lab3_3_01262023

January 26, 2023

[10]:
```
#ASE modules
from ase import Atoms
from ase.visualize import view
from ase.io import read,write
from ase.build import molecule
from ase.calculators.vasp import Vasp

#Python modules
import numpy as np
import matplotlib.pyplot as plt
from scipy.constants import physical_constants
```

[48]:
```
def Calc_Encut(direct, en, atom):

    calc = Vasp(
            directory = direct,
            encut = en, #planewave cutoff
            xc = 'PBE', #exchange-correlation functional
            ismear = 1, #planewave smearing
            sigma = 0.01, #small smearing factor for a molecule
            #kpts = [1,1,1],
            #ediff = 1e-6,
            atoms = atom,
            )

    return calc
```

[58]:
```
d = 1.1

CO = Atoms('CO',
           positions = [ (0,0,0), (0,0, d) ],
           cell = [10,10,10],
           pbc = [1,1,1] #periodic boundary condition
          )

#CO.set_cell([10,10,10])
CO.center()
```

```
view(CO)
```

[58]: <Popen: returncode: None args: ['/afs/.crc.nd.edu/x86_64_linux/p/python/3.10…>

[59]:
```
calc_CO = Calc_Encut('./CO_lab3_3_01262023', 350, CO)

calc_CO.calculate(CO)
```

[67]:
```
calc_CO.read()
CO = calc_CO.get_atoms()

print('Converged? ', calc_CO.converged)
```

```
Converged?  True
```

[68]:
```
#from calc object
print('Energy = {0} eV'.format(calc_CO.get_potential_energy()))
print('Forces (eV/Ang.):')
print(calc_CO.get_forces())
```

```
Energy = -13.13973187 eV
Forces (eV/Ang.):
[[  0.           0.         -27.70951004]
 [ -0.           0.          27.70951004]]
<ase.calculators.vasp.vasp.Vasp object at 0x7fe52666b100>
```

[69]:
```
#from atoms object
print('Energy = {0} eV'.format(CO.get_potential_energy()))
print('Forces (eV/Ang.):')
print(CO.get_forces())
```

```
Energy = -13.13973187 eV
Forces (eV/Ang.):
[[  0.           0.         -27.70951004]
 [ -0.           0.          27.70951004]]
```

[70]:
```
#print status of calculation
print(calc_CO)
```

```
<ase.calculators.vasp.vasp.Vasp object at 0x7fe52666b100>
```

[ ]:
```

```