Find lattice constant

- Find FCC Cu lattice constant
- ASE, ASE-STATE-interface
  - ASE tutorial page: https://wiki.fysik.dtu.dk/ase/tutorials/lattice_constant.html
- Calculated 20 candidates, 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
3.6089 Å	3.6157 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)
```

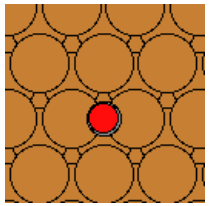
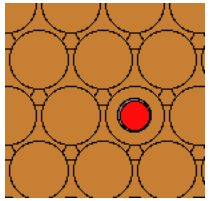
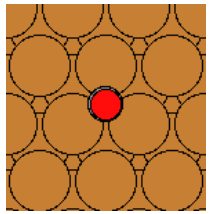
STATE parameters

```
    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'}
                 }
```

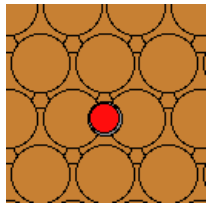
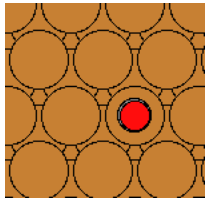
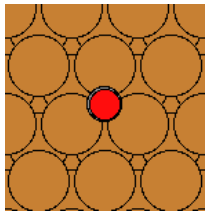
Calculate adsorption energy

- CO on Cu(111)

optb86b-vdw

	bridge	ontop	fcc hollow
			
$E_{abs}(eV)$			
$d_{C-O}(\text{Å})$			
$d_{C_u-C}(\text{Å})$			

rev-vdw-df2

	bridge	ontop	fcc hollow
			
$E_{abs}(eV)$			
$d_{C-O}(\text{Å})$			
$d_{C_u-C}(\text{Å})$			