lab3_4_01292023

January 29, 2023

[1]:
```
#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
```

[14]:
```
def Calc_Encut(direct, en, atom):

    calc = Vasp(
            directory = direct,
            encut = en, #planewave cutoff
            xc = 'PBE', #exchange-correlation functional
            nbands = 8, #number of bands
            ismear = 1, #planewave smearing
            sigma = 0.01, #small smearing factor for a molecule
            kpts = [1,1,1],
            nsw = 20, #number of ionic steps
            ibrion = 2, #conjugate gradient algorithm
            ediff = 1e-6,
            atoms = atom,
            )

    return calc
```

[28]:
```
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.center()

view(CO)
```

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

[29]:
```
calc_CO_geometry = Calc_Encut('./lab3_4_01292023', 350, CO)
calc_CO_geometry.calculate(CO)
```

[30]:
```
calc_CO_geometry.read()
CO = calc_CO_geometry.get_atoms()
print('Converged? ', calc_CO_geometry.converged)
```

```
Converged?  True
```

[34]:
```
print('energy = {0} eV'.format(calc_CO_geometry.get_potential_energy()))
print('number of geometry steps = {0}'.format(calc_CO_geometry.
 ↪read_number_of_ionic_steps()))
print('Forces (eV/Ang.):')
print(calc_CO_geometry.get_forces())
print('Equilibrium Positions (Angs.):')

for atom in CO:
      print(atom.symbol, atom.position)
```

```
energy = -14.81271884 eV
number of geometry steps = 6
Forces (eV/Ang.):
[[ 0.          0.         -0.00951325]
 [-0.          0.          0.00951325]]
Equilibrium Positions (Angs.):
C [5.         5.         4.42810825]
O [5.         5.         5.57189175]
```

[32]:
```
write('./CO-relaxed.png', CO, show_unit_cell = 2, rotation = '60x, -30y, 90z')
```

[ ]: