

Mini-Project 1 - Charlie Janini

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This project seeks to plot the electron densities of some representative molecules (CO₂ and H₂O) as a “fog,” as opposed to the prior representation as a solid.

1 Plot the Electron Density of CO₂ as a “fog”

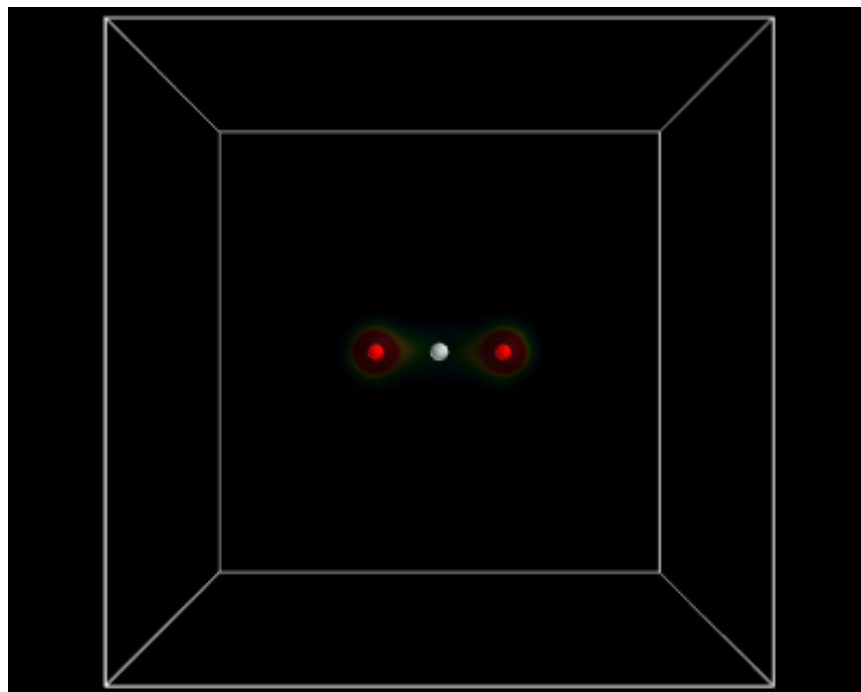
```
1 from jasp import *
2 from enthought.mayavi import mlab
3 from ase.data import vdw_radii
4 from ase.data.colors import cpk_colors
5 from ase import Atoms, Atom
6 import numpy as np
7
8 CO2center = Atoms([Atom('O', [1.8, 2., 2.]),
9                     Atom('C', [2., 2., 2.]),
10                    Atom('O', [3.2, 2., 2.])],
11                  cell = (4, 4, 4))
12
13 CO2center.center()
14
15 with jasp('MiniProject1/CO2Center',
16          encut = 350,
17          xc = 'PBE',
18          atoms = CO2center) as calc:
19     try:
20         calc.calculate()
```

```

21         atoms = calc.get_atoms()
22         x,y,z,cd = calc.get_charge_density()
23     except (VaspSubmitted, VaspQueued):
24         import sys; sys.exit()
25
26     mlab.figure(bgcolor=(0,0,0)) #black background for easier visualization
27
28     # plot atoms as spheres (as seen in dft-book)
29
30     for atom in atoms:
31         mlab.points3d(atom.x,
32                       atom.y,
33                       atom.z,
34                       scale_factor=vdw_radii[atom.number]/5.,
35                       resolution=20,
36                       color = tuple(cpk_colors[atom.number]),
37                       scale_mode='none')
38
39     # construct unit cell (as seen in dft-book)
40
41     a1, a2, a3 = atoms.get_cell()
42     origin = [0,0,0]
43     cell_matrix = [[origin,a1],
44                   [origin,a2],
45                   [origin,a3],
46                   [a1, a1+a2],
47                   [a1, a1+a3],
48                   [a2, a2+a1],
49                   [a2, a2+a3],
50                   [a3, a3+a1],
51                   [a3, a3+a2],
52                   [a1+a2, a1+a2+a3],
53                   [a2+a3, a1+a2+a3],
54                   [a1+a3, a1+a2+a3]]
55
56     # connect corners of unit cell with tubes (as seen in dft-book)
57
58     for p1,p2 in cell_matrix:
59         mlab.plot3d([p1[0],p2[0]],
60                    [p1[1],p2[1]],
61                    [p1[2],p2[2]],
62                    tube_radius=0.02)
63
64     # map x, y, z, and cd (outputs from calc.get_charge_density) into scalar_field to allow for plotting
65     data = mlab.pipeline.scalar_field(x,y,z,cd)
66
67     # plot charge density as a fog
68     mlab.pipeline.volume(data, vmin = .5, vmax = 3.5)
69     # vmin and vmax parameters must be optimized for best visualization
70     mlab.view(azimuth=90, elevation=90, distance = 'auto')
71     # view angle must also be optimized for best viewing of electron density
72     mlab.savefig('CO2ChargeFog.png')
73     mlab.show()
74
75     print min
76     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 CO₂.

2 Plot the Electron Density of H₂O as a “fog”

Code very similar to plotting of CO₂, 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.]),
```

```

11             Atom('H',[1.25,2.,1.42]),
12             Atom('H',[2.75,2.,2.58])),
13             cell = (4,4,4))
14
15
16 with jasp('MiniProject1/H2OCenter',
17           encut = 350,
18           xc = 'PBE',
19           atoms = H2Ocenter) as calc:
20     try:
21         calc.calculate()
22         atoms = calc.get_atoms()
23         x,y,z,cd = calc.get_charge_density()
24     except (VaspSubmitted, VaspQueued):
25         import sys; sys.exit()
26
27 mlab.figure(bgcolor=(0,0,0))
28
29 # plot atoms as spheres
30
31 for atom in atoms:
32     mlab.points3d(atom.x,
33                  atom.y,
34                  atom.z,
35                  scale_factor=vdw_radii[atom.number]/5.,
36                  resolution=20,
37                  color = tuple(cpk_colors[atom.number]),
38                  scale_mode='none')
39
40 # construct unit cell
41
42 a1, a2, a3 = atoms.get_cell()
43 origin = [0,0,0]
44 cell_matrix = [[origin,a1],
45                [origin,a2],
46                [origin,a3],
47                [a1, a1+a2],
48                [a1, a1+a3],
49                [a2, a2+a1],
50                [a2, a2+a3],
51                [a3, a3+a1],
52                [a3, a3+a2],
53                [a1+a2, a1+a2+a3],
54                [a2+a3, a1+a2+a3],
55                [a1+a3, a1+a2+a3]]
56
57 # connect corners of unit cell with tubes
58
59 for p1,p2 in cell_matrix:
60     mlab.plot3d([p1[0],p2[0]],
61                 [p1[1],p2[1]],
62                 [p1[2],p2[2]],
63                 tube_radius=0.02)
64
65 # map x, y, z, and charge density into scalar_field to allow for plotting
66 data = mlab.pipeline.scalar_field(x,y,z,cd)

```

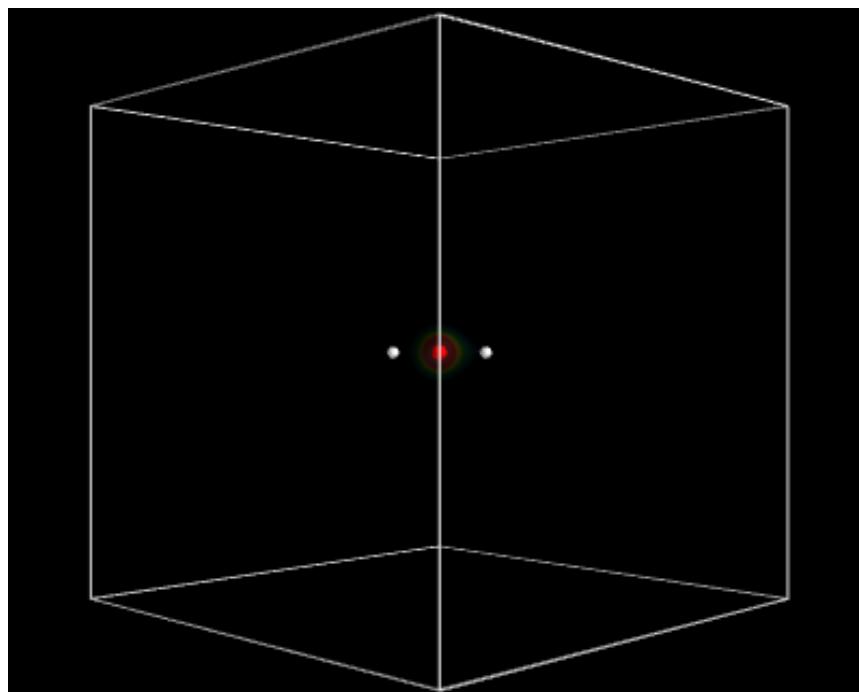
```

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 CH₃Cl 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

```

```

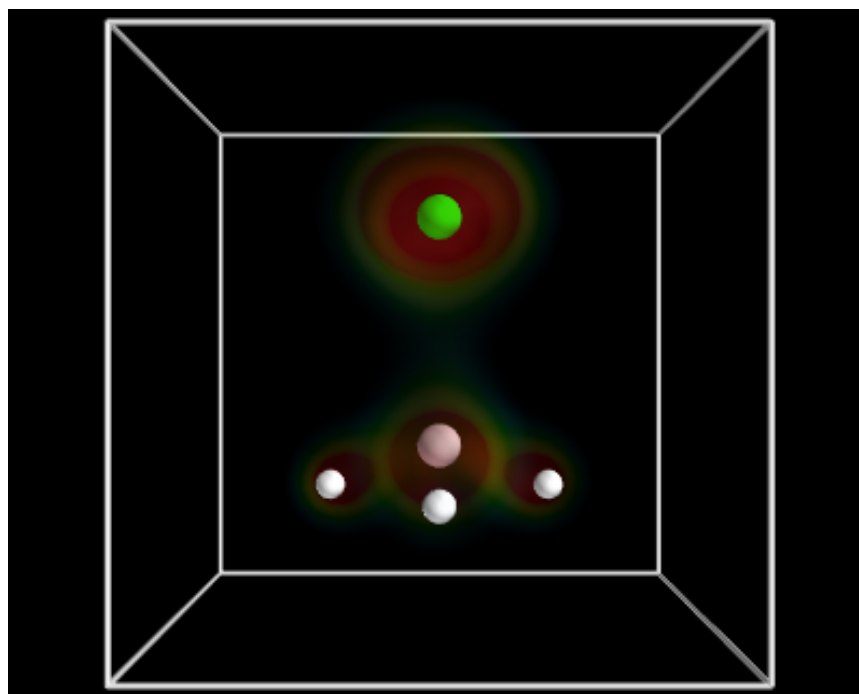
5  from ase.data.molecules import molecule
6  import numpy as np
7
8  # Input H2O atom with experimental bond lengths in center of cell
9
10 CH3Clcenter = molecule('CH3Cl', cell = (4,4,4))
11 CH3Clcenter.center()
12
13
14 with jasp('MiniProject1/CH3ClCenter',
15          encut = 350,
16          xc = 'PBE',
17          atoms = CH3Clcenter) as calc:
18     try:
19         calc.calculate()
20         atoms = calc.get_atoms()
21         x,y,z,cd = calc.get_charge_density()
22     except (VaspSubmitted, VaspQueued):
23         import sys; sys.exit()
24
25 mlab.figure(bgcolor=(0,0,0))
26
27 # plot atoms as spheres
28
29 for atom in atoms:
30     mlab.points3d(atom.x,
31                  atom.y,
32                  atom.z,
33                  scale_factor=vdw_radii[atom.number]/5.,
34                  resolution=20,
35                  color = tuple(cpk_colors[atom.number]),
36                  scale_mode='none')
37
38 # construct unit cell
39
40 a1, a2, a3 = atoms.get_cell()
41 origin = [0,0,0]
42 cell_matrix = [[origin,a1],
43               [origin,a2],
44               [origin,a3],
45               [a1, a1+a2],
46               [a1, a1+a3],
47               [a2, a2+a1],
48               [a2, a2+a3],
49               [a3, a3+a1],
50               [a3, a3+a2],
51               [a1+a2, a1+a2+a3],
52               [a2+a3, a1+a2+a3],
53               [a1+a3, a1+a2+a3]]
54
55 # connect corners of unit cell with tubes
56
57 for p1,p2 in cell_matrix:
58     mlab.plot3d([p1[0],p2[0]],
59                [p1[1],p2[1]],
60                [p1[2],p2[2]],

```

```

61         tube_radius=0.02)
62
63     # map x, y, z, and charge density into scalar_field to allow for plotting
64     data = mlab.pipeline.scalar_field(x,y,z,cd)
65
66     #plot charge density as a fog
67     mlab.pipeline.volume(data, vmin = 0.5, vmax = 1.5) #changed vmin and vmax from CO_{2} example above
68     mlab.view(azimuth=90, elevation=90, distance = 'auto') #changed view to make visualization better
69     mlab.savefig('CH3ClChargeFog.png')
70     mlab.show()

```



As the figure shows, the majority of the electron density for chloromethane lies on the chlorine atom. Chlorine is highly electronegative 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.