Mini-Project 1 - Charlie Janini

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Contents

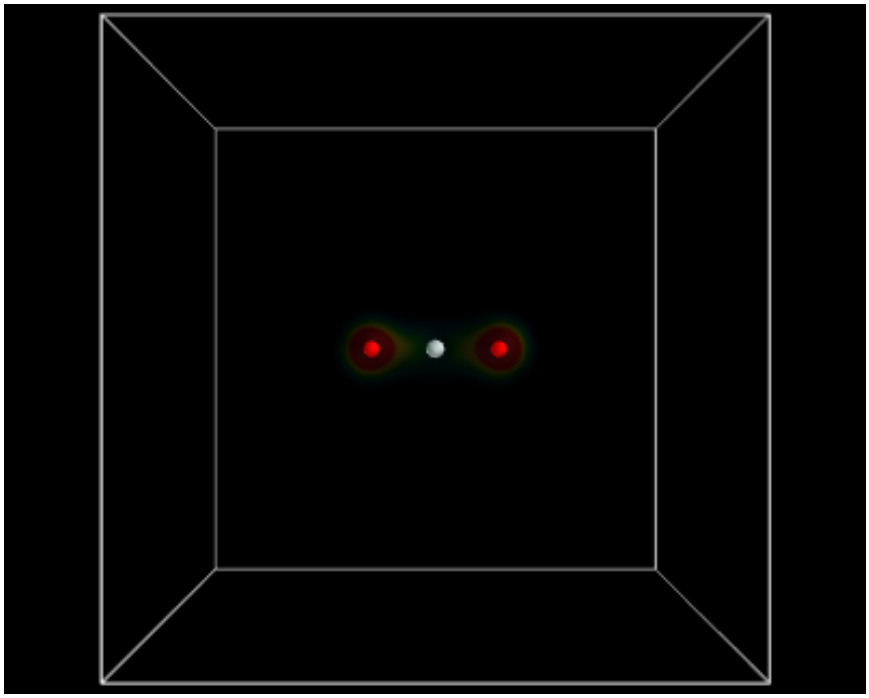
This project seeks to plot the electron densities of some representative molecules (CO_2 and H_2O) as a "fog," as opposed to the prior representation as a solid.

1 Plot the Electron Density of CO_2 as a "fog"

```
from jasp import *
from enthought.mayavi import mlab
from ase.data import vdw_radii
from ase.data.colors import cpk_colors
from ase import Atoms, Atom
import numpy as np

CO2center = Atoms([Atom('O',[1.8,2.,2.]),
              Atom('C',[2.,2.,2.]),
              Atom('O',[3.2,2.,2.])],
              cell = (4,4,4))

CO2center.center()

with jasp('MiniProject1/CO2Center',
          encut = 350,
          xc = 'PBE',
          atoms = CO2center) as calc:
    try:
        calc.calculate()
```

```
        atoms = calc.get_atoms()
        x,y,z,cd = calc.get_charge_density()
    except (VaspSubmitted, VaspQueued):
        import sys; sys.exit()

mlab.figure(bgcolor=(0,0,0)) #black background for easier visualization

# plot atoms as spheres (as seen in dft-book)

for atom in atoms:
    mlab.points3d(atom.x,
                  atom.y,
                  atom.z,
                  scale_factor=vdw_radii[atom.number]/5.,
                  resolution=20,
                  color = tuple(cpk_colors[atom.number]),
                  scale_mode='none')

# construct unit cell (as seen in dft-book)

a1, a2, a3 = atoms.get_cell()
origin = [0,0,0]
cell_matrix = [[origin,a1],
               [origin,a2],
               [origin,a3],
               [a1,    a1+a2],
               [a1,    a1+a3],
               [a2,    a2+a1],
               [a2,    a2+a3],
               [a3,    a3+a1],
               [a3,    a3+a2],
               [a1+a2, a1+a2+a3],
               [a2+a3, a1+a2+a3],
               [a1+a3, a1+a2+a3]]

# connect corners of unit cell with tubes (as seen in dft-book)

for p1,p2 in cell_matrix:
    mlab.plot3d([p1[0],p2[0]],
                [p1[1],p2[1]],
                [p1[2],p2[2]],
                tube_radius=0.02)

# map x, y, z, and cd (outputs from calc.get_charge_density) into scalar_field to allow for plotting
data = mlab.pipeline.scalar_field(x,y,z,cd)

# plot charge density as a fog
mlab.pipeline.volume(data, vmin = .5, vmax = 3.5)
# vmin and vmax parameters must be optimized for best visualization
mlab.view(azimuth=90, elevation=90, distance = 'auto')
# view angle must also be optimized for best viewing of electron density
mlab.savefig('CO2ChargeFog.png')
mlab.show()

print min
print max
```

```
<built-in function min>
<built-in function max>
```



Electron density is concentrated on the oxygen atoms, which makes sense because oxygen is more electronegative than carbon. Thus, the oxygen serves as an electron sink while the carbon serves as an electron source to the bonding of CO_2.

2 Plot the Electron Density of H_2O as a "fog"

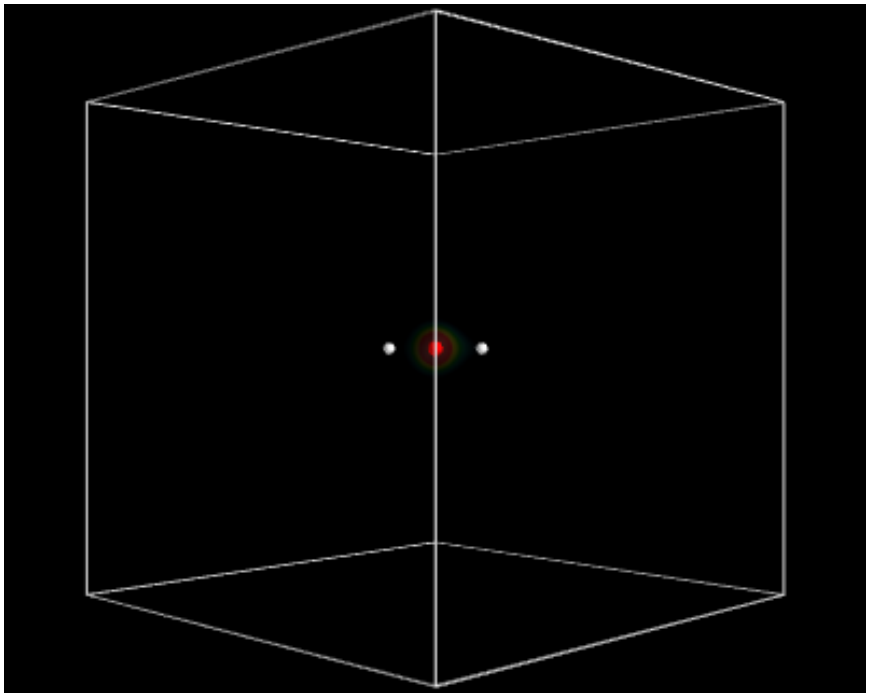
Code very similar to plotting of CO_2, changed Atoms object, vmin, vmax, and view of visualization.

```
1  from jasp import *
2  from enthought.mayavi import mlab
3  from ase.data import vdw_radii
4  from ase.data.colors import cpk_colors
5  from ase import Atoms, Atom
6  import numpy as np
7
8  # Input H2O atom with experimental bond lengths in center of cell
9
10 H2Ocenter = Atoms([Atom('O',[2.,2.,2.]),
```

```
                    Atom('H',[1.25,2.,1.42]),
                    Atom('H',[2.75,2.,2.58])],
                    cell = (4,4,4))


with jasp('MiniProject1/H2OCenter',
          encut = 350,
          xc = 'PBE',
          atoms = H2Ocenter) as calc:
    try:
        calc.calculate()
        atoms = calc.get_atoms()
        x,y,z,cd = calc.get_charge_density()
    except (VaspSubmitted, VaspQueued):
        import sys; sys.exit()

mlab.figure(bgcolor=(0,0,0))

# plot atoms as spheres

for atom in atoms:
    mlab.points3d(atom.x,
                  atom.y,
                  atom.z,
                  scale_factor=vdw_radii[atom.number]/5.,
                  resolution=20,
                  color = tuple(cpk_colors[atom.number]),
                  scale_mode='none')

# construct unit cell

a1, a2, a3 = atoms.get_cell()
origin = [0,0,0]
cell_matrix = [[origin,a1],
               [origin,a2],
               [origin,a3],
               [a1,    a1+a2],
               [a1,    a1+a3],
               [a2,    a2+a1],
               [a2,    a2+a3],
               [a3,    a3+a1],
               [a3,    a3+a2],
               [a1+a2, a1+a2+a3],
               [a2+a3, a1+a2+a3],
               [a1+a3, a1+a2+a3]]

# connect corners of unit cell with tubes

for p1,p2 in cell_matrix:
    mlab.plot3d([p1[0],p2[0]],
                [p1[1],p2[1]],
                [p1[2],p2[2]],
                tube_radius=0.02)

# map x, y, z, and charge density into scalar_field to allow for plotting
data = mlab.pipeline.scalar_field(x,y,z,cd)
```

```
67
68  #plot charge density as a fog
69  mlab.pipeline.volume(data, vmin = 1, vmax = 3) #changed vmin and vmax from CO_{2} example above
70  mlab.view(azimuth=135, elevation=90, distance = 'auto') #changed view to make visualization better
71  mlab.savefig('H2OChargeFog.png')
72  mlab.show()
73
74  print min
75  print max
```

```
-0.0013805
7.9041
```



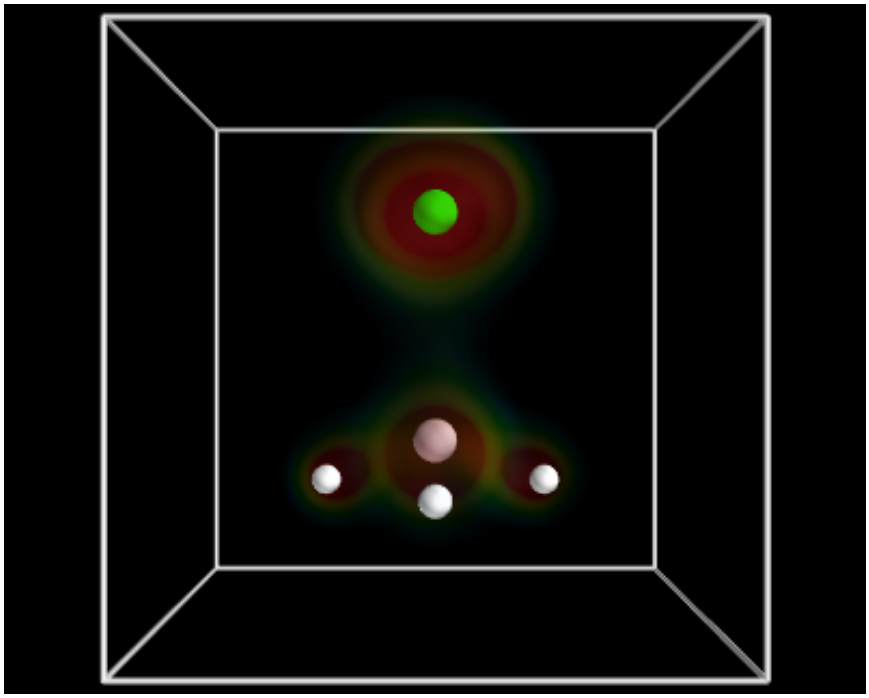
As can be seen in the plot, the electron density around water is concentrated on the oxygen molecule. This makes sense because oxygen is much more electronegative than hydrogen.

3 Plot the Electron Density of CH_3Cl as a "fog"

```
1  from jasp import *
2  from enthought.mayavi import mlab
3  from ase.data import vdw_radii
4  from ase.data.colors import cpk_colors
```

```
from ase.data.molecules import molecule
import numpy as np

# Input H2O atom with experimental bond lengths in center of cell

CH3Clcenter = molecule('CH3Cl', cell = (4,4,4))
CH3Clcenter.center()


with jasp('MiniProject1/CH3ClCenter',
          encut = 350,
          xc = 'PBE',
          atoms = CH3Clcenter) as calc:
    try:
        calc.calculate()
        atoms = calc.get_atoms()
        x,y,z,cd = calc.get_charge_density()
    except (VaspSubmitted, VaspQueued):
        import sys; sys.exit()

mlab.figure(bgcolor=(0,0,0))

# plot atoms as spheres

for atom in atoms:
    mlab.points3d(atom.x,
                  atom.y,
                  atom.z,
                  scale_factor=vdw_radii[atom.number]/5.,
                  resolution=20,
                  color = tuple(cpk_colors[atom.number]),
                  scale_mode='none')

# construct unit cell

a1, a2, a3 = atoms.get_cell()
origin = [0,0,0]
cell_matrix = [[origin,a1],
               [origin,a2],
               [origin,a3],
               [a1,    a1+a2],
               [a1,    a1+a3],
               [a2,    a2+a1],
               [a2,    a2+a3],
               [a3,    a3+a1],
               [a3,    a3+a2],
               [a1+a2, a1+a2+a3],
               [a2+a3, a1+a2+a3],
               [a1+a3, a1+a2+a3]]

# connect corners of unit cell with tubes

for p1,p2 in cell_matrix:
    mlab.plot3d([p1[0],p2[0]],
                [p1[1],p2[1]],
                [p1[2],p2[2]],
```

```
                tube_radius=0.02)

# map x, y, z, and charge density into scalar_field to allow for plotting
data = mlab.pipeline.scalar_field(x,y,z,cd)

#plot charge density as a fog
mlab.pipeline.volume(data, vmin = 0.5, vmax = 1.5) #changed vmin and vmax from CO_{2} example above
mlab.view(azimuth=90, elevation=90, distance = 'auto') #changed view to make visualization better
mlab.savefig('CH3ClChargeFog.png')
mlab.show()
```



As the figure shows, the majority of the electron density for chloromethane lies on the chlorine atom. Chlorine is highly elecrtonegative compared to carbon and hydrogen. This electron density plot agrees with the experimental fact that chloromethane has a large dipole moment, with the negative end at the chlorine atom.