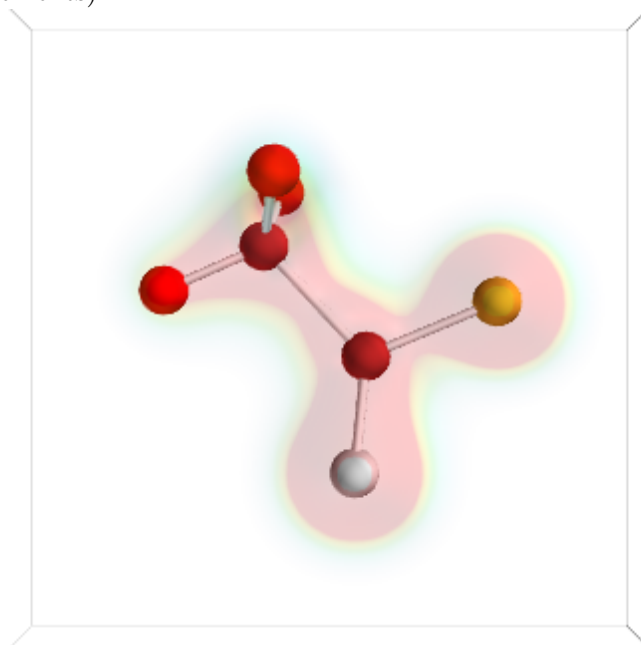
ENCUT = 400

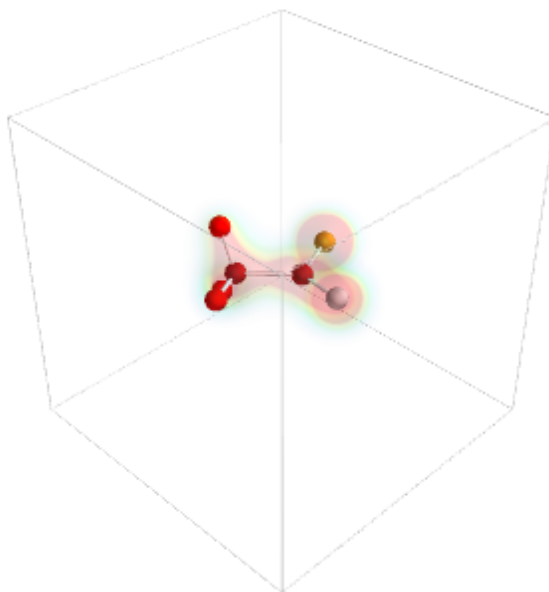
There is a difference in the electron density. The difference itself is

not shown in a single plot as the electron density grid for $\text{ENCUT} = 400$ is more finely divided than $\text{ENCUT} = 100$. This creates a need to interpolate between the points for $\text{ENCUT} = 100$ 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.

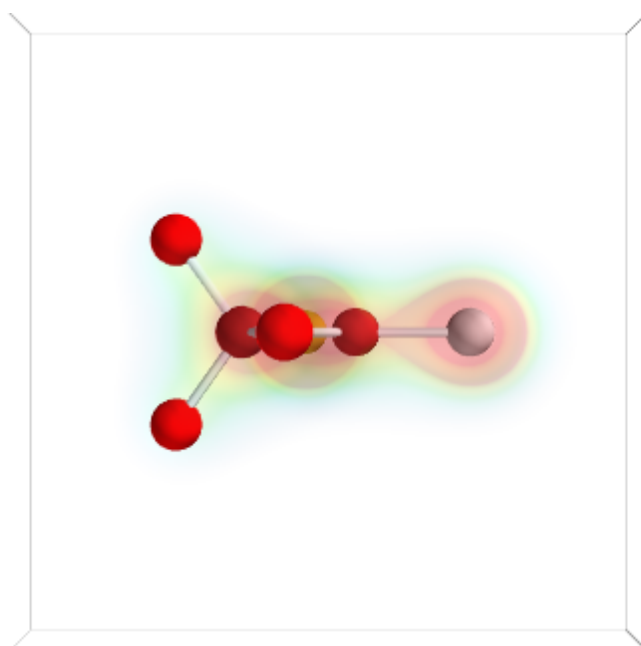
- CH_3COF (4 elements)

Top view

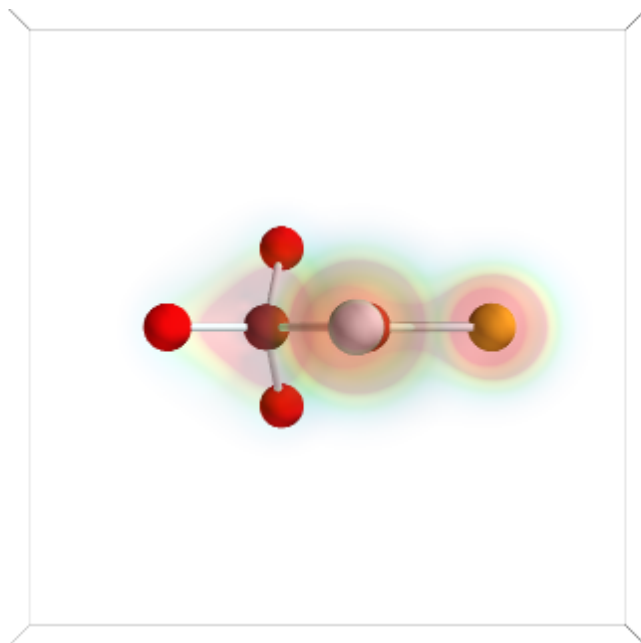




Iso view



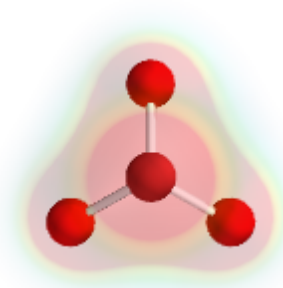
Side view



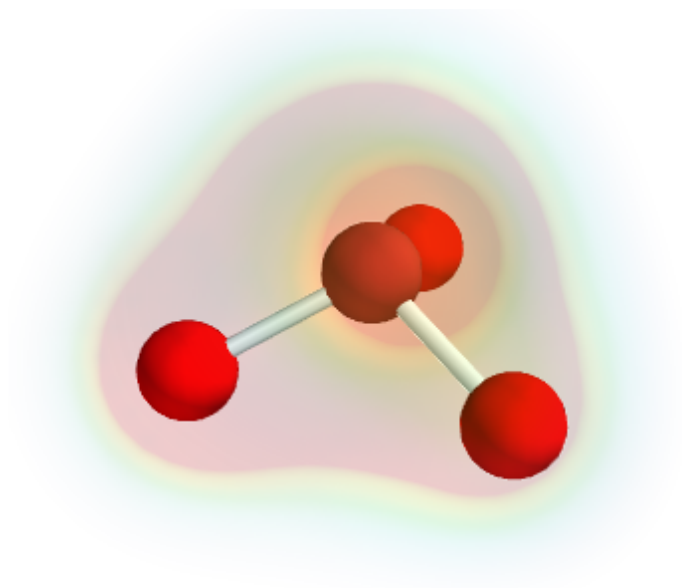
Front view

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

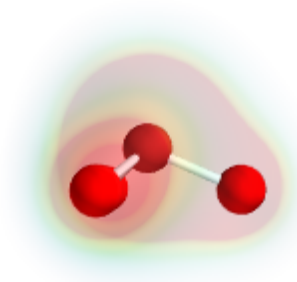
- NH₃ (Lone pair of electrons)



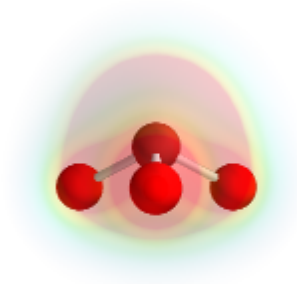
Top view



Iso view



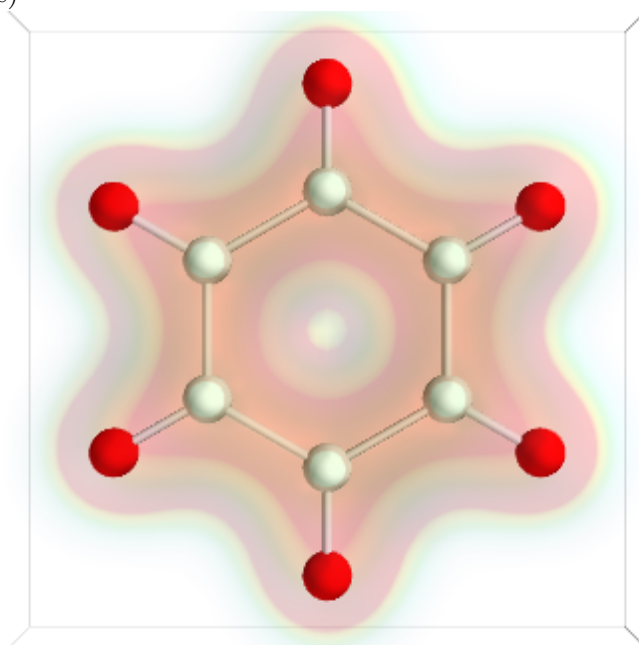
Side view



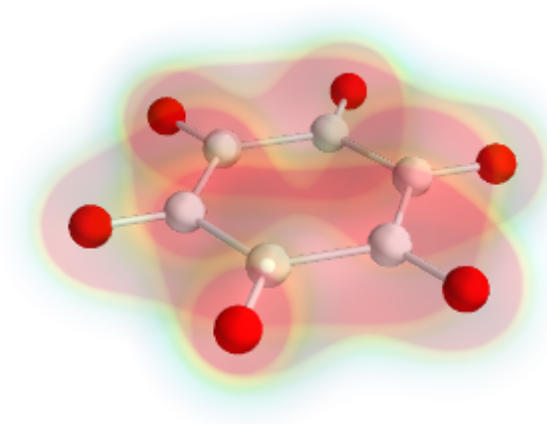
Front view

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

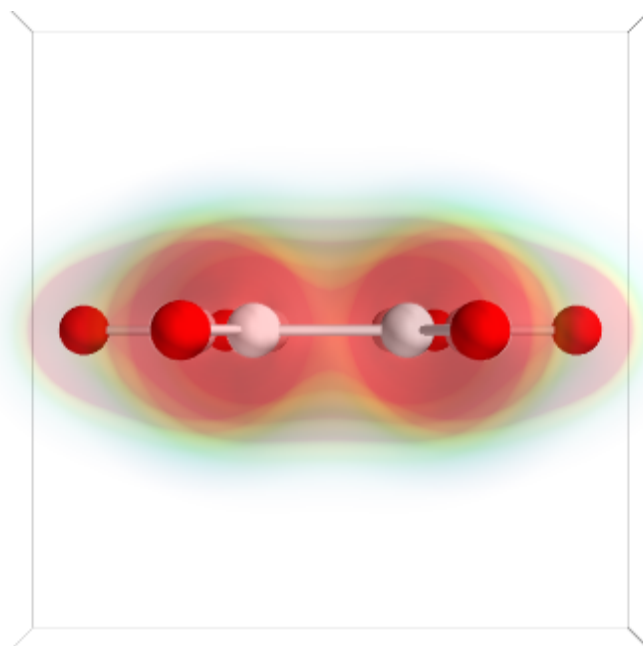
- C₆H₆ (Benzene)



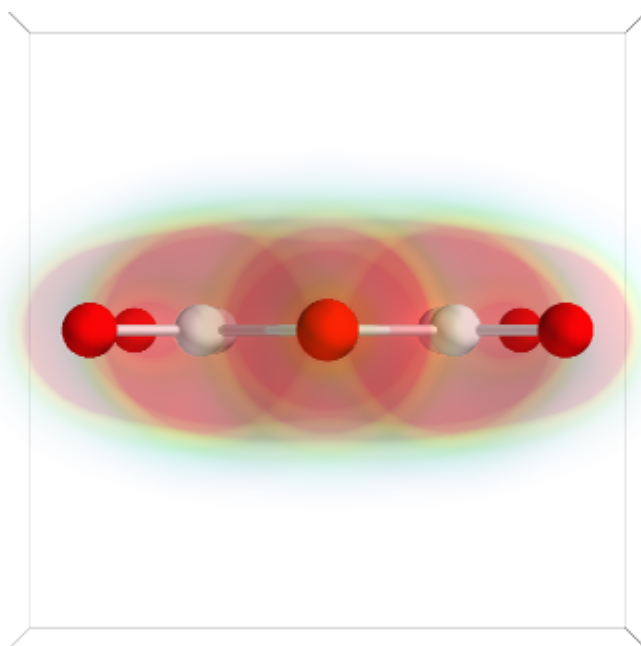
Top view



Iso view



Side view

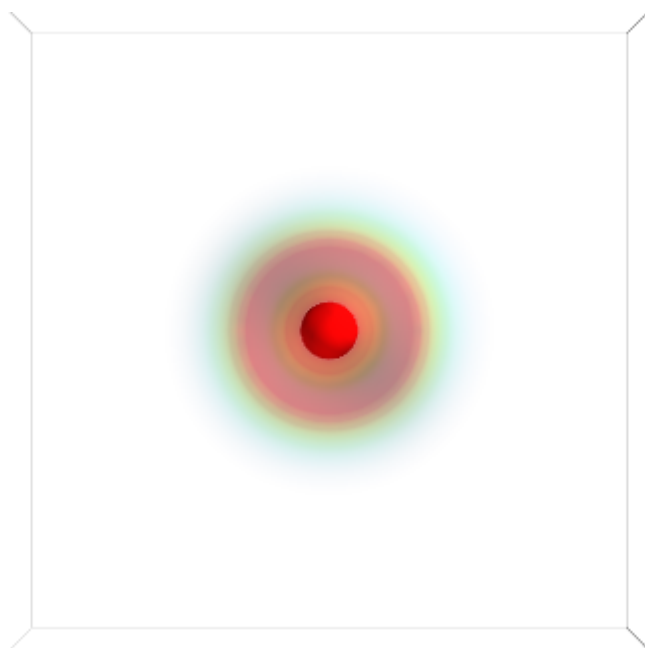


Front view

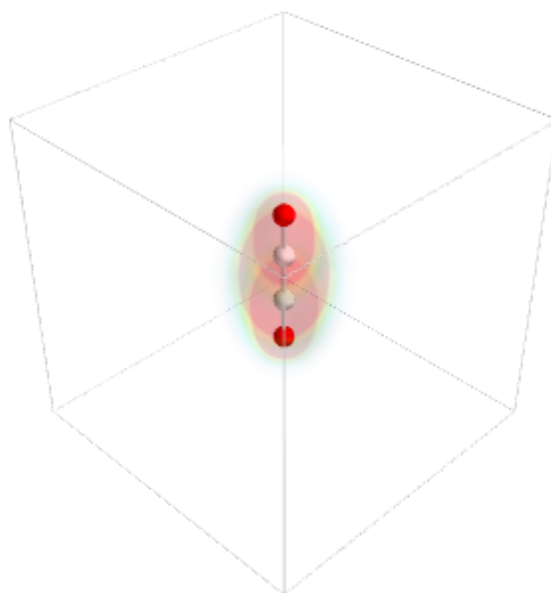
There is a concentration of electron density along the carbon backbone forming a ring. A lack of electron density in the center is observed. This mirrors the bonding nature in benzene.

- C₂H₂ (Triple Bond in carbon chain)

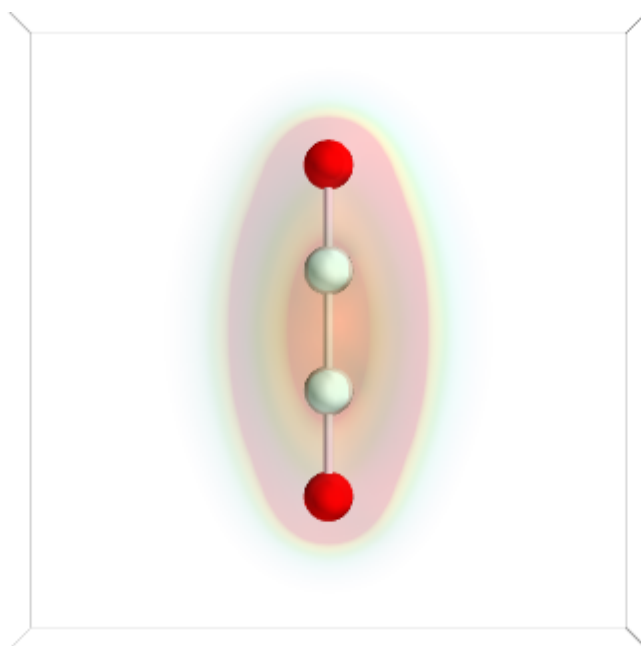
Top view



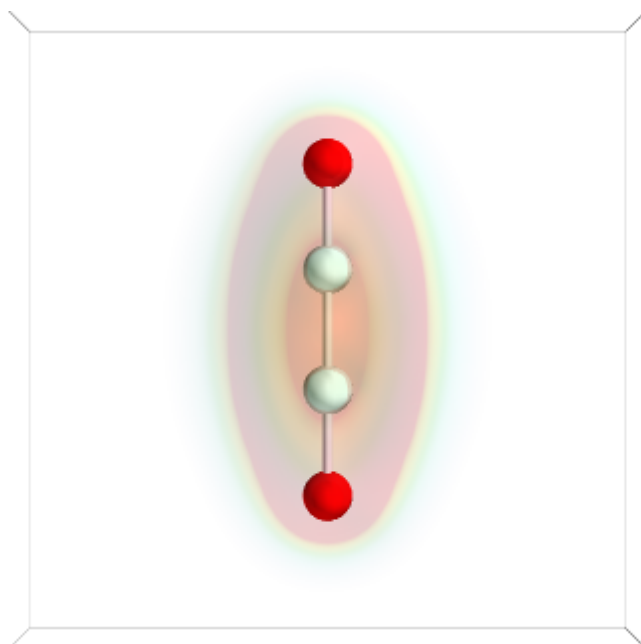
Iso view



Side view

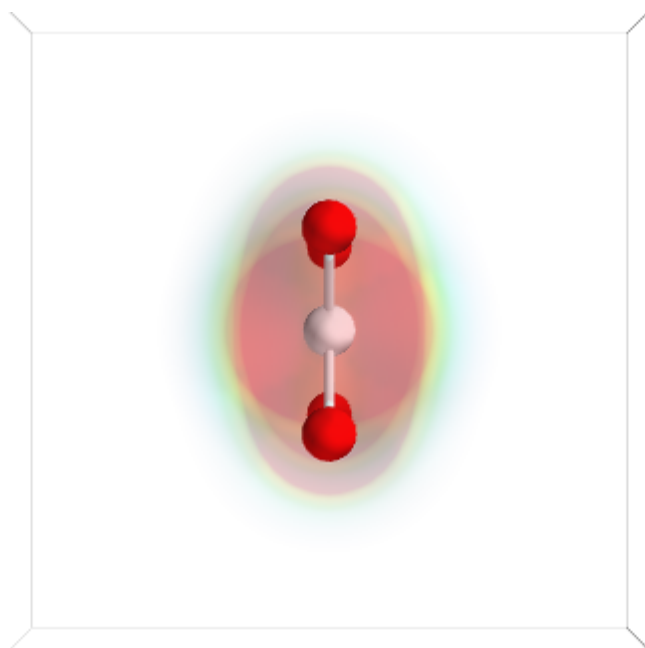


Front view

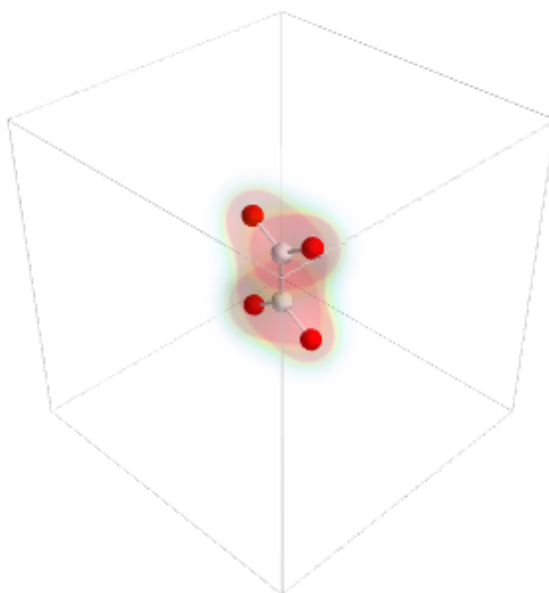


- C2H4 (Double Bond in carbon chain)

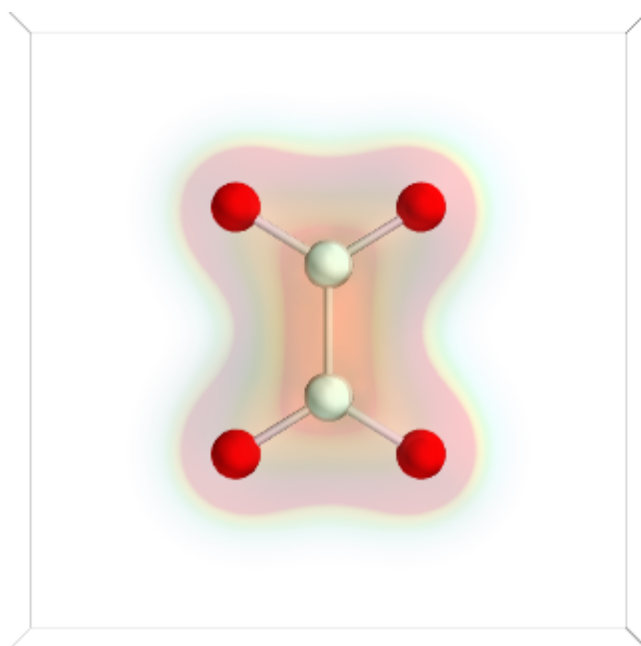
Top view



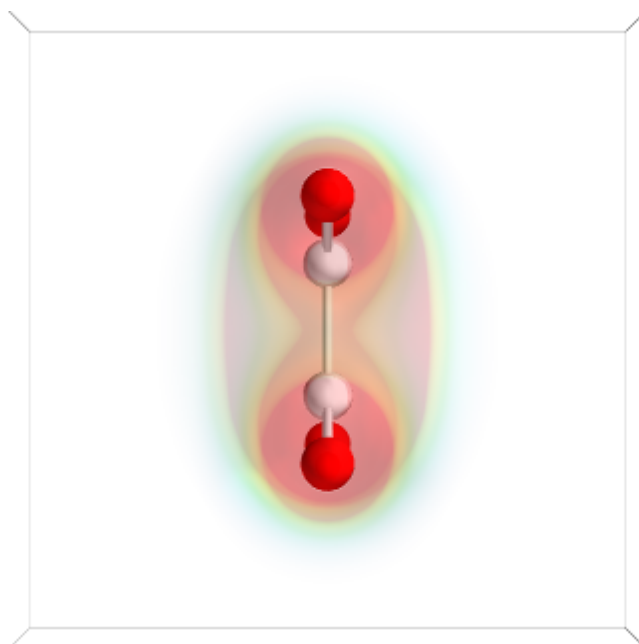
Iso view



Side view

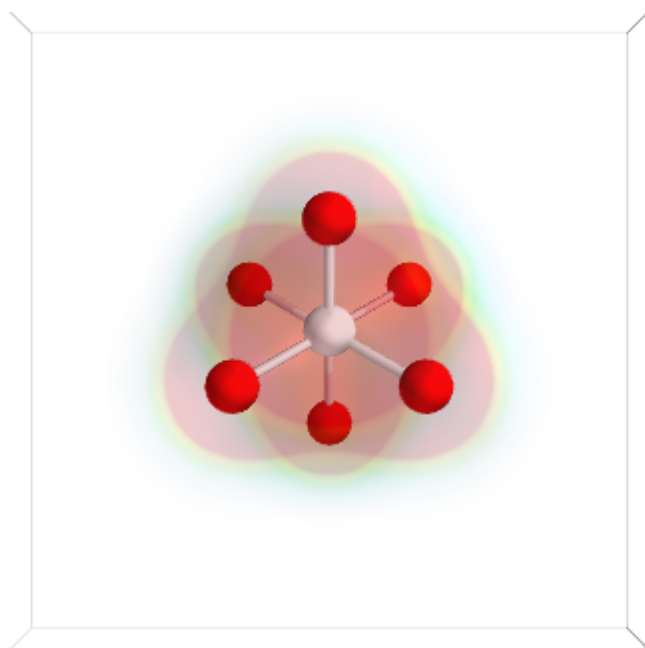


Front view

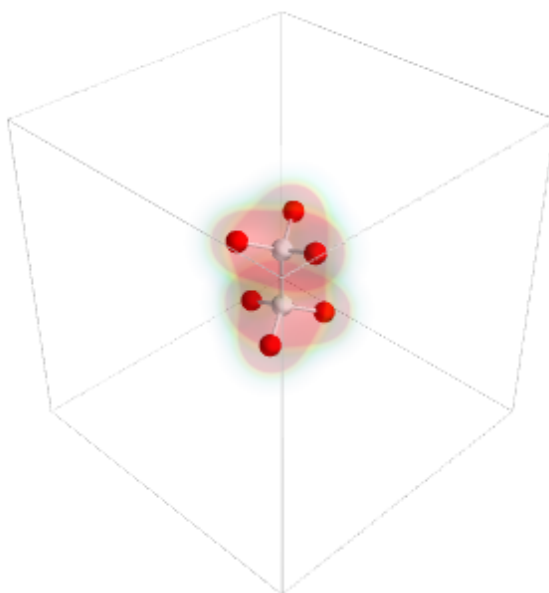


- C_2H_6 (Single Bond in carbon chain)

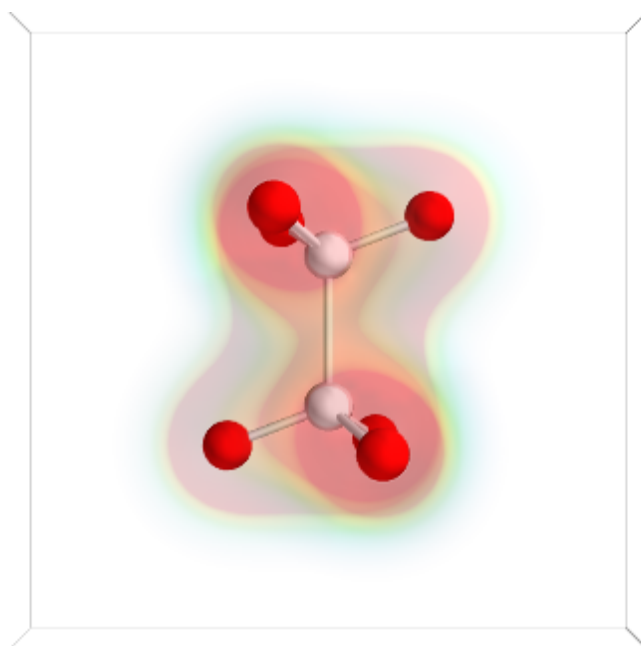
Top view



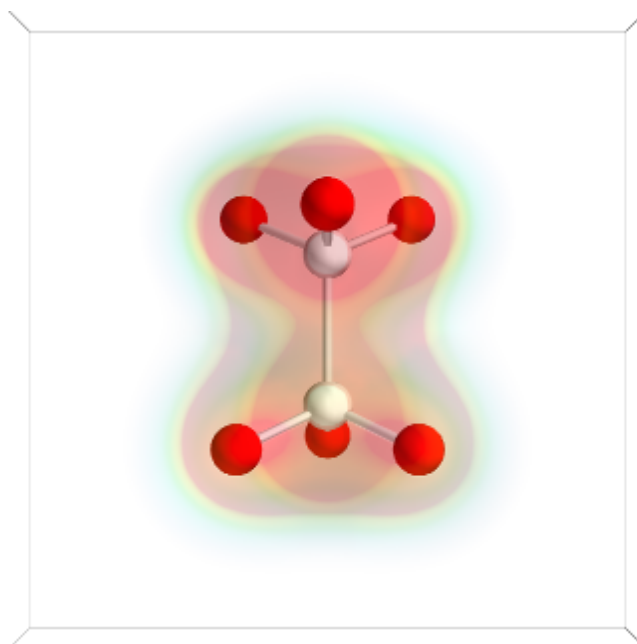
Iso view



Side view



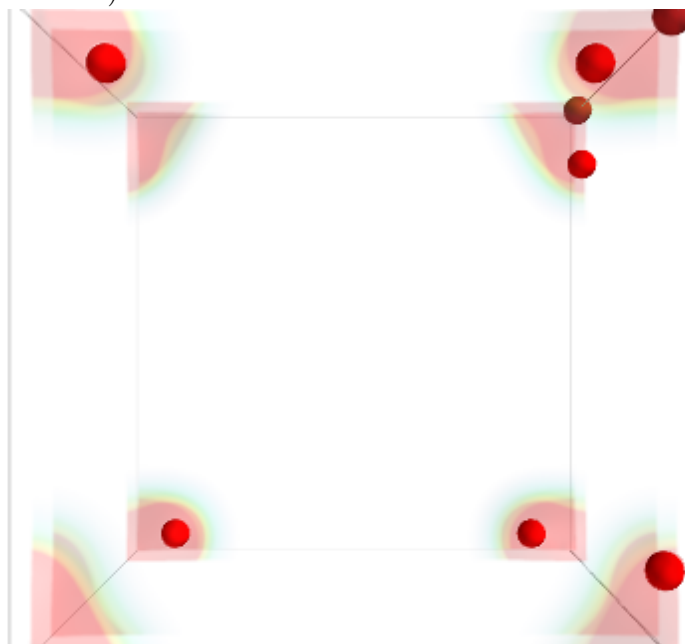
Front view



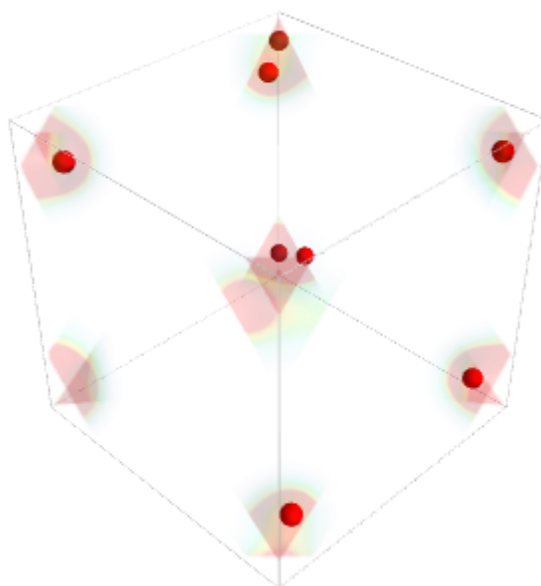
Comparison between images of C_2H_2 , C_2H_4 and C_2H_6 showed a higher electron density between the carbon pair for C_2H_2 and C_2H_4 than for C_2H_6 . This is due to the presence of the double and triple

bond.

- C₂H₆ (Not Centered)

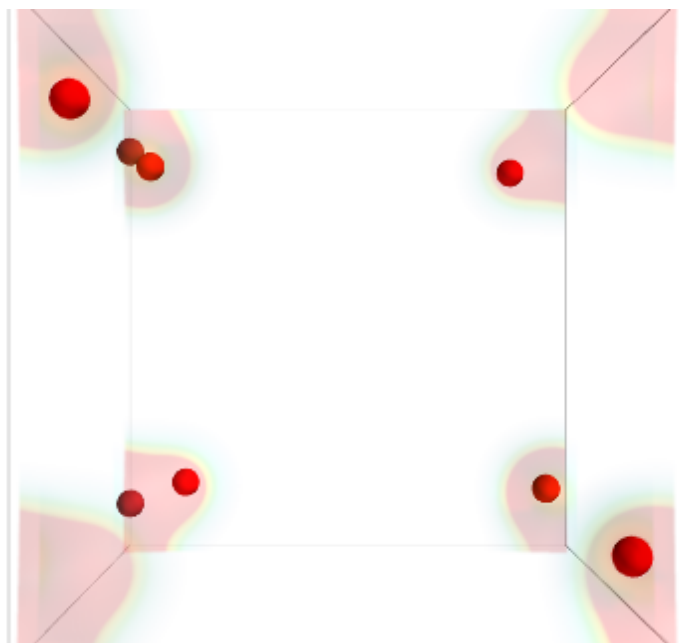


Top view

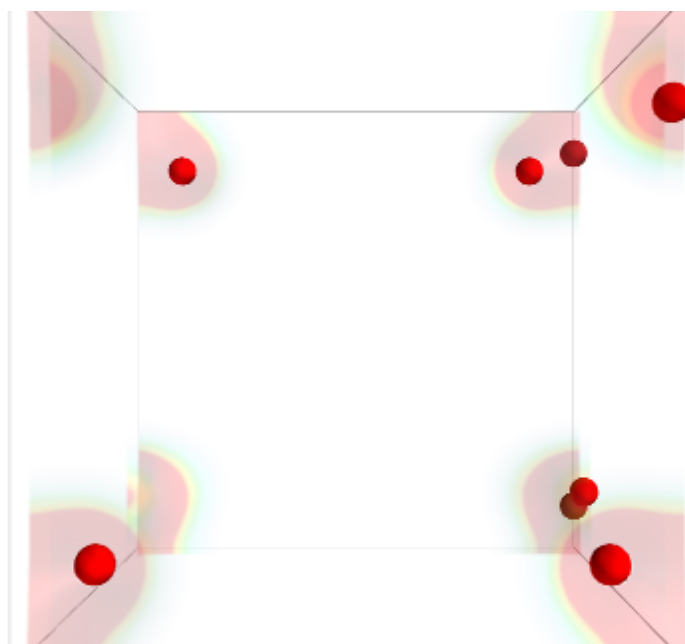


Iso view

Side view

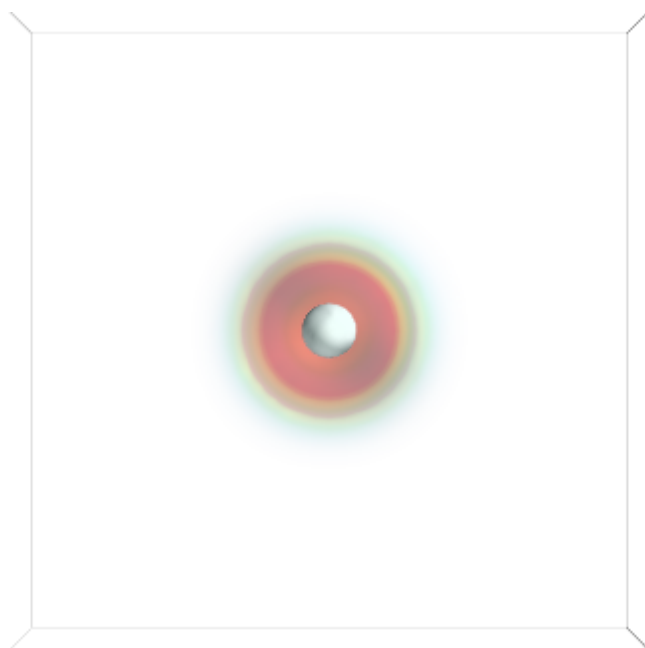


Front view

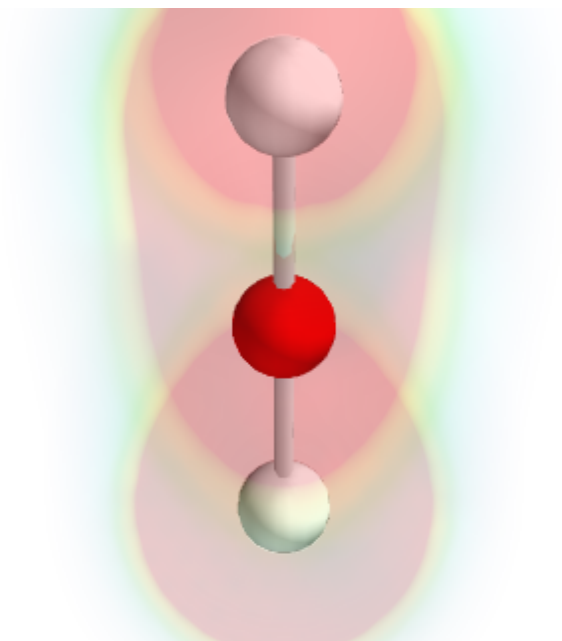


• CO2

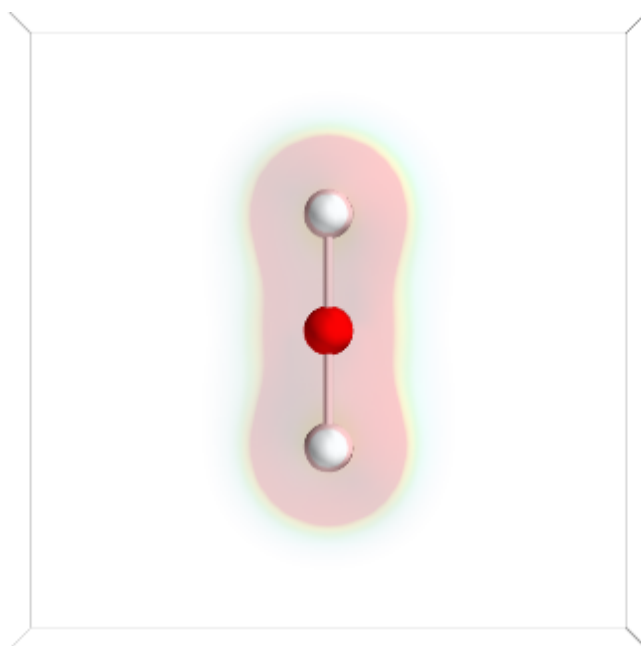
Top view



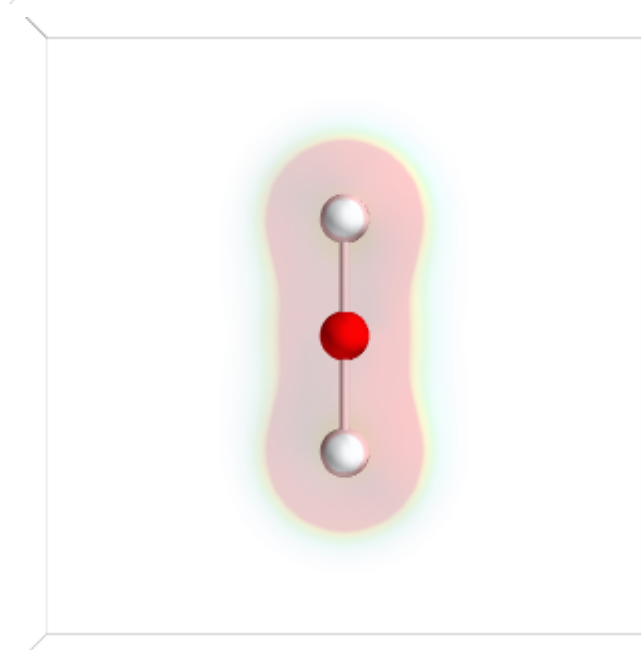
Iso view



Side view

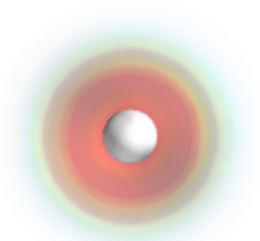


Front view

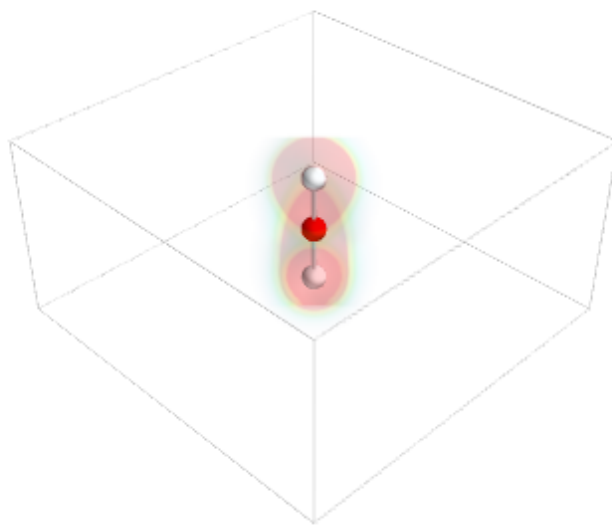


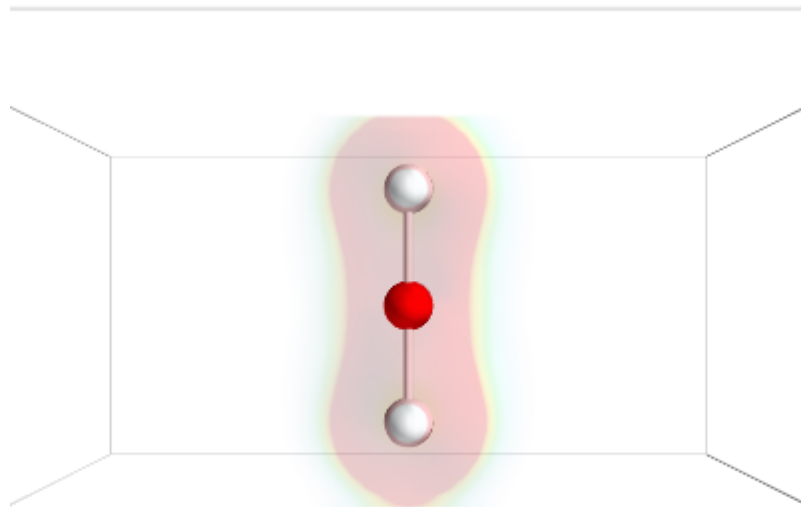
- CO₂ (Non-uniform simulation cubic cell)

Top view

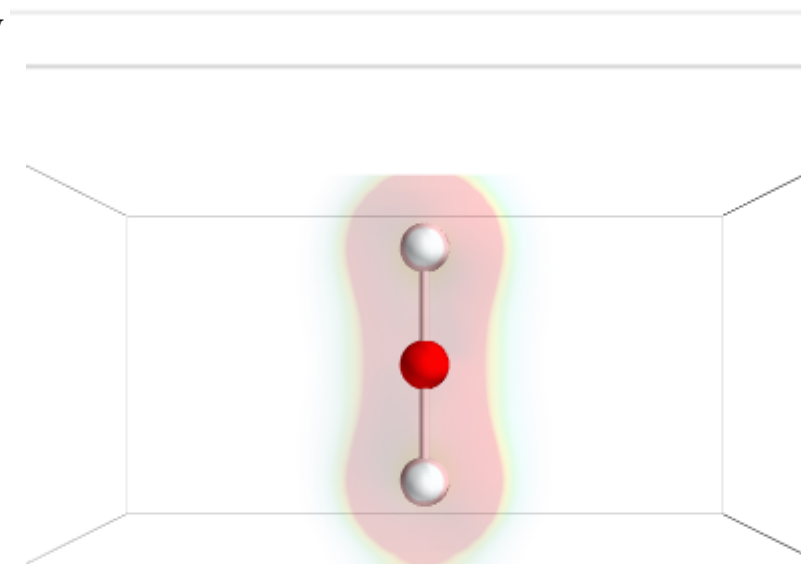


Iso view





Side view

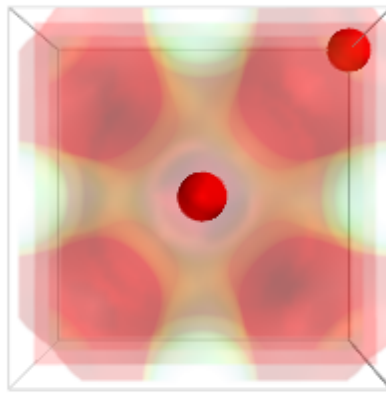


Front view

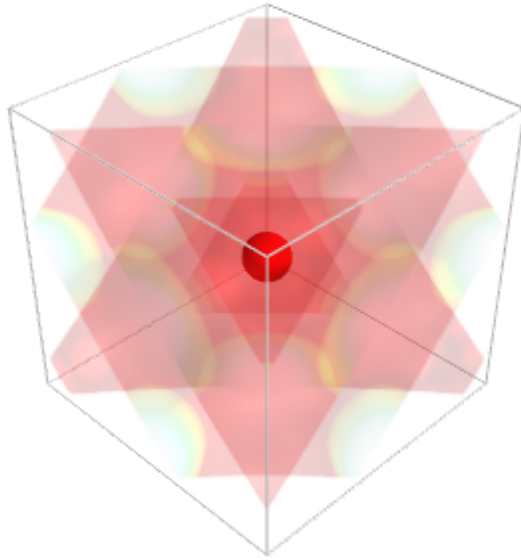
1.6.2 Periodic structures

The periodic nature of these cells results in plots of electron density not being itself enclosed but spread across the cell boundary.

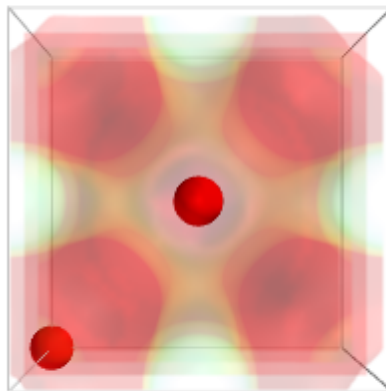
- Ta (BCC Metal)



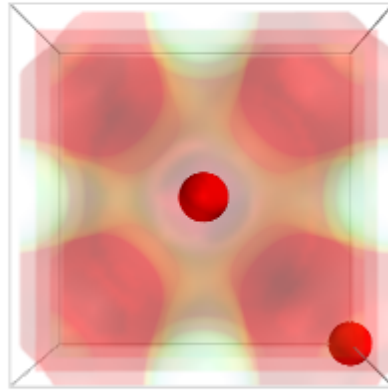
Top view



Iso view



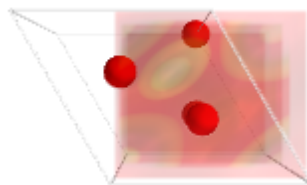
Side view



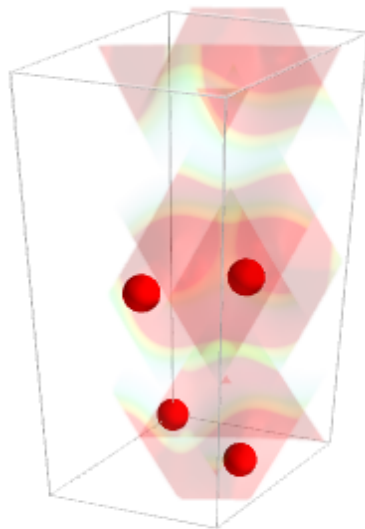
Front view

The electron cloud tends to cluster near to the center and vertices of the cell as compared to a FCC structure as shown below for TaC.

- Graphite (Planar hexagonal)



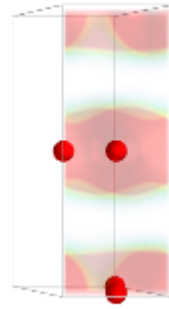
Top view



Iso view



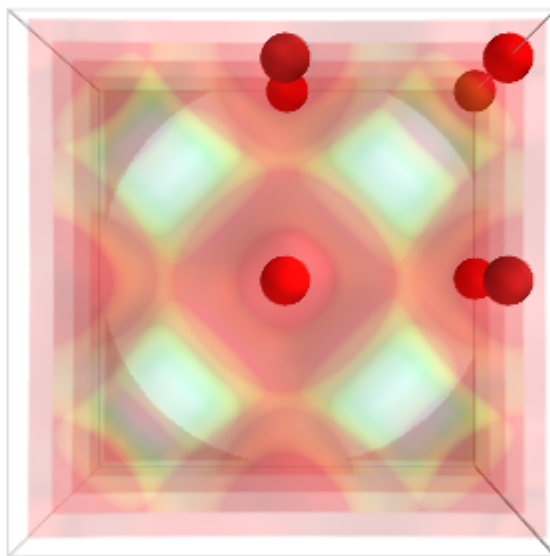
Side view



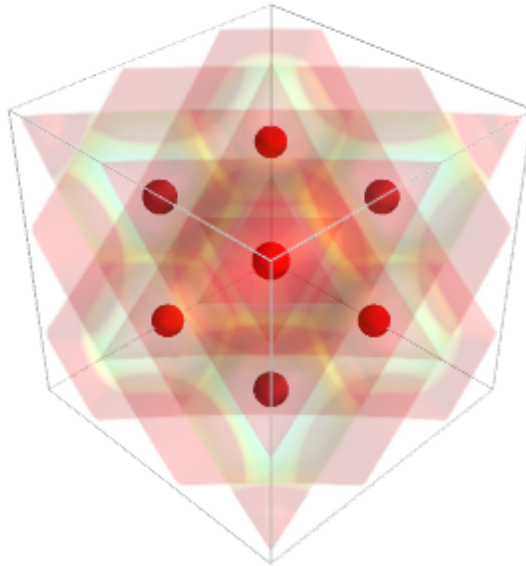
Front view

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

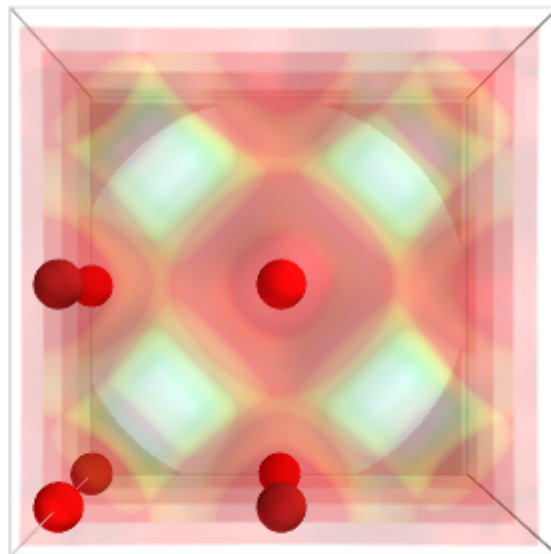
- TaC (rock-salt structure)



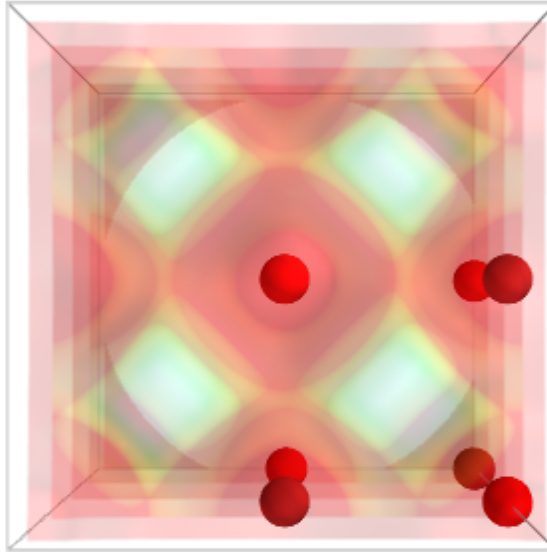
Top view



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. A possible reason is the physical density and arrangement of the atoms in FCC differ from BCC, pulling electrons closer around each atom.