Find lattice constant

- Find FCC Cu lattice constant
- Using ASE, ASE-STATE-interface
  - ASE tutorial page: https://wiki.fysik.dtu.dk/ase/tutorials/lattice_constant.html
- Calculated 10 candidates of lattice constant, shifting gradually from the initial value 3.6 Å

Fit the energy using this expression(a: lattice constant)

$$E(a) = p_0 + p_1 a + p_2 a^2$$

optb86b-vdw	rev-vdw-df2	rebpbe-d2	rpbe-d2
3.6089 Å	3.6157 Å	3.6048 Å	3.6173 Å

Code

```
from state_interface.state import STATE
import os
import sys
from ase.build import bulk
from ase.io import Trajectory, read
import numpy as np

a0 = 3.6
eps = 0.01
traj = Trajectory('Cu.traj', 'w')
n_cpus = int(sys.argv[1])

energies = []
for i, a in enumerate(a0 * np.linspace(1 - eps, 1 + eps, 20)):
    slab = bulk('Cu', 'fcc', a=a)
    label = f'Cu{i}'
    input_file = f'{label}.in'
    output_file = f'{label}.out'
    pw_loc = './STATE'

    os.environ['ASE_STATE_COMMAND'] = f'mpirun -np {n_cpus} {pw_loc} < {input_file} > {output_file}'


    dft_calc = STATE(label=label, input_data=input_data)
    slab.calc = dft_calc
    energies.append(slab.get_potential_energy())
    traj.write(slab)

print(energies)
configs = read('Cu.traj@:')
a = np.array([2*config.cell[0, 1] for config in configs])
print(a)
# f(a) = p0 + p1*a + p2*a**2
functions = np.array([a**0, a, a**2])
p = np.linalg.lstsq(functions.T, energies, rcond=-1)[0]
#f'(a) = p1 + 2*p2*a
p1 = p[1]
p2 = 2*p[2]
a0 = -p1/p2
print(a0)
```

STATE parameters

```
    input_data = {'WF_OPT'       :    'DAV' ,
                  'TYPE'         :      0  ,
                  'NSPG'         :      1  ,
                  'VERBOSITY'    :     'MEDIUM',
                  'GMAX'         :     6.00 ,
                  'GMAXP'        :     20.00 ,
                  'KPOINT_MESH'  : [16, 16, 16],
                  'KPOINT_SHIFT' : ['OFF', 'OFF', 'OFF'],
                  'NEG'          : 12,
                  'NSCF'         : 200,
                  'NSTEP'        : 200,
                  'TASK'         : 'SCF',
                  'WAY_MIX'      : 6,
                  'MIX_WHAT'     : 1,
                  'KBXMIX'       : 30,
                  'MIX_ALPHA'    : 0.5,
                  'DTIO'         : 100,
                  'IMDALG'       : 2,
                  'WIDTH'        : -0.0020,
                  'FORCCR'       : '1.00D-03',
                  'XCTYPE'        : 'optb86b',
                  'DESTM'        : 1.00,
                  'EDELTA'       : '1.00D-09',
                  'PSEUDOS'      : [
                                      ['Cu', 63.55, 'pot.Cu_pbe1'],
                                   ],
                  'VDW-DF'       : {'QCUT' : 10, 'NQ' : '20'}
                }
```

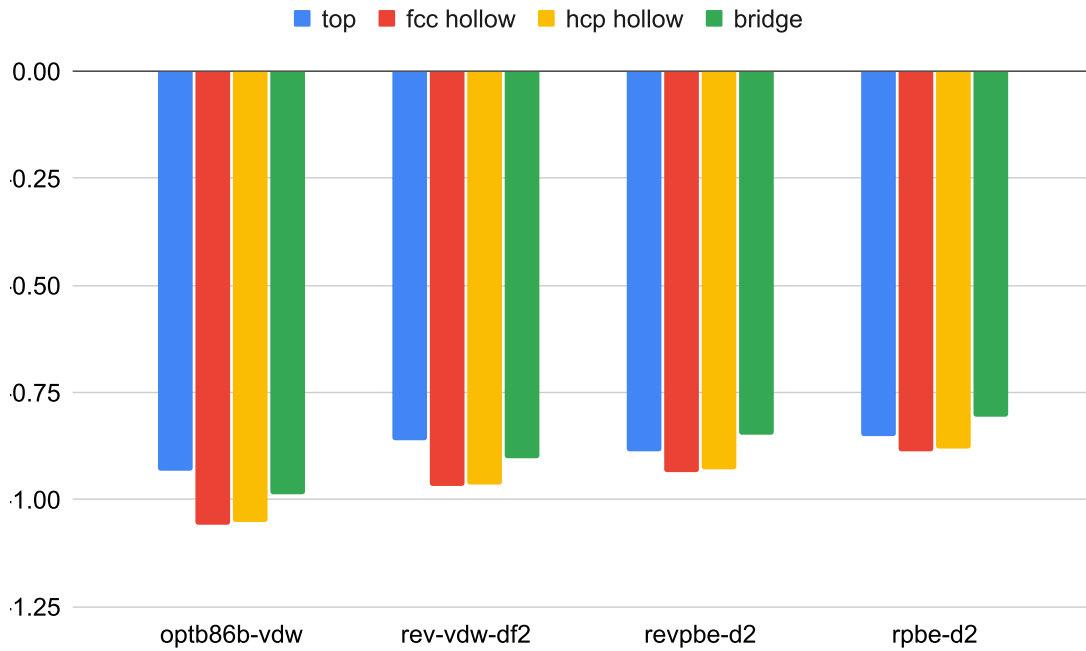
Calculate adsorption energy

- CO on Cu(111)

$$E_{\text{ads}}^{\text{CO}} = E_{\text{tot}}(\text{sys}) - [E_{\text{tot}}(\text{subs}) + E_{\text{tot}}(\text{CO})]$$

CO adsorption energy on Cu(111) surface [eV]

	ontop	fcc hollow	hcp hollow	bridge
optb86b-vdw	-0.93	-1.06	-1.05	-0.99
rev-vdw-df2	-0.86	-0.97	-0.96	-0.90
revpbe-d2	-0.89	-0.94	-0.93	-0.85
rev-vdw-df2	-0.85	-0.89	-0.88	-0.81



For the GGA calculations, the CO adsorption energies are defined as

$$E_{ads}^{CO} = E_{tot}(sys) - [E_{tot}(subs) + E_{tot}(CO)], \quad (1)$$

where $E_{tot}(sys)$, $E_{tot}(subs)$, and $E_{tot}(CO)$ represent the total energies of the adsorbed system, the clean relaxed substrate, and gas phase CO, respectively. The CO adsorption energies obtained from the vdW-DF calculations followed the reported prescriptions to eliminate error due to the "egg-box effect," i.e., the dependence of the total energies on the positions of atoms relative to the fast Fourier transform (FFT) grid points:[30,31]

$$\begin{aligned} E_{ads}^{CO} = {} & E_{tot}^{vdW}(sys) - E_{fix}^{vdW}(subs) - E_{fix}^{vdW}(ads) \\ & + \left[E_{fix}^{GGA}(subs) - E_{tot}^{GGA}(subs)\right] \\ & + \left[E_{fix}^{GGA}(ads) - E_{tot}^{GGA}(ads)\right], \end{aligned} \quad (2)$$

where $E_{tot}^{vdW}(sys)$, $E_{tot}^{GGA}(subs)$, and $E_{tot}^{GGA}(ads)$ represent the total energies of the adsorbed system, the isolated clean substrate, and the gas phase adsorbate, respectively. The $E_{fix}^{GGA/vdW}(subs)$ and $E_{fix}^{GGA/vdW}(ads)$ represent the total energies of the clean substrate and the gas phase adsorbate with their geometries fixed to those in the optimized adsorbed systems. The superscripts "GGA" and "vdW" mean