lab3_5_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
```

[2]:
```
def Calc_Encut(direct, en, atom):

    calc = Vasp(
            directory = direct,
            encut = en, #planewave cutoff
            xc = 'PBE', #exchange-correlation functional
            atoms = atom,
            )

    return calc
```

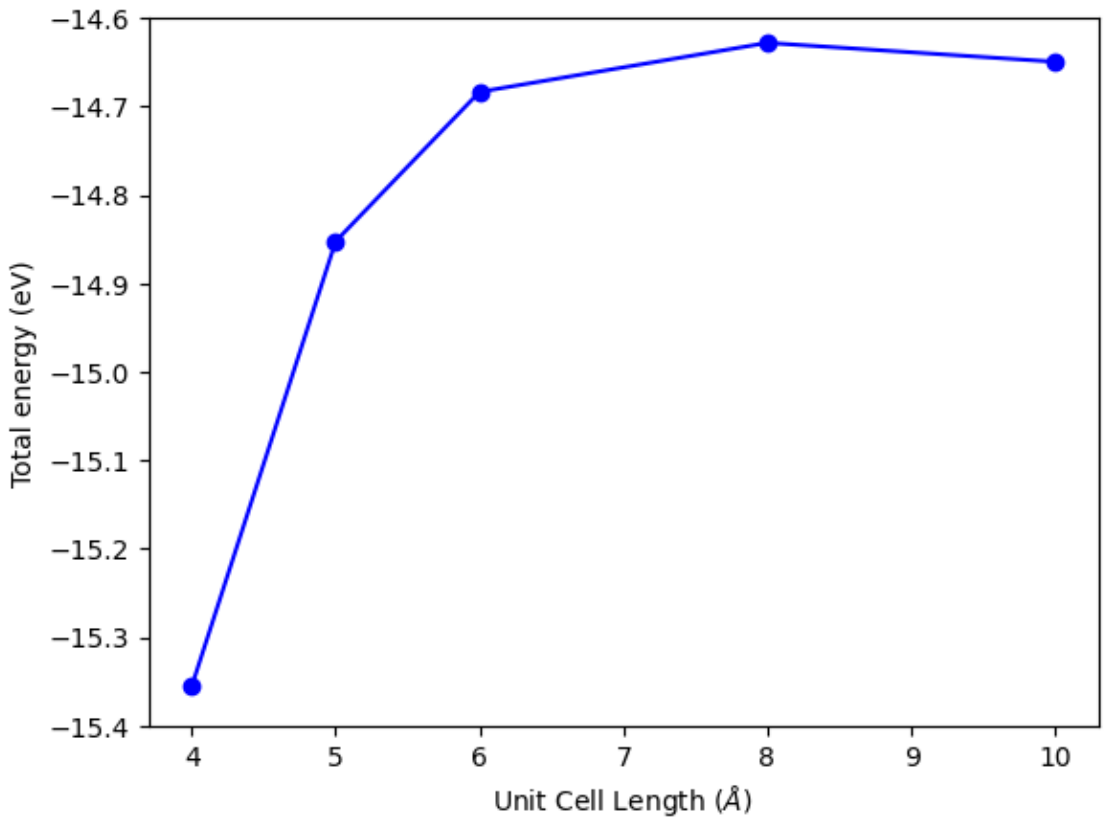
[4]:
```
atoms = Atoms('CO',
              positions = [(0,0,0), (1.2,0,0)],
              pbc = [1,1,1],
             )

#view(atoms)
```

[14]:
```
L = [4,5,6,8,10]
energies = []

for a in L:
    atoms.set_cell([a,a,a], scale_atoms = False)
    atoms.center()
    #view(atoms)
```

```
    calc = Calc_Encut('./lab3_5_012923/co-L-{0}'.format(a), 350, atoms)
    print(calc)
    calc.calculate(atoms)
    calc.read()

    energies.append(calc.get_potential_energy())
```

```
<ase.calculators.vasp.vasp.Vasp object at 0x7fd3c5d91cc0>
<ase.calculators.vasp.vasp.Vasp object at 0x7fd3c6582b90>
<ase.calculators.vasp.vasp.Vasp object at 0x7fd3c6d177f0>
<ase.calculators.vasp.vasp.Vasp object at 0x7fd3c6d17820>
<ase.calculators.vasp.vasp.Vasp object at 0x7fd3c5f19210>
```

[19]:
```
plt.plot(L, energies, 'bo-')
plt.xlabel('Unit Cell Length ($\AA$)')
plt.ylabel('Total energy (eV)')
plt.savefig('./lab3_5_012923/co-e-v.png')
plt.ylim([-15.4, -14.6])
plt.show()
```



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