

# Mini-Project 1 - Charlie Janini

Charles Janini

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This project seeks to plot the electron densities of some representative molecules (CO<sub>2</sub> and H<sub>2</sub>O) as a “fog,” as opposed to the prior representation as a solid.

## 1 Plot the Electron Density of CO<sub>2</sub> 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()
```

```

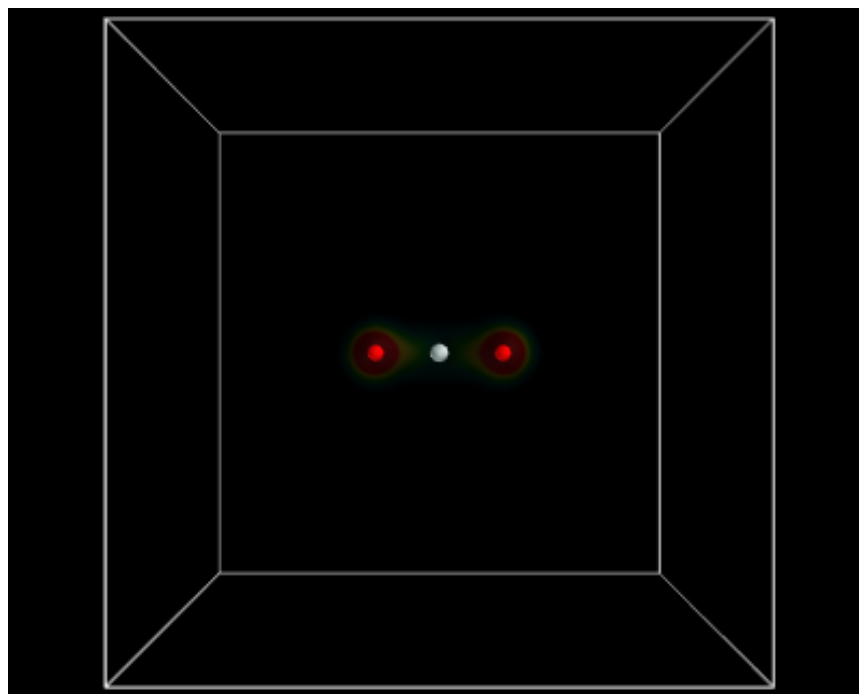
23     except (VaspSubmitted, VaspQueued):
24         import sys; sys.exit()
25
26     mlab.figure(bgcolor=(0,0,0)) #black background for easier visualization
27
28     # plot atoms as spheres (as seen in dft-book)
29
30     for atom in atoms:
31         mlab.points3d(atom.x,
32                       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('C02ChargeFog.png')
73     mlab.show()
74
75     print min
76     print max

```

---

-0.001544

8.0754



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<sub>2</sub>.

## 2 Plot the Electron Density of H<sub>2</sub>O as a “fog”

Code very similar to plotting of CO<sub>2</sub>, 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

```

```

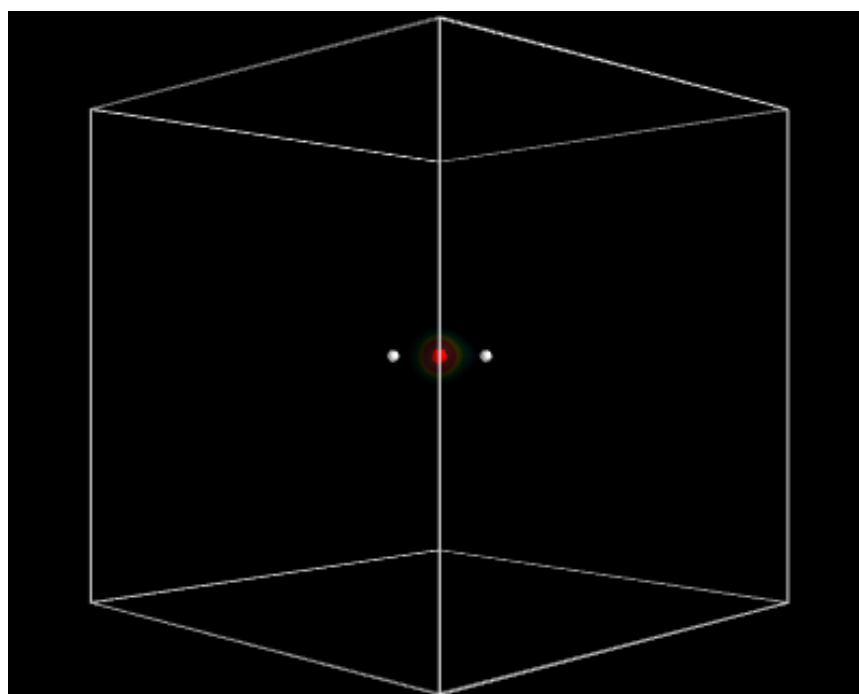
69 mlab.pipeline.volume(data, vmin = 1, vmax = 3) #changed vmin and vmax from CO_{2} example above
70 mlab.view(azimuth=135, elevation=90, distance = 'auto') #changed view to make visualization better
71 mlab.savefig('H2OChargeFog.png')
72 mlab.show()
73
74 print min
75 print max

```

---

-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.