

Project #1: Maximizing D(0)

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Visual Python Project #1, 2014550025, Sang-Woo Lee

```
## importing
import pybinding as pb
import numpy as np
import matplotlib.pyplot as plt
from math import sqrt, pi
from pybinding.repository import graphene

pb.pltutils.use_style()
%matplotlib inline

plt.rcParams.update({'font.size':16, 'font.family':'serif', 'figure.figsize':[16,9]})
```

Part-(a): Investigate edge effect through nanoribbon model

Purpose: Which edge is better for value of DOS at 0 energy?

How to make the model

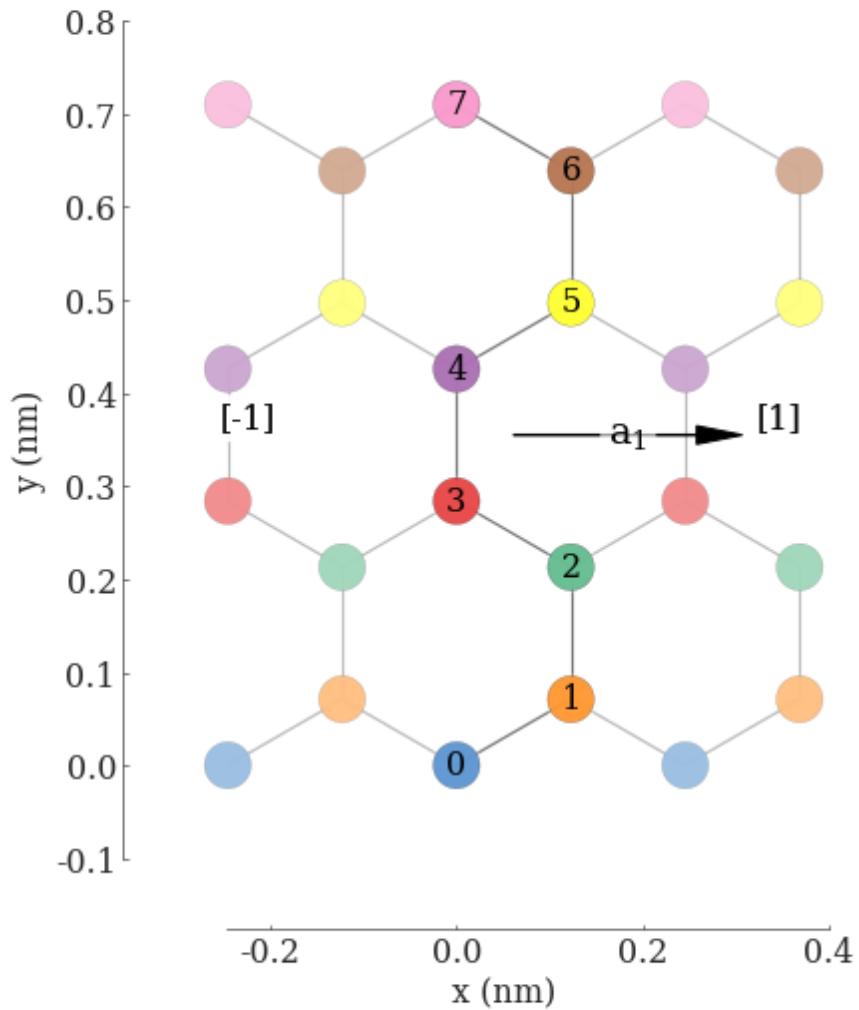
```
#make lattice for the model
def zigzag_nanoribbon():
    #a = 0.24595 # [nm] unit cell length
    #a_cc = 0.142 # [nm] carbon-carbon distance
    d = 0.142 # [nm] carbon-carbon distance
    t = -2.8 # [eV] nearest neighbour hopping

    lat = pb.Lattice(a1=[d*sqrt(3), 0])
    lat.add_sublattices(('0', [0, 0]),
                        ('1', [d*sqrt(3)/2, d/2]),
                        ('2', [d*sqrt(3)/2, d*3/2]),
                        ('3', [0, d*2]),
                        ('4', [0, d*3]),
                        ('5', [d*sqrt(3)/2, d*7/2]),
                        ('6', [d*sqrt(3)/2, d*9/2]),
                        ('7', [0, d*5]))
    )
    lat.add_hoppings(
        # inside the main cell
        ([0, 0], '0', '1', t),
        ([0, 0], '1', '2', t),
        ([0, 0], '2', '3', t),
        ([0, 0], '3', '4', t),
        ([0, 0], '4', '5', t),
        ([0, 0], '5', '6', t),
        ([0, 0], '6', '7', t),
        # between neighboring cells
        ([-1, 0], '0', '1', t),
        ([1, 0], '2', '3', t),
        ([-1, 0], '4', '5', t),
        ([1, 0], '6', '7', t)
    )
    return lat

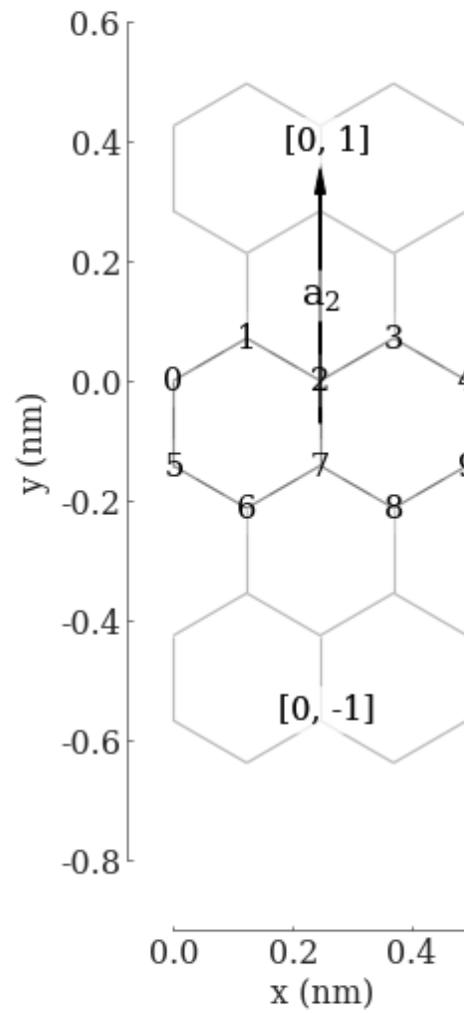
lattice = zigzag_nanoribbon()
lattice.plot()
plt.title('Model system')
```

Models: zigzag and armchair

Model system



Model system



How to calculate

```
#set up the model
model = pb.Model(
    zigzag_nanoribbon(),
    pb.translational_symmetry(a1=True, a2=False)
)
solver = pb.solver.lapack(model)

#Band structure
plt.subplot(131)
bands = solver.calc_bands(-pi/graphene.a, pi/graphene.a) #in the first Brillouin zone
bands.plot()
plt.title('Band structure')

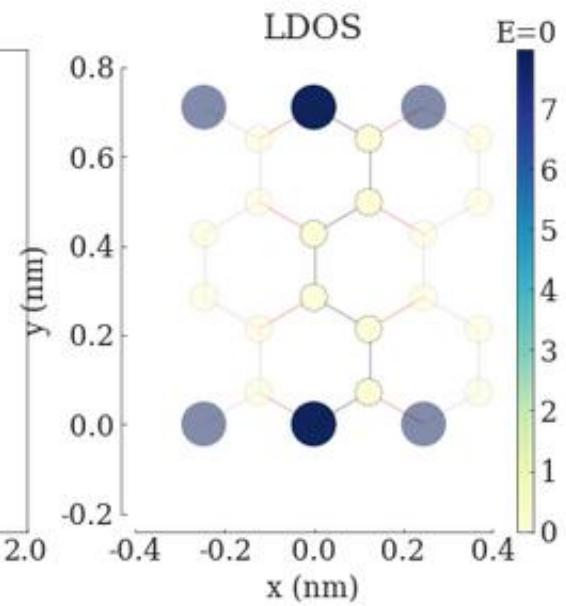
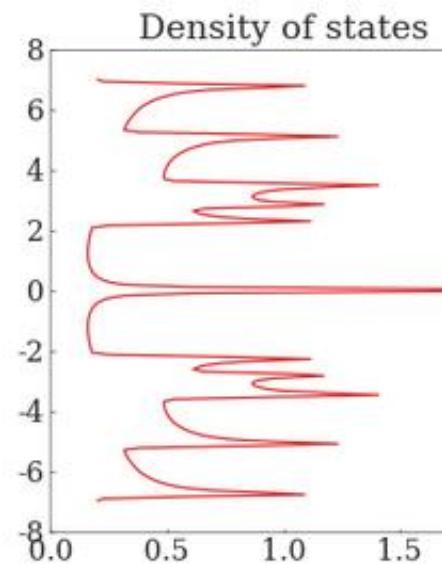
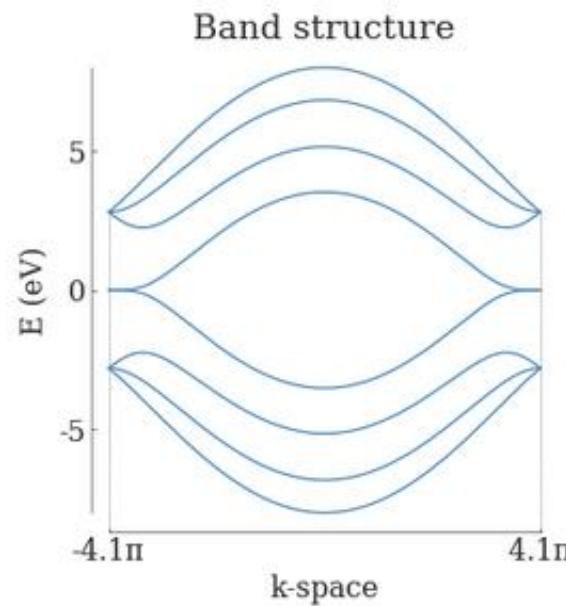
#Average density of states
kx=np.linspace(-pi/(graphene.a), pi/(graphene.a),200)
solver.set_wave_vector([0,0])
lapack_dos = solver.calc_dos(np.linspace(-7, 7, 200), broadening=0.05)
data1=lapack_dos.data
for i in range(0,200):
    solver = pb.solver.lapack(model)
    solver.set_wave_vector([kx[i],0])
    lapack_dos = solver.calc_dos(np.linspace(-7, 7, 200), broadening=0.05)
    data1+=lapack_dos.data
data1=data1/200
plt.subplot(132)
plt.plot(data1, np.linspace(-7, 7, 200)) # To switch the x and y axis
plt.title('Density of states')
print('Value of dos at 0 energy',data1[100])

#Local density of states
plt.subplot(133)
reference_energy=0
ldos_map = solver.calc_spatial_ldos(energy=reference_energy, broadening=0.05) # [eV]
ldos_map.plot()
pb=pltutils.colorbar(label='E=%d'%reference_energy)
plt.title('LDOS')
```

Zigzag

Value of dos at 0 energy 1.7422411608371775

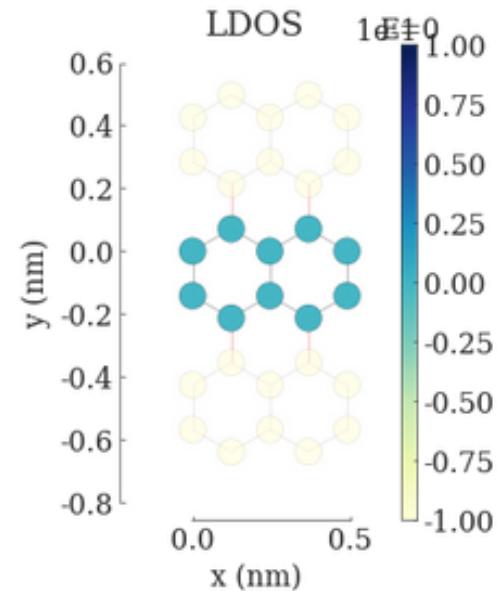
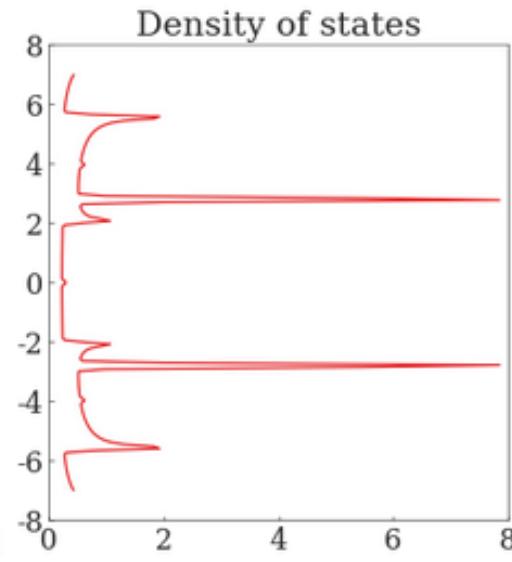
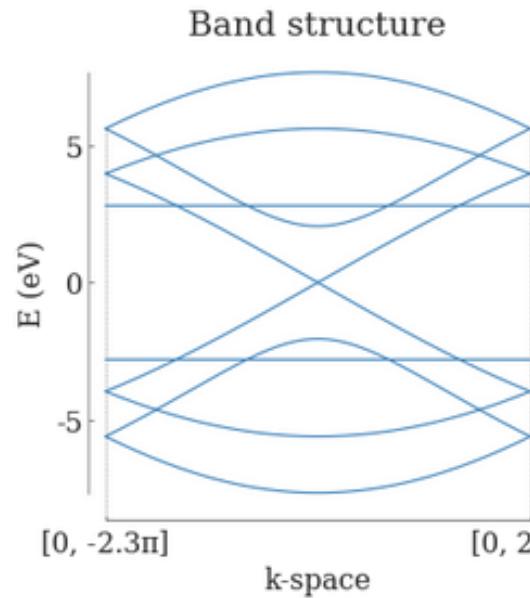
Text(0.5, 1.0, 'LDOS')



Armchair

Value of dos at 0 energy 0.28853516506295024

Text(0.5, 1.0, 'LDOS')



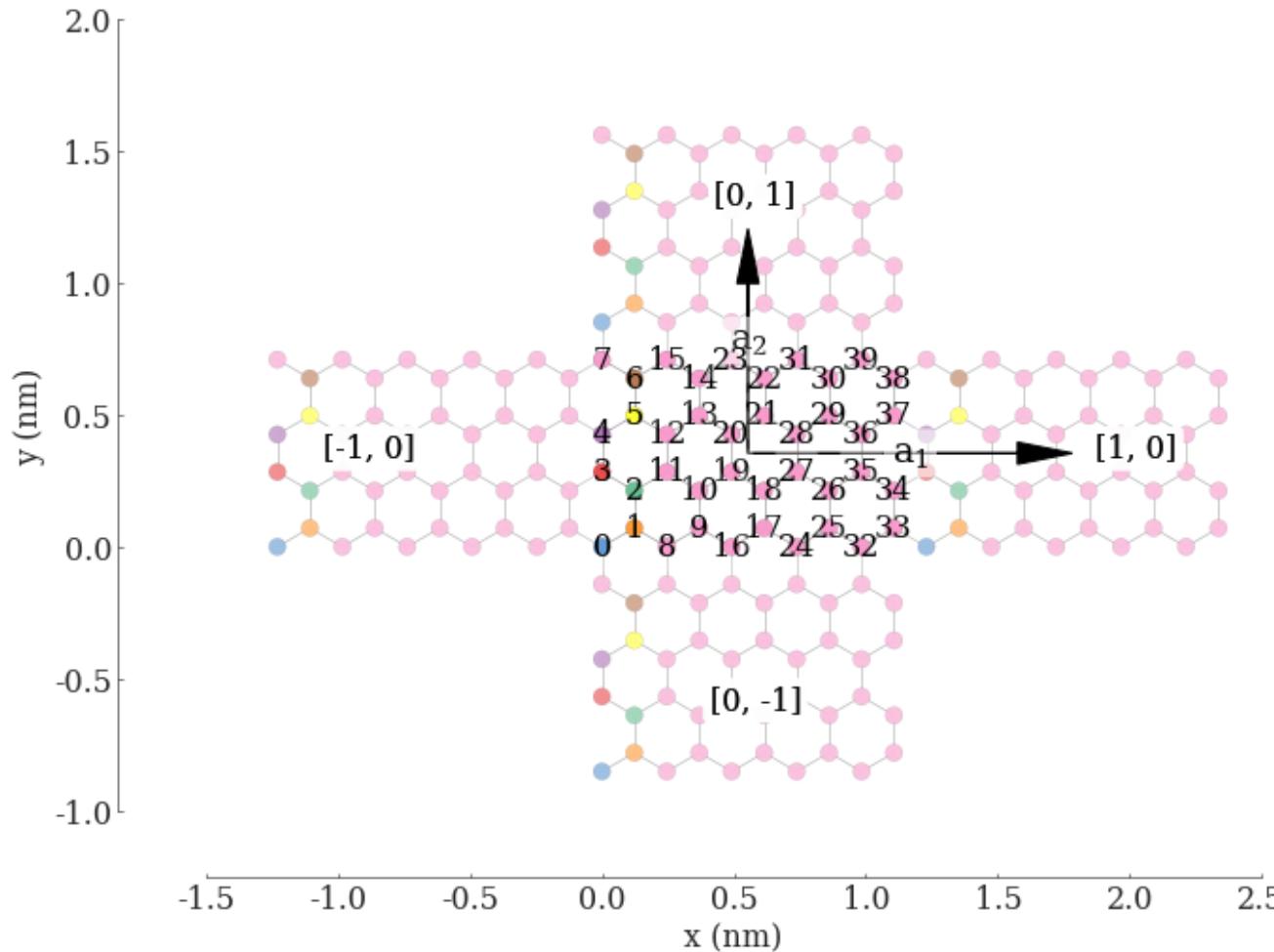
Conclusion of (a) :

The zigzag edge bring larger value of DOS at 0 energy than the armchair edge

How about Graphene sheet?

Part-(b): DOS for graphene sheet through unit cell model.

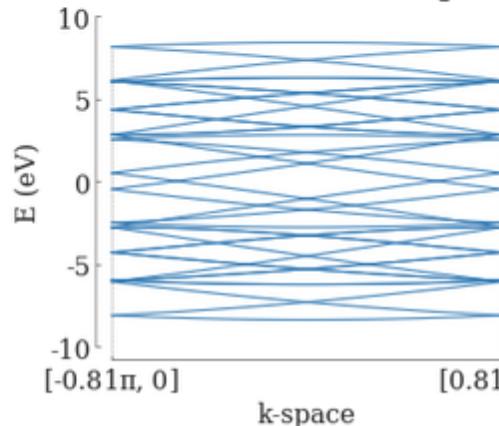
Purpose: Which model is better for value of DOS at 0 energy?



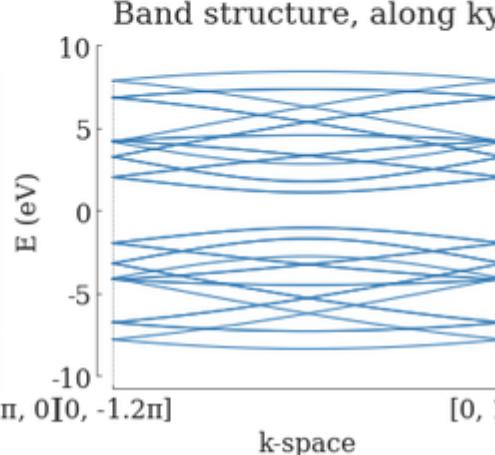
Pristine Graphene

Value of dos at 0 energy $8.829815120240424e-54$

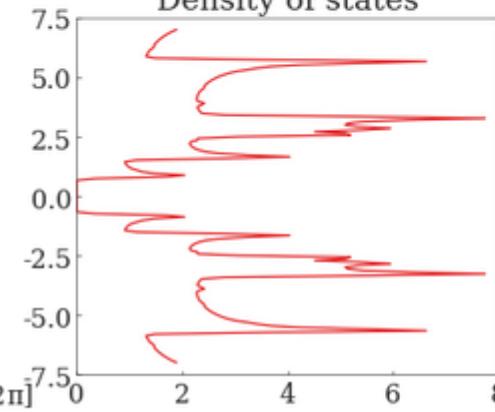
Band structure, along kx



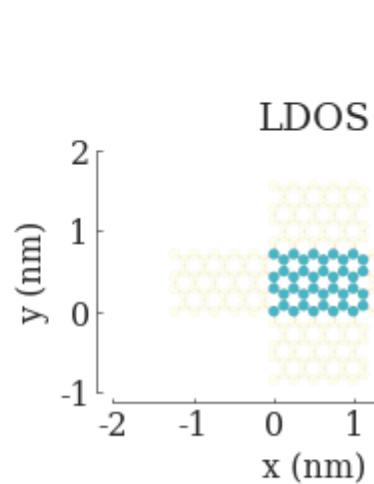
Band structure, along ky



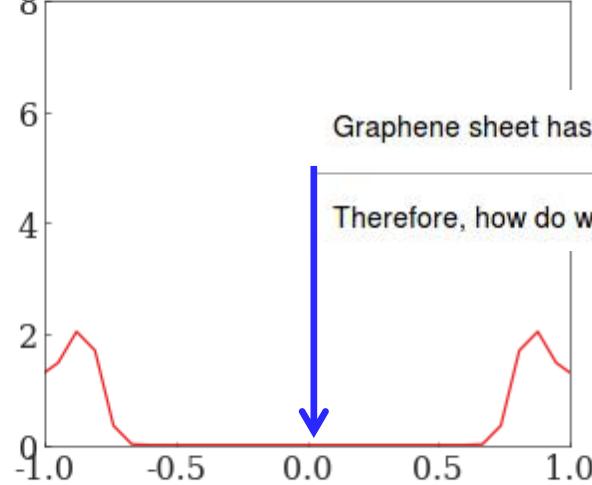
Density of states



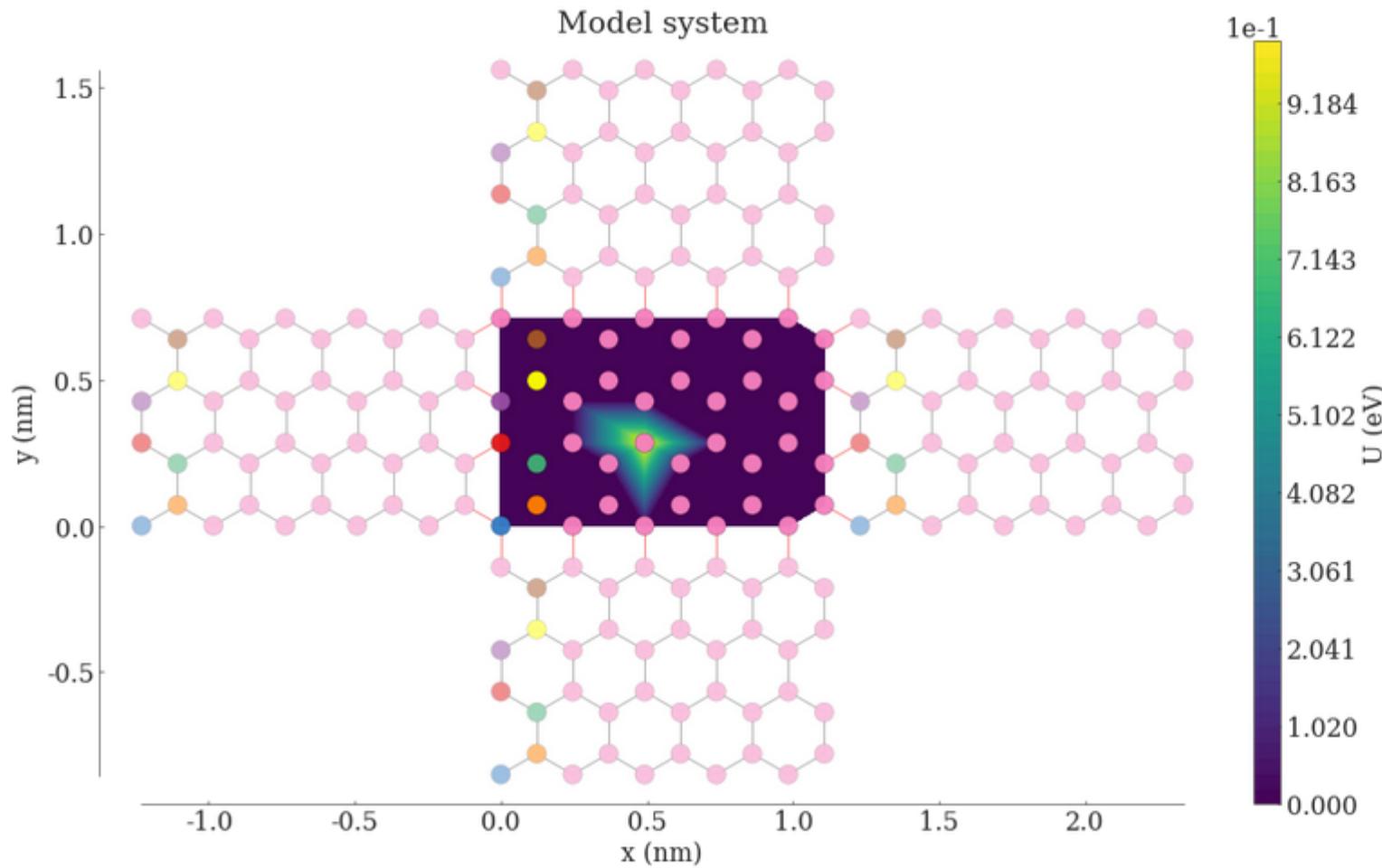
(-1, 1)



Density of states near 0 energy

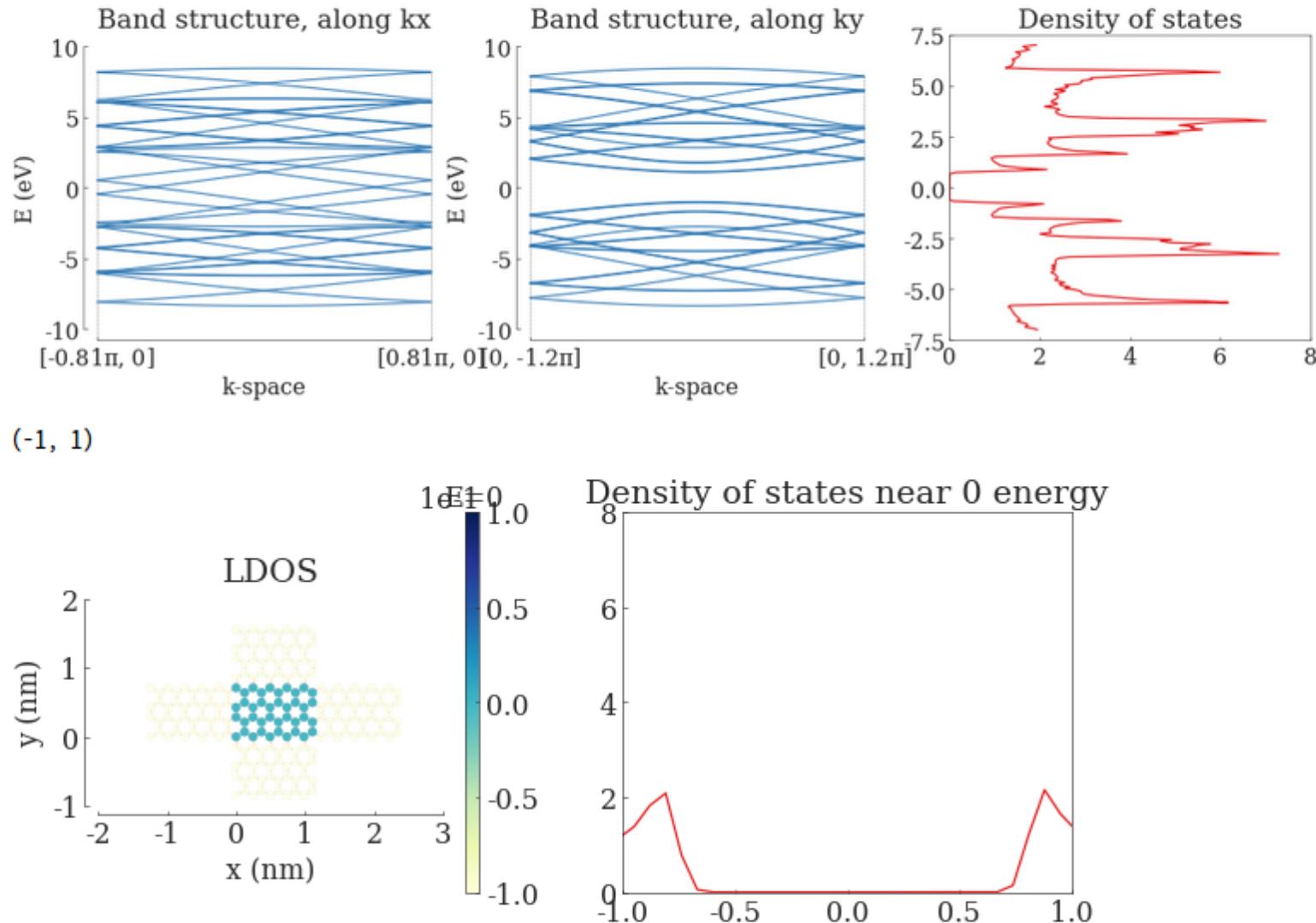


Addition or Substitution



Addition or Substitution

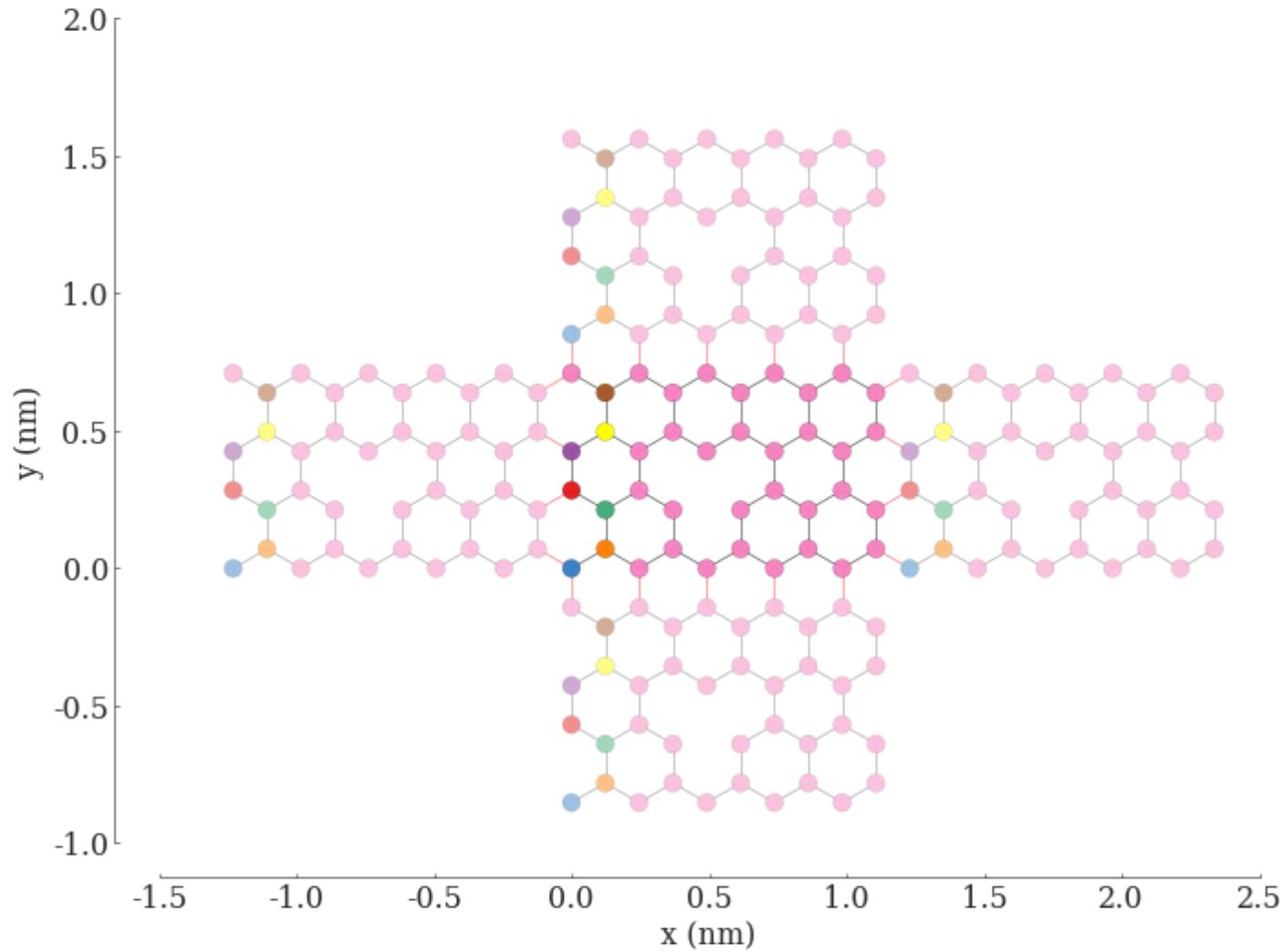
Value of dos at 0 energy 5.832706209386134e-57



By adding or substituting, the value is not changed well, in fact.

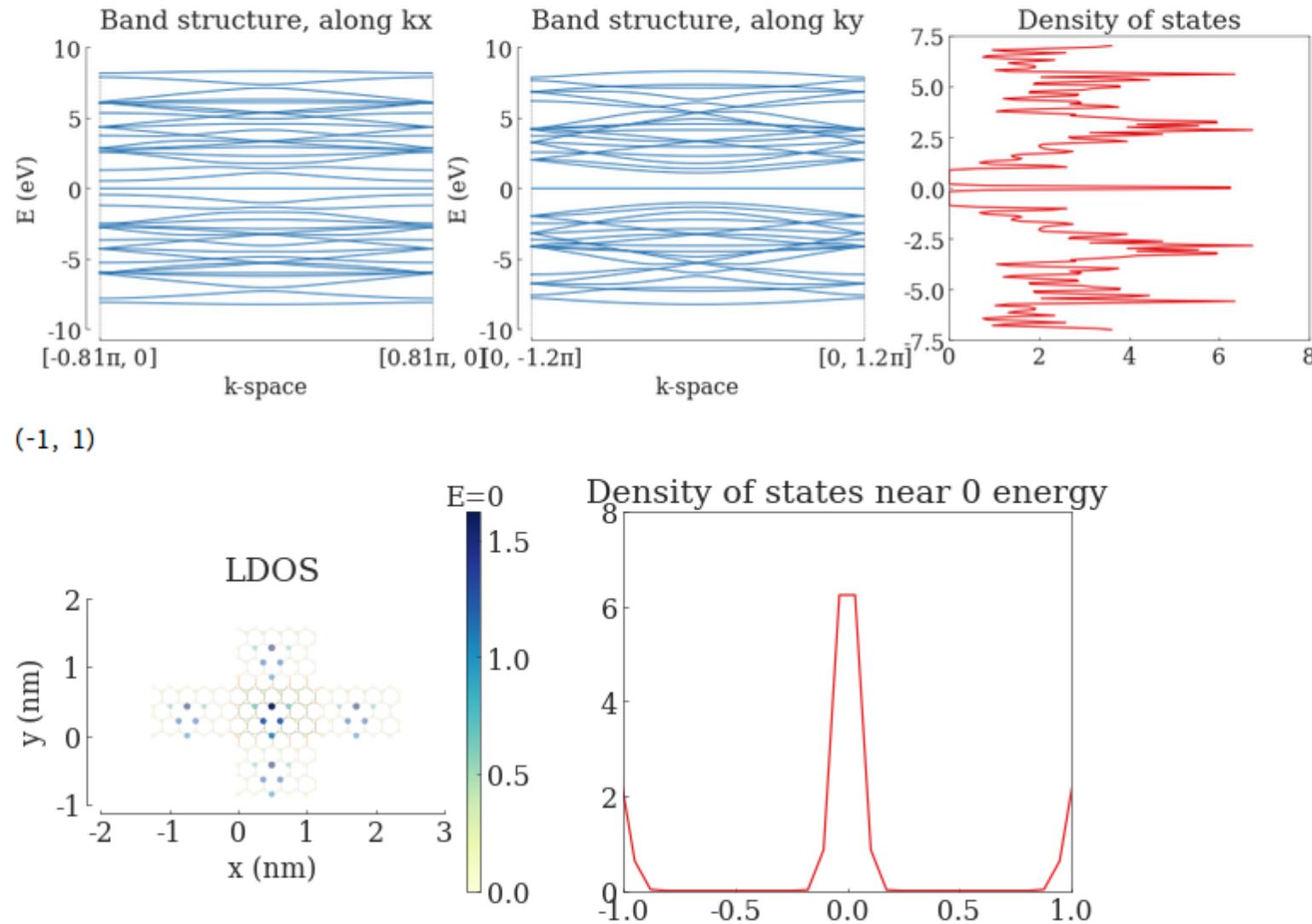
Make a vacancy

Model system



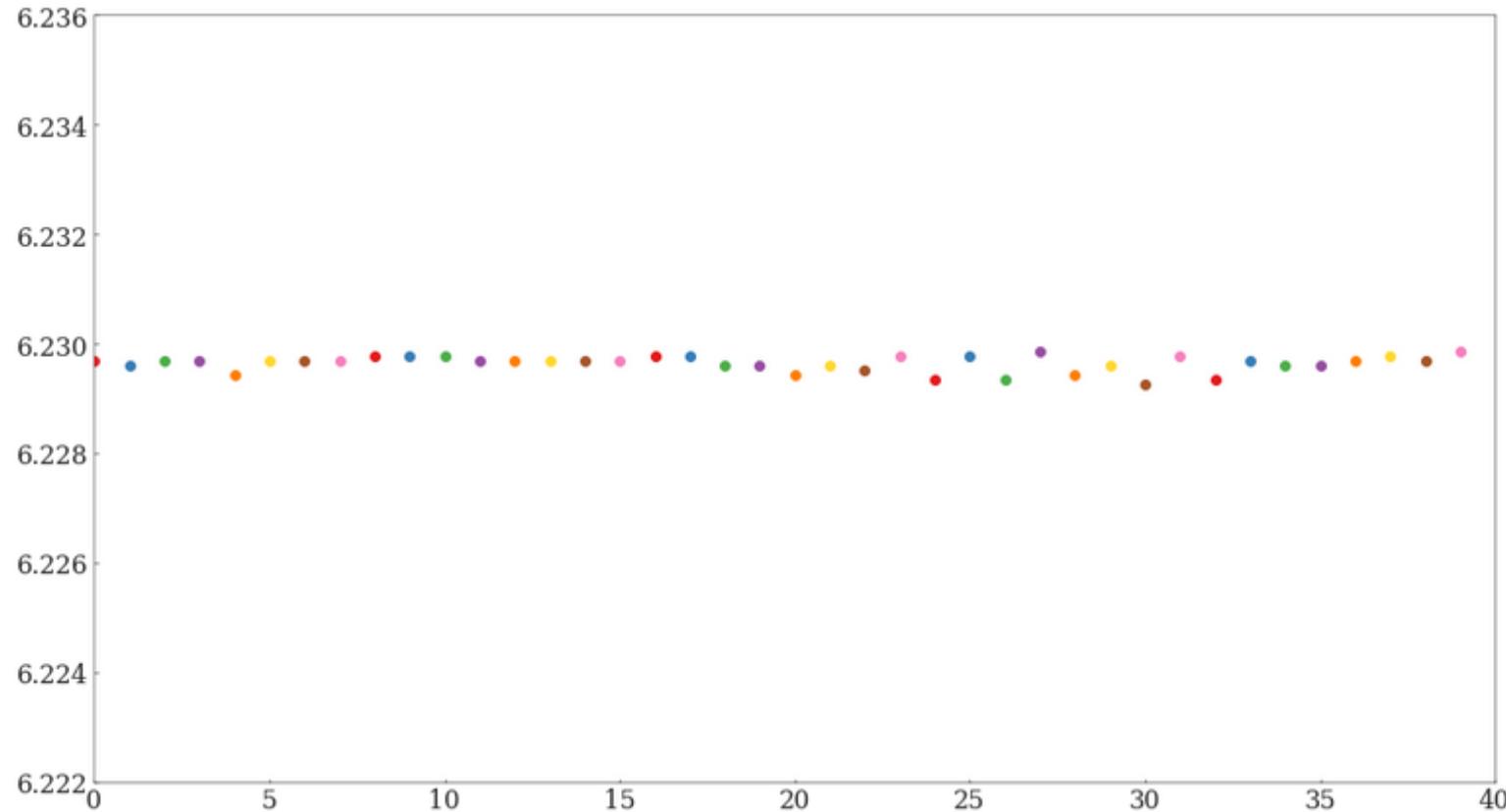
Value of dos at 0 energy 6.245272217194619

Make a vacancy



By making a vacancy, the value is changed significantly.

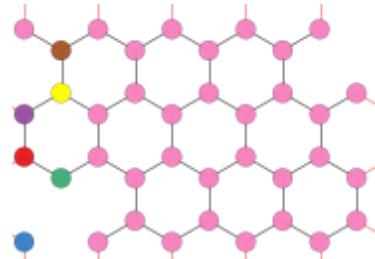
Dependence on the specific site



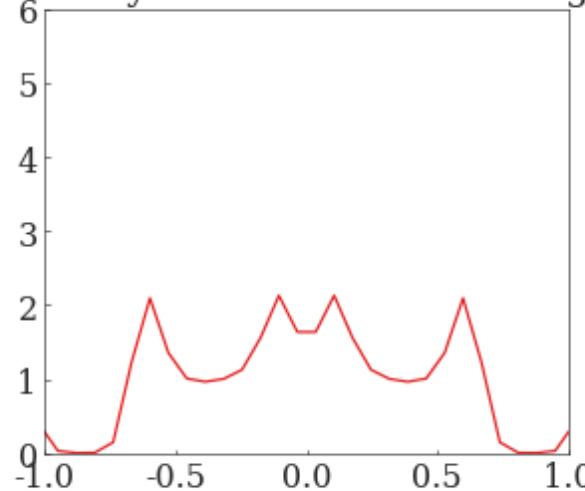
For making only one vacancy, the specific site does not matter.

Make two vacancies

Sites 1, 38

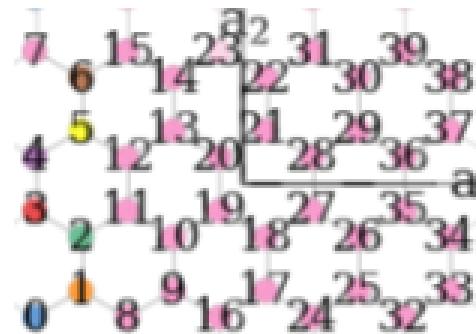


Density of states near 0 energy

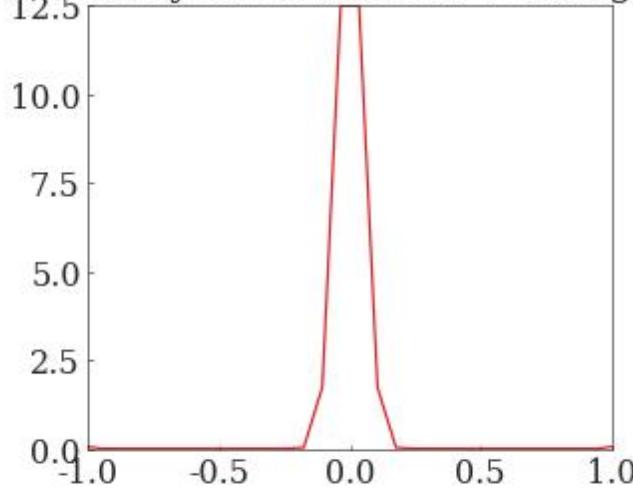


The value at 0 : 1.638

Sites 1, 37



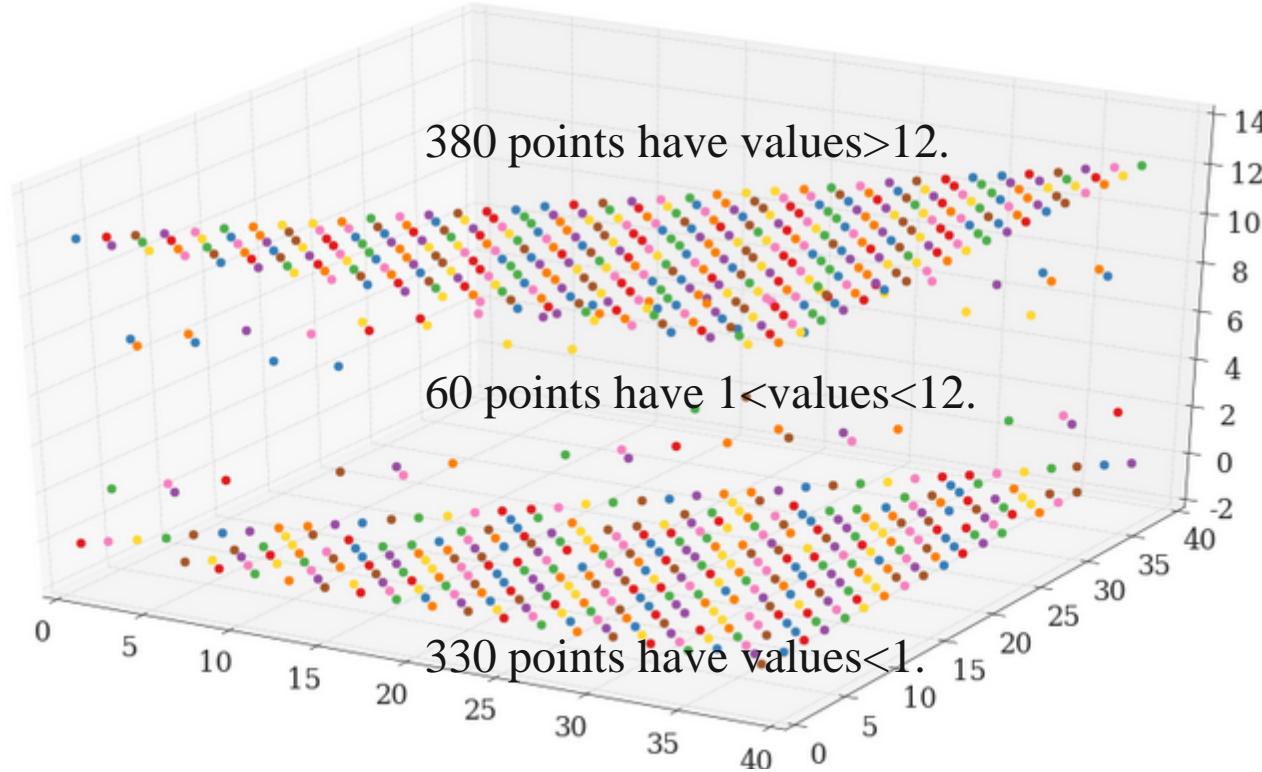
Density of states near 0 energy



The value at 0 : 12.50

In case of this, even if the selection is slightly different,
a huge difference is can be obtained!

Dependence on the specific site combination



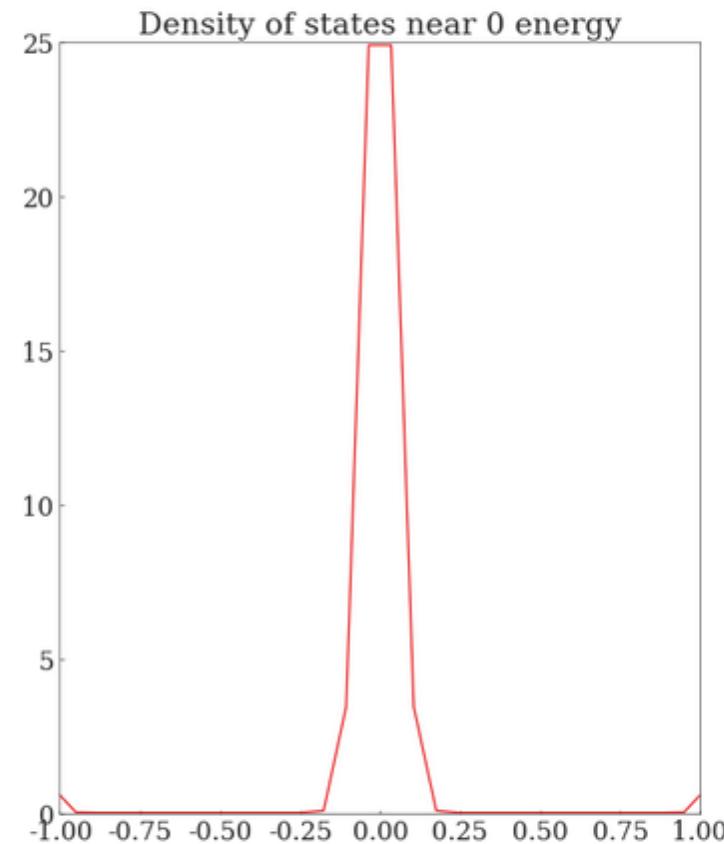
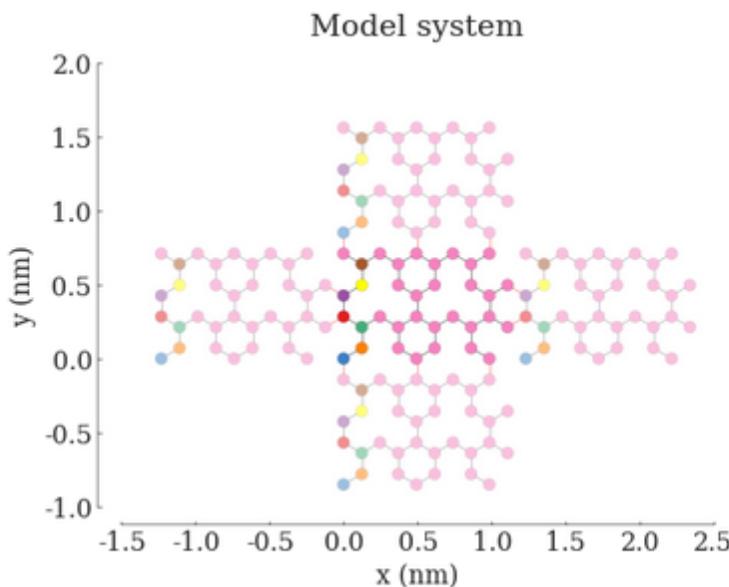
{2: 38, 4: 36, 6: 34, 8: 32, 10: 30, 12: 28, 14: 26, 16: 24, 18: 22, 20: 20, 22: 18, 24: 16, 26: 14, 28: 12, 30: 10, 32: 8, 34: 6, 36: 4, 38: 2}

dict_keys([2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38])

The maximizing condition is that the number of connections between given points is an even number. In terms of Network theory(or Graph theory), the number of links of path between given nodes is an even number!

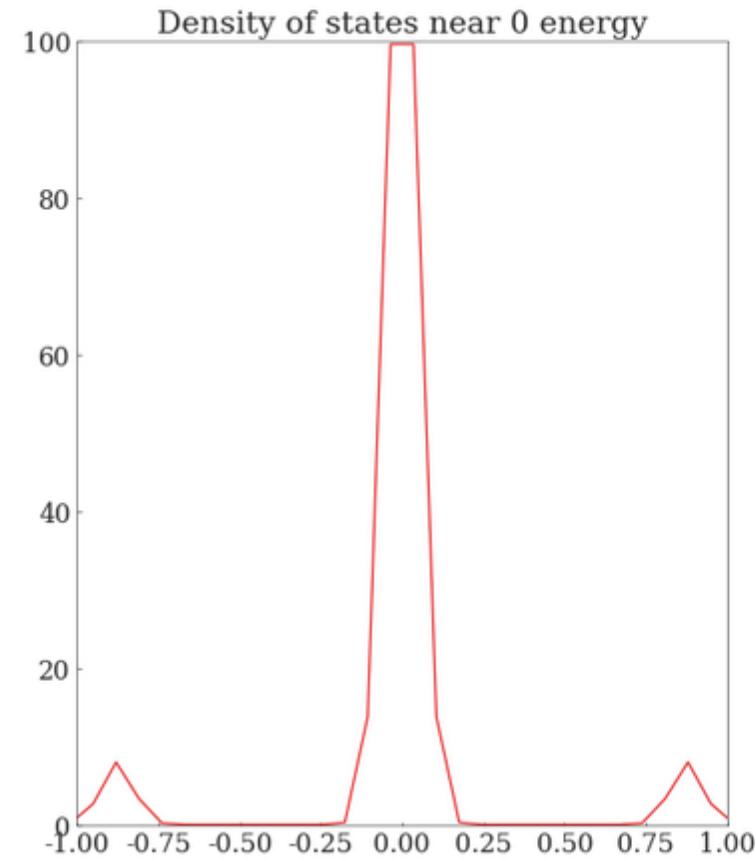
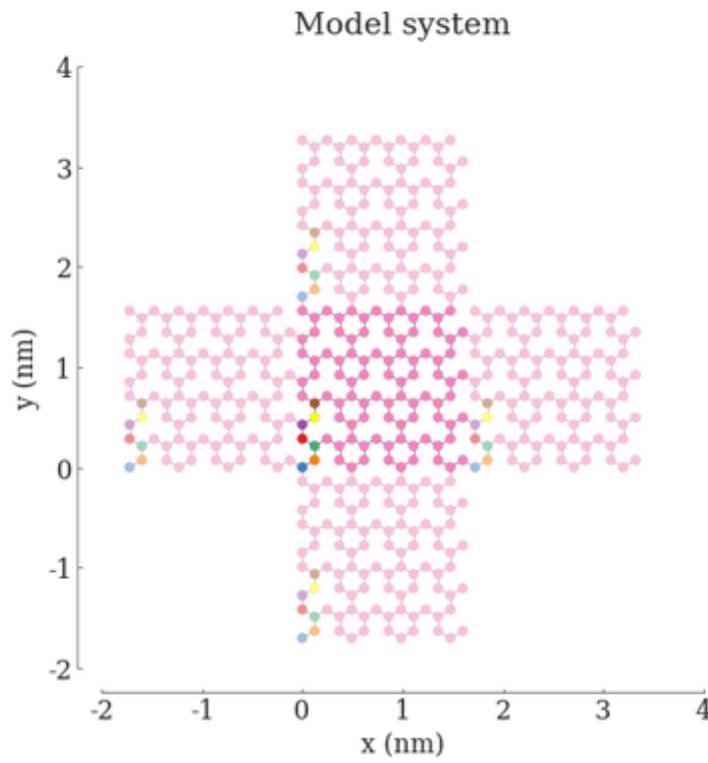
Conclusion of (b) & Sugestion unit cell defect distribution:

By adding hydrogen atom or substituting by nitrogen atom, the value is not changed, in fact. The value is changed significantly by making vacancies. More vacancies are not always better. There is specific the maximizing rule that the number of links between given nodes is an even number.



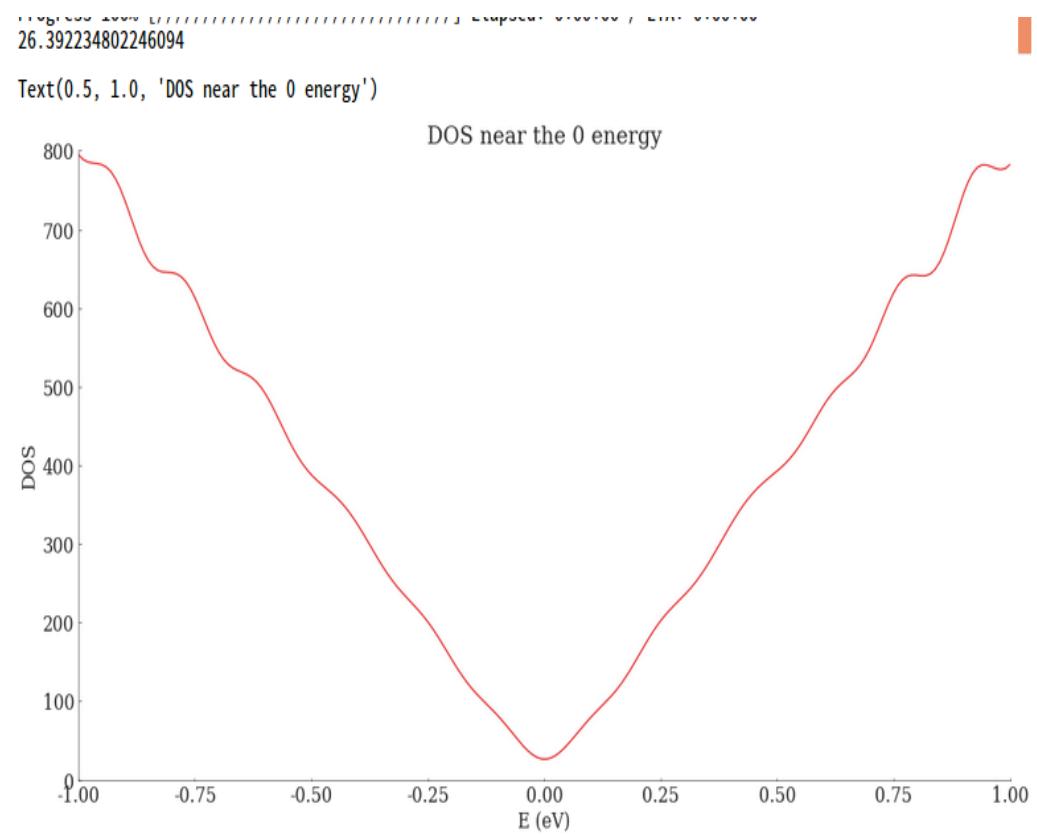
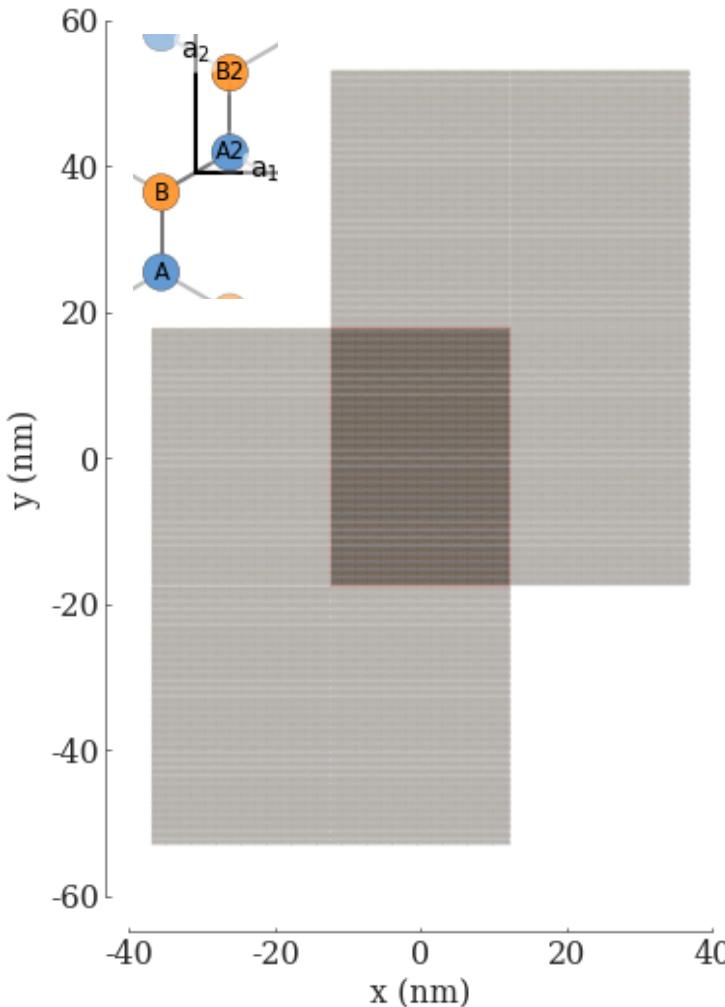
Valid for larger unit cell model

Value of dos at 0 energy 99.67460722744867



Part-(c): DOS for graphene sheet through large cell model.

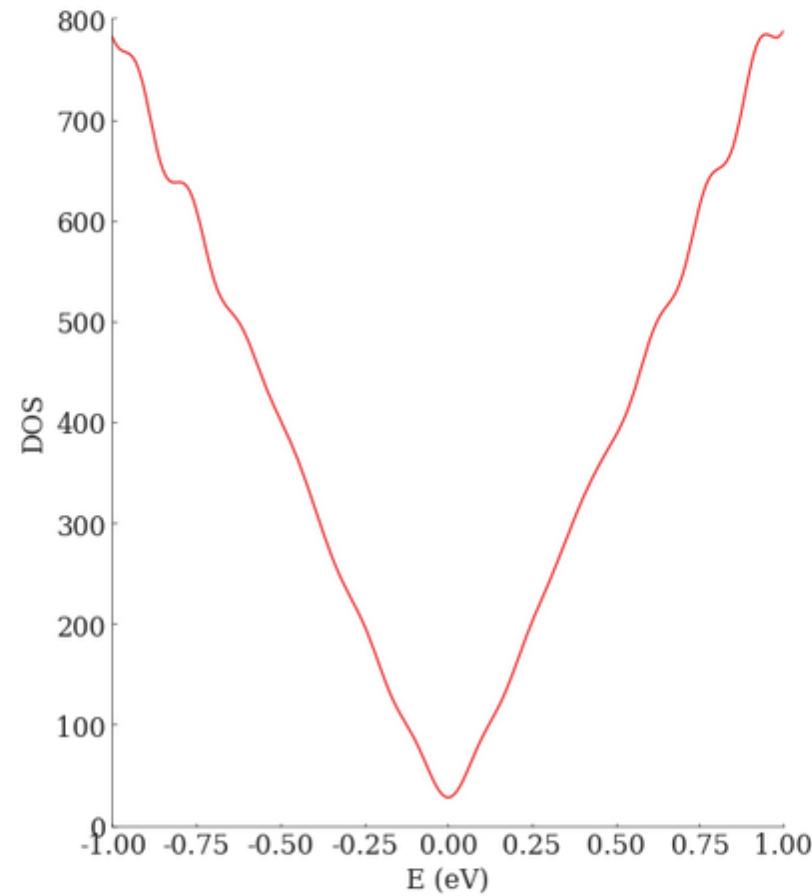
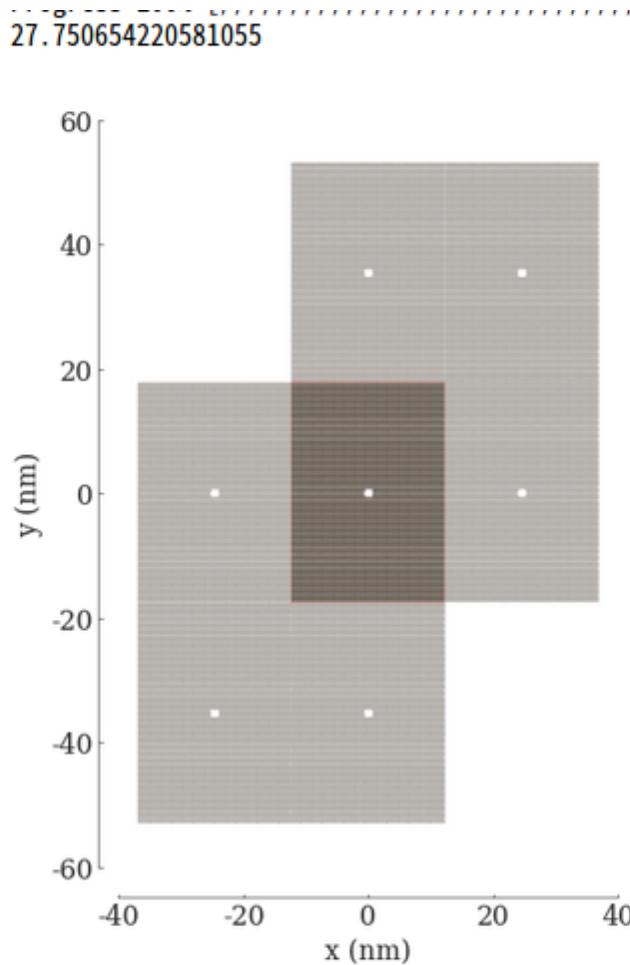
Model system



Of course, the value is extremely small

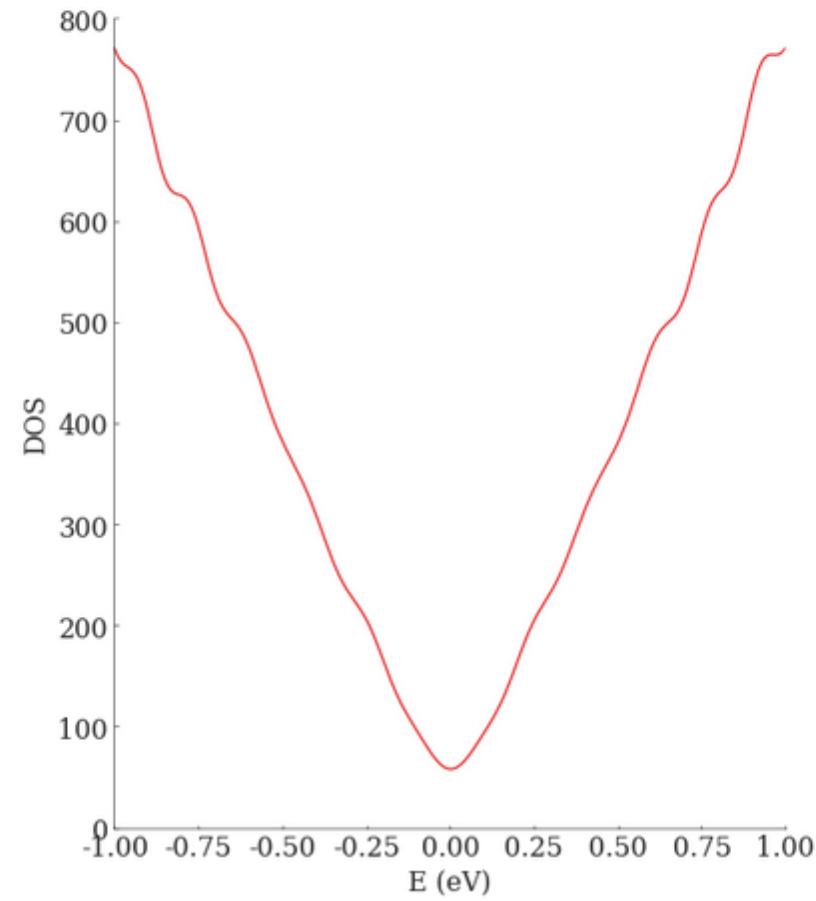
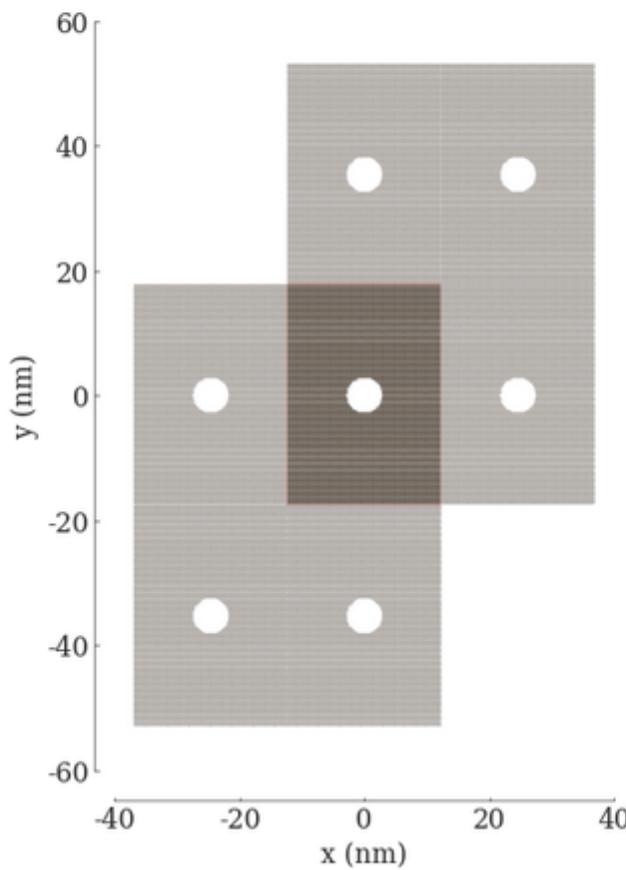
Hole defect

27.750654220581055



Hole defect

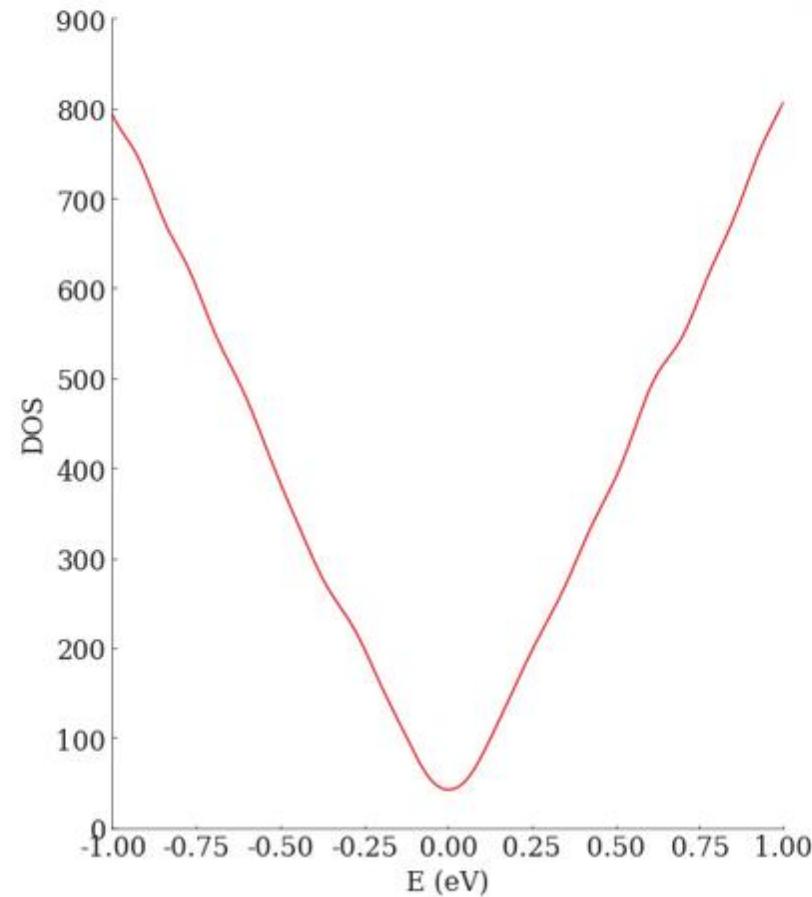
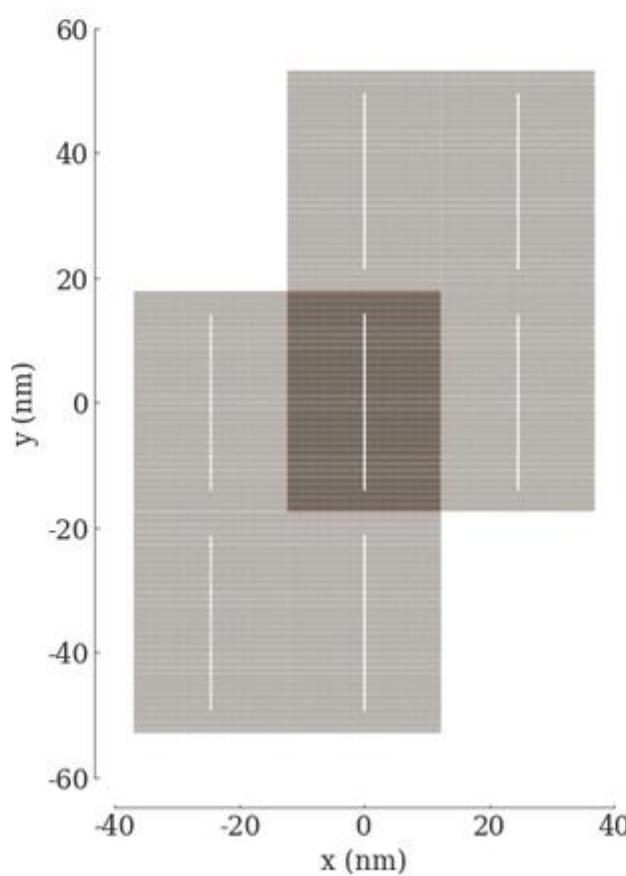
57.86277389526367



The larger hole is better, ordinary.

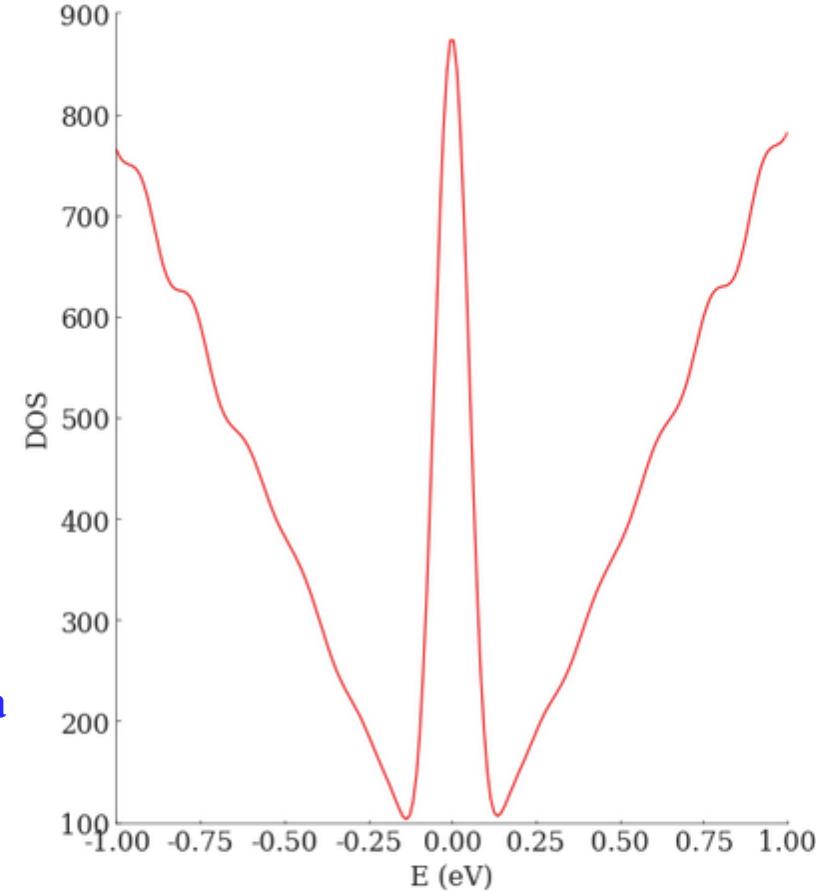
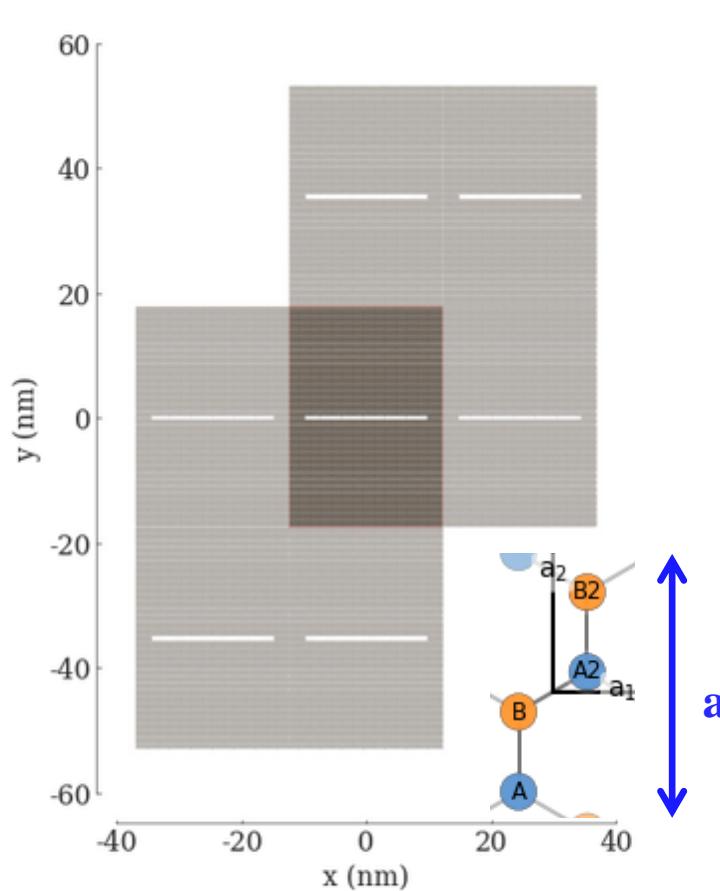
Line defect-vertical

42.07976531982422



The vertical line defect is not good.

Line defect-horizontal

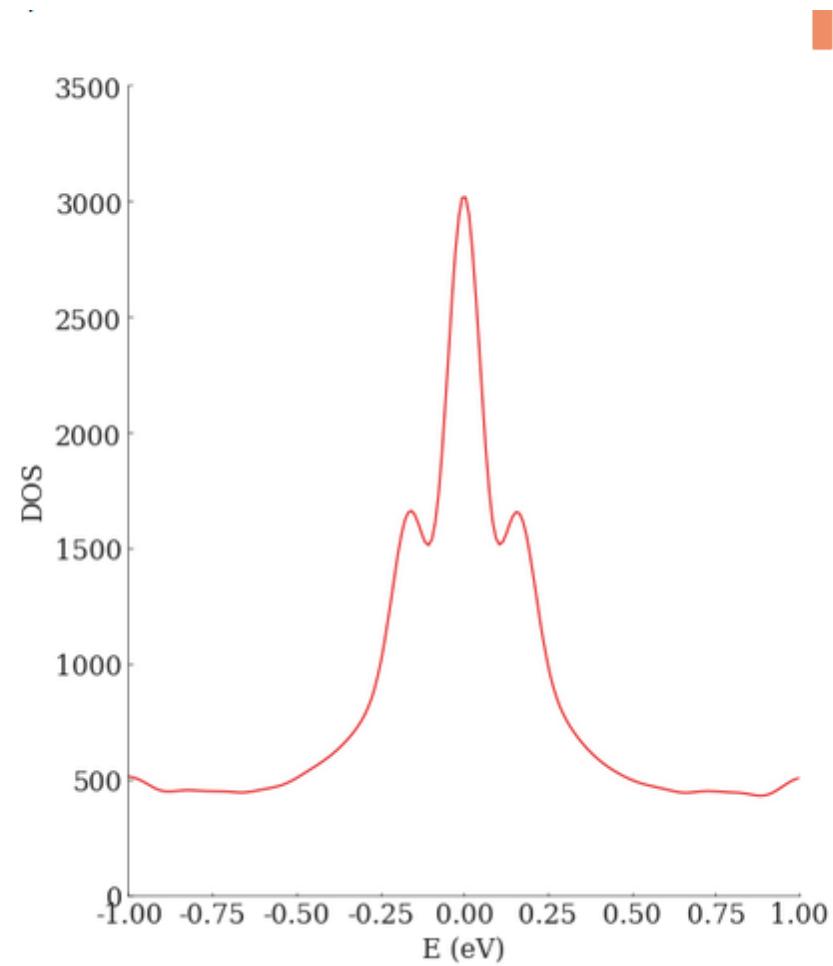
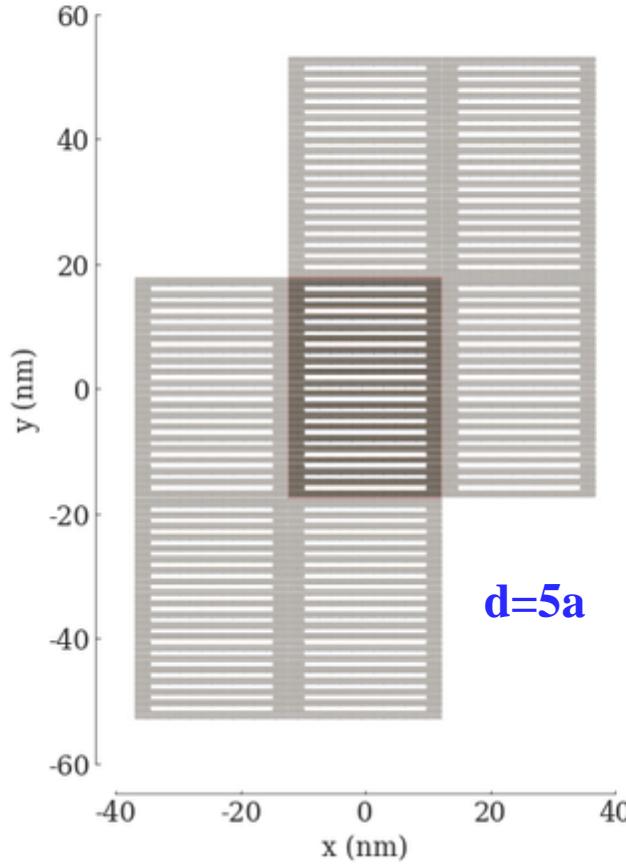


The horizontal line defect is so good!

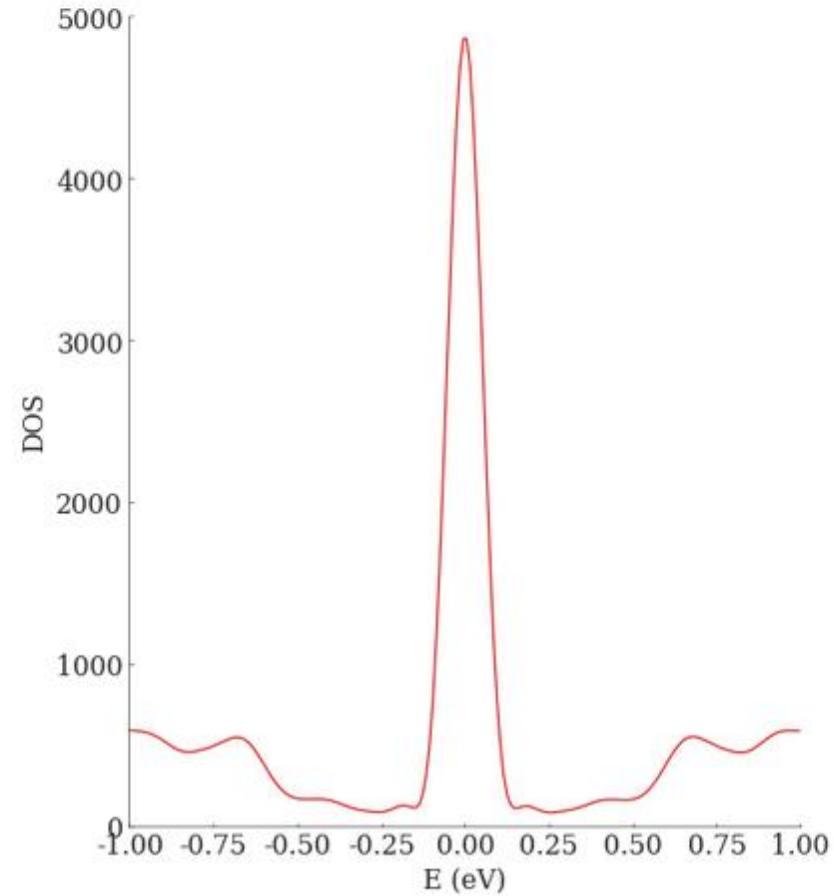
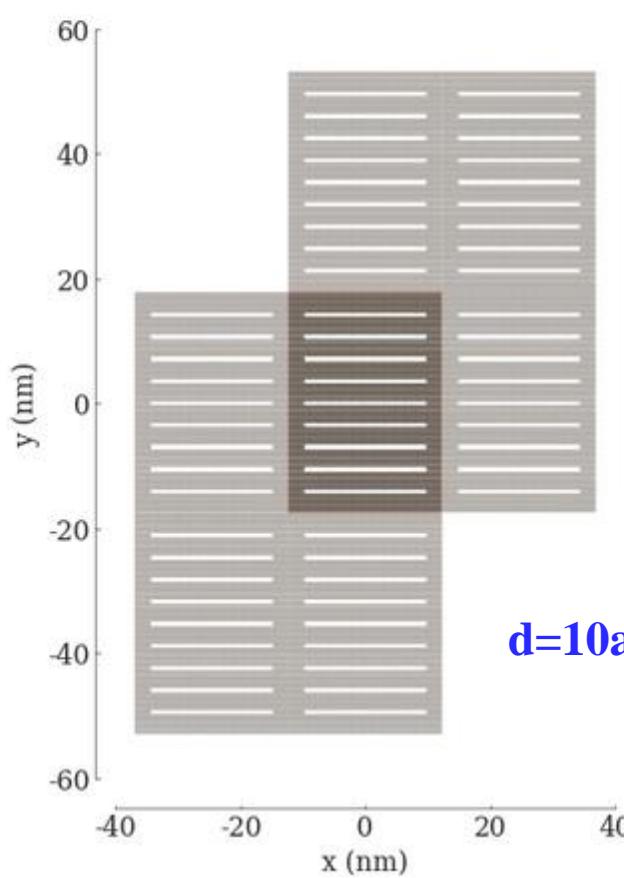
This result is explained by the fact that getted at part(a). The zigzag edge is very effective, so the horizontal shape has large value at 0.

Many line defects

3016.600341796875



Many line defects

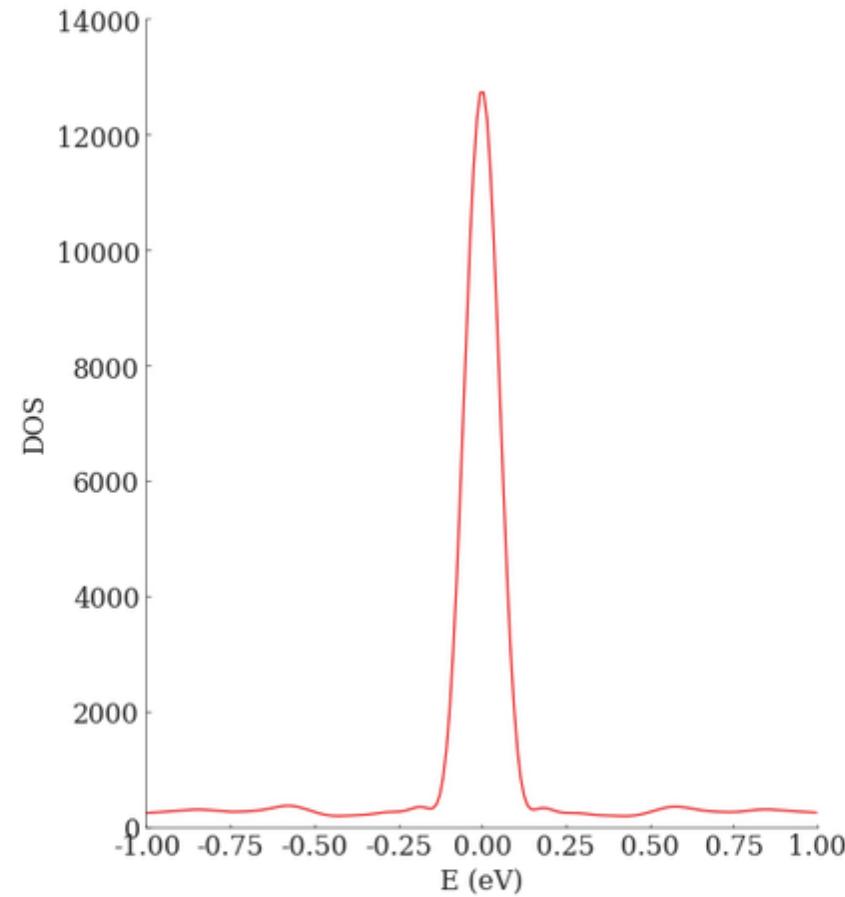
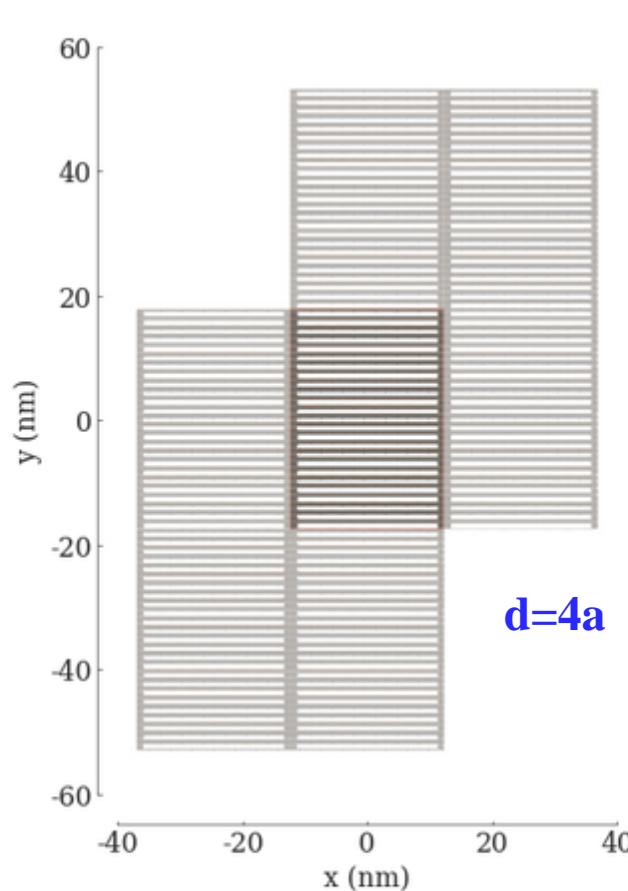


However, many horizon lines are not always good. This case has smaller lines than above case, but has the larger value.

This result is explained by the fact that getted at part(b). The spacing between lines should be even times of cell size!

Conclusion: My final ideal model for maximizing value of DOS at 0 energy

12729.0263671875



This model has very large value at 0!

Thanks