

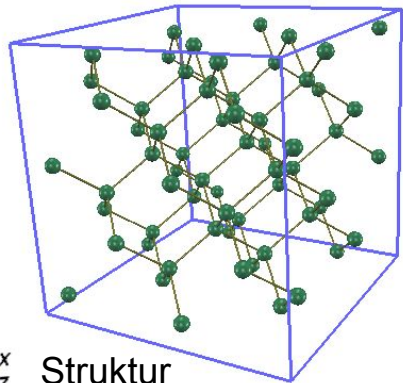
Struktur Elektronik: Silicon (3D) & Silicene (2D)

Zohan Syah Fatomi

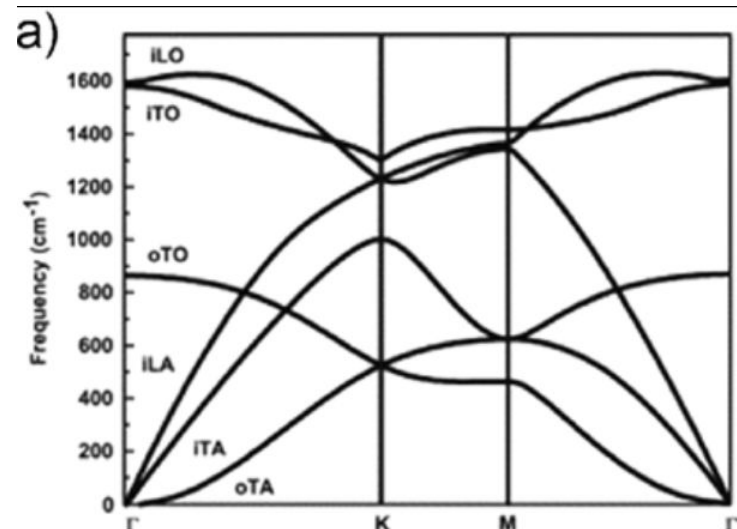
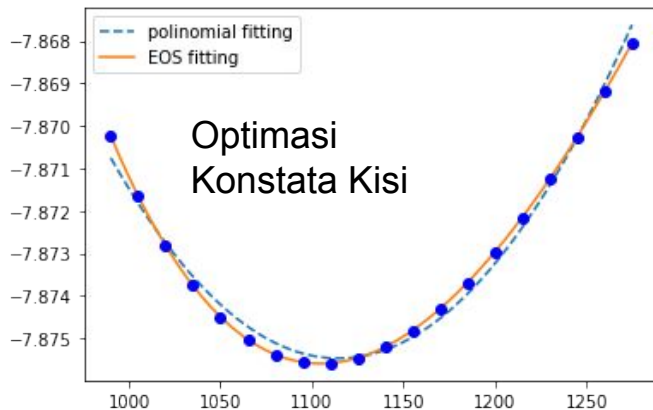


Jurusan Fisika
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Jenderal Soedirman

Rekayasa Komputasi Material



Struktur kristal

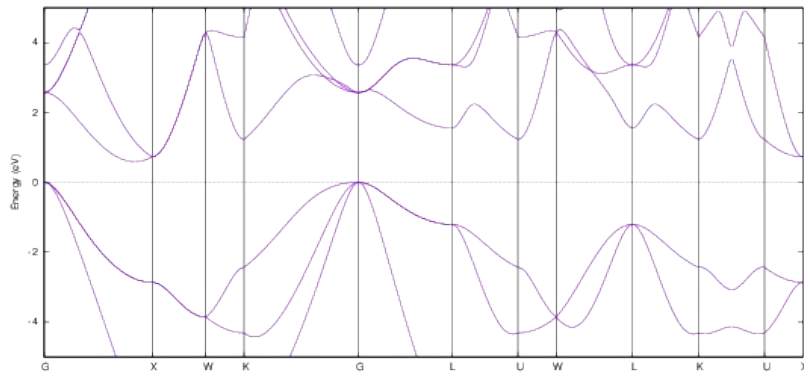


Sifat vibrasi
(phonon dispersion)

**Density Functional
Theory (DFT) +
Komputasi Numerik
+ Komputer**

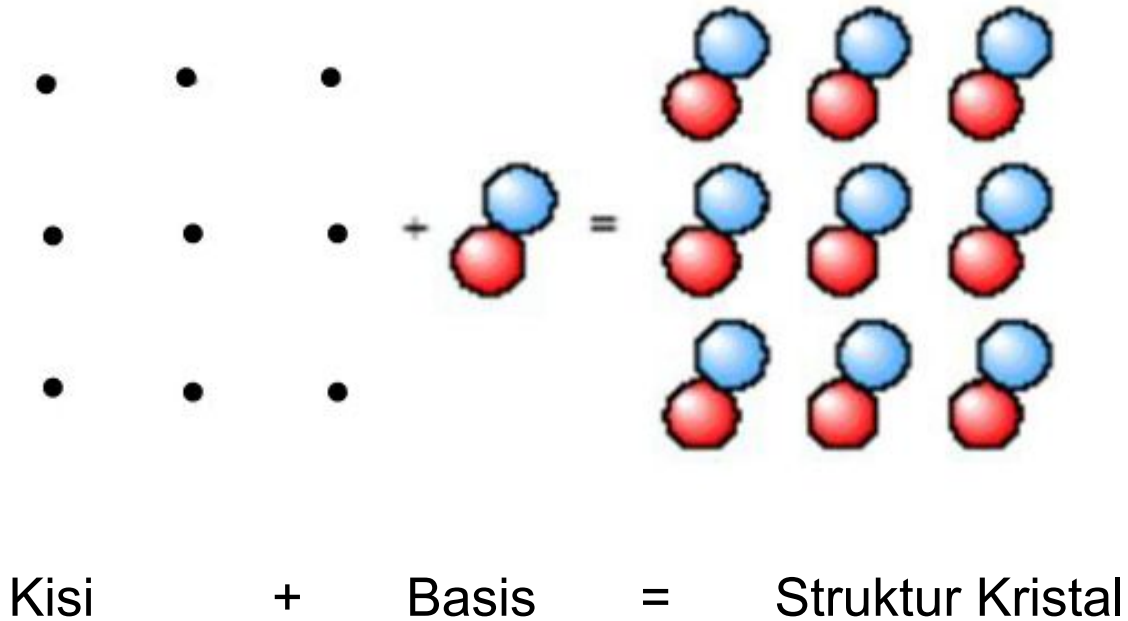
Input:
Koordinat atomik

Output:
Sifat elektronik,
Optik, Magnetik,
dlsb

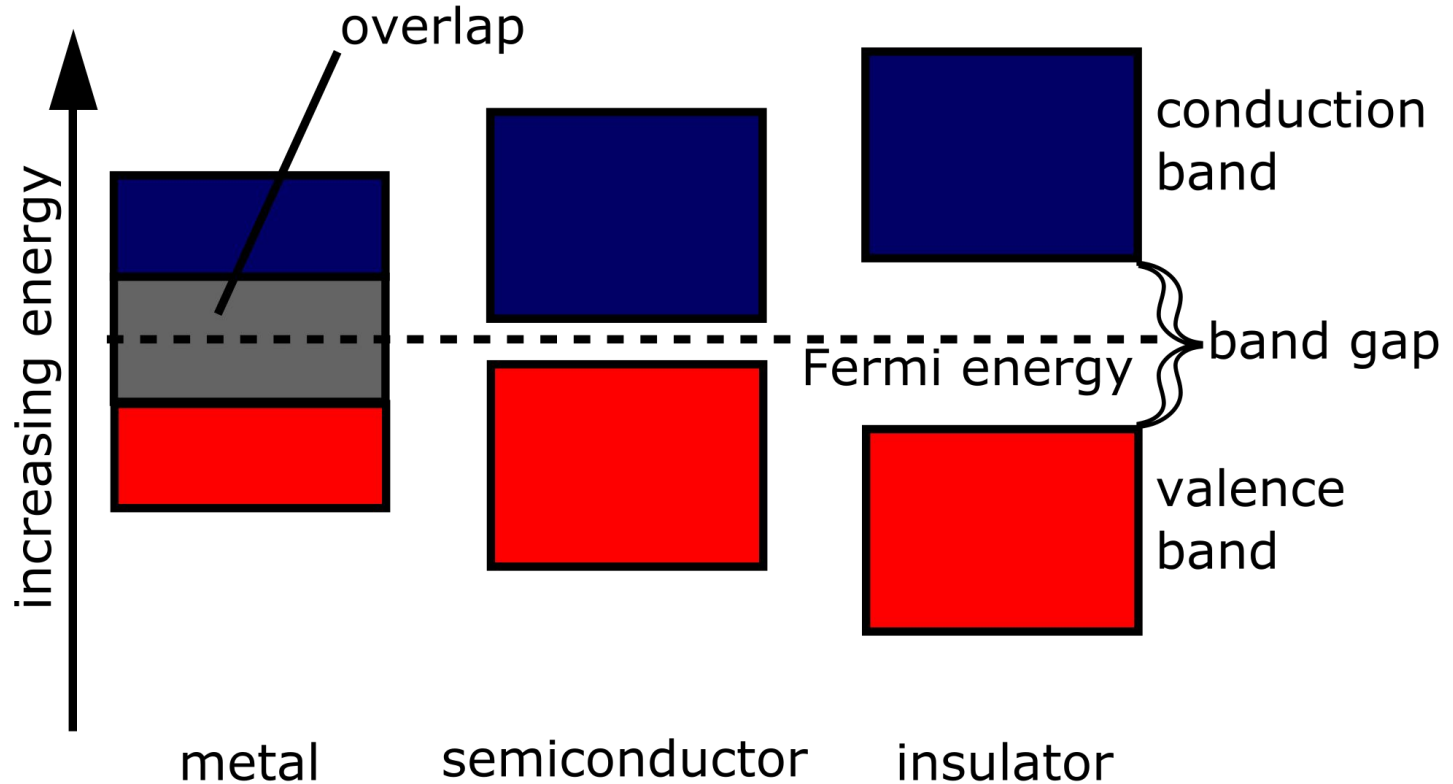


Struktur elektronik

Sistem Kristal



Struktur Band



Sifat Elektronik pada Material

Berdasarkan kemagnetannya material dibedakan menjadi 3:

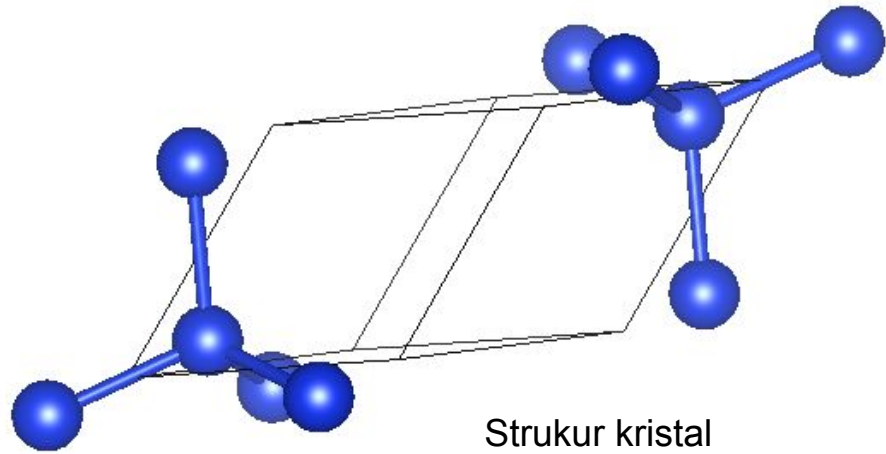
1. **Konduktor** : *conduction band & valence band* tumpang tindih (*overlap*).
Contoh: besi (Fe), tembaga (Cu) dll.
2. **Semikonduktor** : memiliki band gap sedang (0.1 - 4.0 eV).
Contoh: Silicon, Germanium dll.
3. **Isolator** : memiliki band gap besar (> 4.0 eV)
Contoh: Diamond, kaca

Silicone (3D)

Struktur kristal unit sel Si (3D) adalah diamond FCC.

**Berapa atom
Atom Si di unit
sel?**

**Berapa lattice
constant pada
Si?**



Struktur kristal primitiv Silicon

$$a_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$a_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

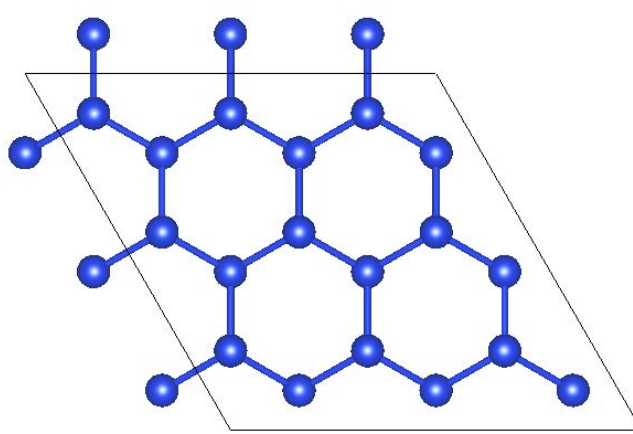
$$a_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

Silicene (2D)

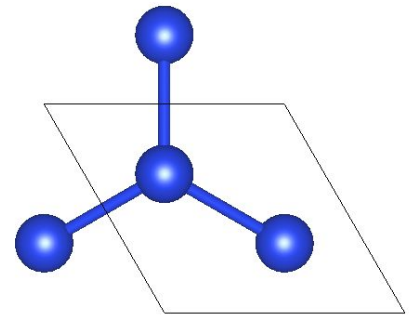
Struktur kristal unit sel Si (3D) adalah diamond FCC.

Berapa atom Atom Si di unit sel?

Berapa lattice constant pada Silicene?



Super sel 3x3x1
silicene

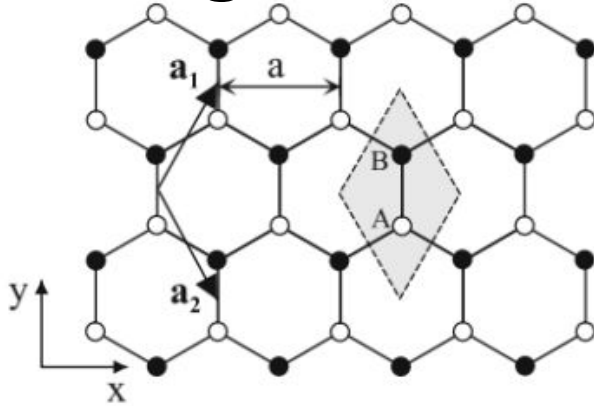


Struktur kristal primitif silicene

$$\vec{b}_1 = a_0(1.\vec{x} + 0.\vec{y})$$

$$\vec{b}_2 = a_0\left(-\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y}\right)$$

Hexagonal Lattice Structure



Primitive Lattice Vector I

$$\vec{a}_1 = a_0 \left(\frac{1}{2} \vec{x} + \frac{\sqrt{3}}{2} \vec{y} \right)$$

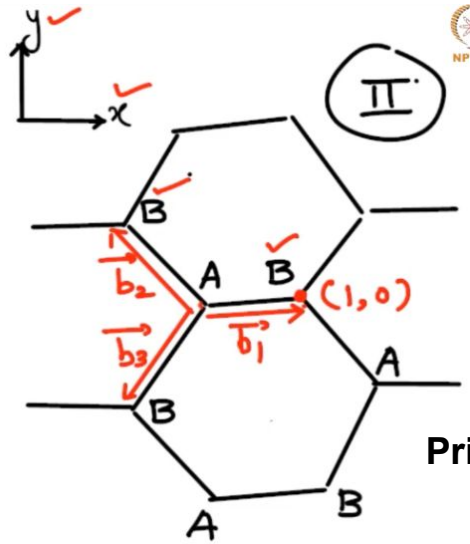
$$\vec{a}_2 = a_0 \left(\frac{1}{2} \vec{x} - \frac{\sqrt{3}}{2} \vec{y} \right)$$

a_0 = konstanta kisi graphene

Primitive Lattice Vector II

$$\vec{b}_1 = a_0 (1 \cdot \vec{x} + 0 \cdot \vec{y})$$

$$\vec{b}_2 = a_0 \left(-\frac{1}{2} \vec{x} + \frac{\sqrt{3}}{2} \vec{y} \right)$$



Primitive Unit Cell Graphene

Kalkulasi DFT PHASE0

Untuk melakukan kalkulasi DFT pada PHASE0 dibutuhkan 3 file utama:

1. **Filenames.data** -> deklarasi penamaan file.
2. **Input.data** -> konfigurasi perhitungan dan sistem kristal
3. **Pseudopotential.data** -> file pseudo potential

Silahkan download kode pada url berikut!

<https://github.com/zohansyahfatomi/struktur-elektronik>

filenames.data

```
Open  ▾  📄  ~/1_Research/0_UNSOED_Research  
1 &fnames  
2 F_INP = './nfinp.data'  
3 F_POT(1) = 'Si_ggapbe_nc_01.pp'  
4 F_DYNM = './nfdynm.data'  
5 F_ENF = './nfefn.data'  
6 F_CHR = './nfchr.cube'  
7 F_WANNIER = './nfwannier.cube'  
8 F_WFk = './nfwfk.cube'
```

filenames.data digunakan untuk mengidentifikasi file **input** dan **pseudopotential**.

Ubah nama file pada **F_POT(1)** dengan nama **Pseudopotential** yang sesuai (**Si_ggapbe_nc_01.pp**)

nfnp.data

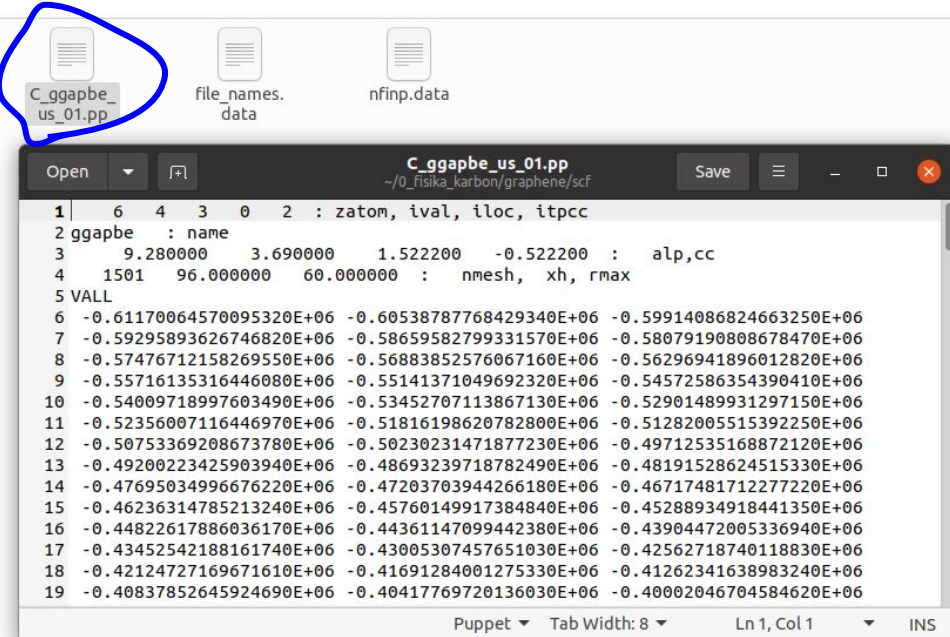
```
1 Control{
2     cpumax = 3600 sec
3     condition = Initial
4 }
5 accuracy{
6     cutoff_wf = 25.00 rydberg
7     cutoff_cd = 225.00 rydberg
8     num_bands = 16
9     ksampling{
10         mesh{
11             nx = 2
12             ny = 2
13             nz = 1
14         }
15     }
16 }
17 structure{
18     unit_cell_type = primitive
19     unit_cell{
20         a_vector = 4.6646320985 0.00 0.00
21         b_vector = -2.3323160493 4.0396898966 0.00
22         c_vector = 0.00 0.00 18.895488655
23     }
24     atom_list{
25         atoms{
26             #tag element rx ry rz mobile
27             C 0.66666667 0.33333333 0.0 1
28             C 0.33333333 0.66666667 0.0 1
29         }
30     }
31     element_list{
32         #tag element atomicnumber mass zeta deviation
33         C 6 21894.5796 0.0 1.83
34     }
35 }
```

Block **Control**: mengatur **kondisi** kalkulasi (maksimal waktu kalkulasi, jenis kalkulasi dlsb)

Block **Accuracy**: mengatur **akurasi** kalkulasi (energi cut-off, jumlah band, jumlah kpoint dlsb)

Block **Structure**: pengaturan **konfigurasi** struktur kristal, apakah kristal itu **Silicon**, **Silicene** dlsb, tergantung konfigurasi pada block tsb.

File pseudopotential



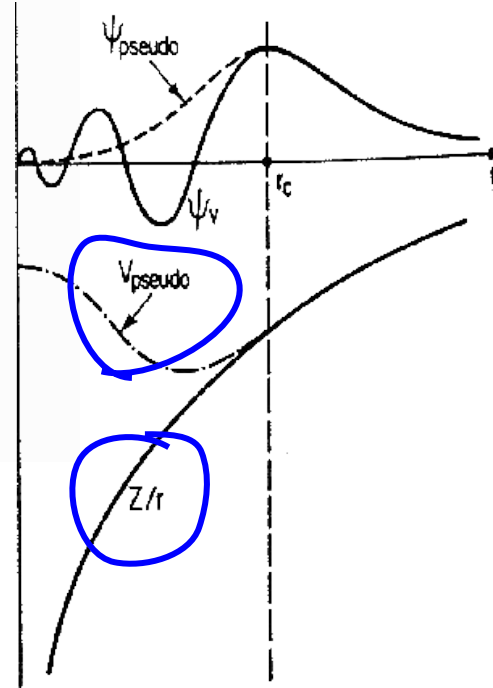
The image shows a file manager window with three files: 'C_ggapbe_us_01.pp' (circled in blue), 'file_names.data', and 'nfinp.data'. Below it is a text editor window titled 'C_ggapbe_us_01.pp' showing the contents of the pseudopotential file. The file contains a header section with parameters like 'name', 'zatom', 'ival', 'iloc', 'itpc', 'name', 'alp', 'cc', 'nmesh', 'xh', 'rmax', and 'VALL'. The main body of the file consists of a large table of numerical values representing the pseudopotential.

```
1 6 4 3 0 2 : zatom, ival, iloc, itpc
2 ggapbe : name
3 9.280000 3.690000 1.522200 -0.522200 : alp, cc
4 1501 96.000000 60.000000 : nmesh, xh, rmax
5 VALL
6 -0.61170064570095320E+06 -0.60538787768429340E+06 -0.59914086824663250E+06
7 -0.59295893626746820E+06 -0.58659582799331570E+06 -0.58079190808678470E+06
8 -0.57476712158269550E+06 -0.56883852576067160E+06 -0.56296941896012820E+06
9 -0.55716135316446080E+06 -0.55141371049692320E+06 -0.54572586354390410E+06
10 -0.54009718997603490E+06 -0.53452707113867130E+06 -0.52901489931297150E+06
11 -0.52356007116446970E+06 -0.51816198620782800E+06 -0.51282005515392250E+06
12 -0.50753369208673780E+06 -0.50230231471877230E+06 -0.49712535168872120E+06
13 -0.49200223425903940E+06 -0.48693239718782490E+06 -0.48191528624515330E+06
14 -0.47695034996676220E+06 -0.47203703944266180E+06 -0.46717481712277220E+06
15 -0.46236314785213240E+06 -0.45760149917384840E+06 -0.45288934918441350E+06
16 -0.44822617886036170E+06 -0.44361147099442380E+06 -0.43904472005336940E+06
17 -0.43452542188161740E+06 -0.43005307457651030E+06 -0.42562718740118830E+06
18 -0.42124727169671610E+06 -0.41691284001275330E+06 -0.41262341638983240E+06
19 -0.40837852645924690E+06 -0.40417769720136030E+06 -0.40002046704584620E+06
```

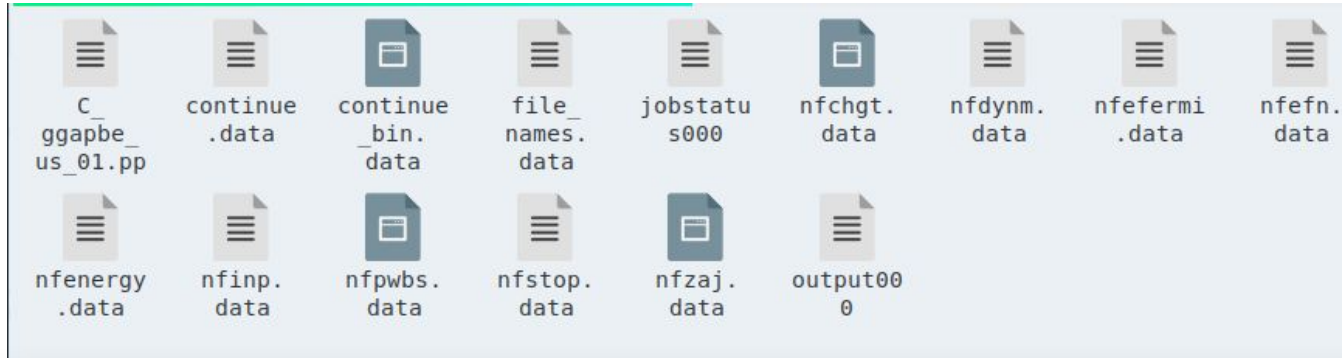
File pseudopotential ada di **phase/samples**

Pseudopotential digunakan untuk mengaproksimasi bentuk potensial yang ekstrim.

Setiap **Unsur** memiliki **pseudopotential sendiri**.



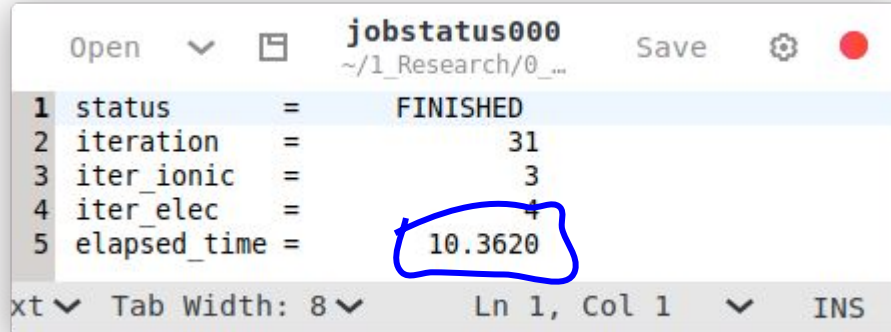
SCF



```
graphene ls
C_ggapbe_us_01.pp file_names.data nfinp.data
graphene mpirun -np 2 phase
```

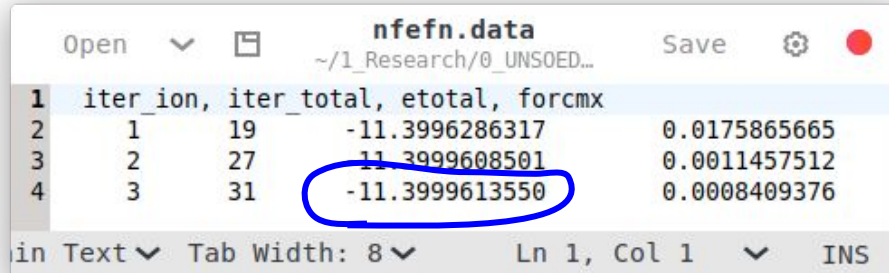
mpirun -np 2 phase

Kalkulasi SCF



jobstatus000	
~/1_Research/0_...	
1	status = FINISHED
2	iteration = 31
3	iter_ionic = 3
4	iter_elec = 4
5	elapsed_time = 10.3620

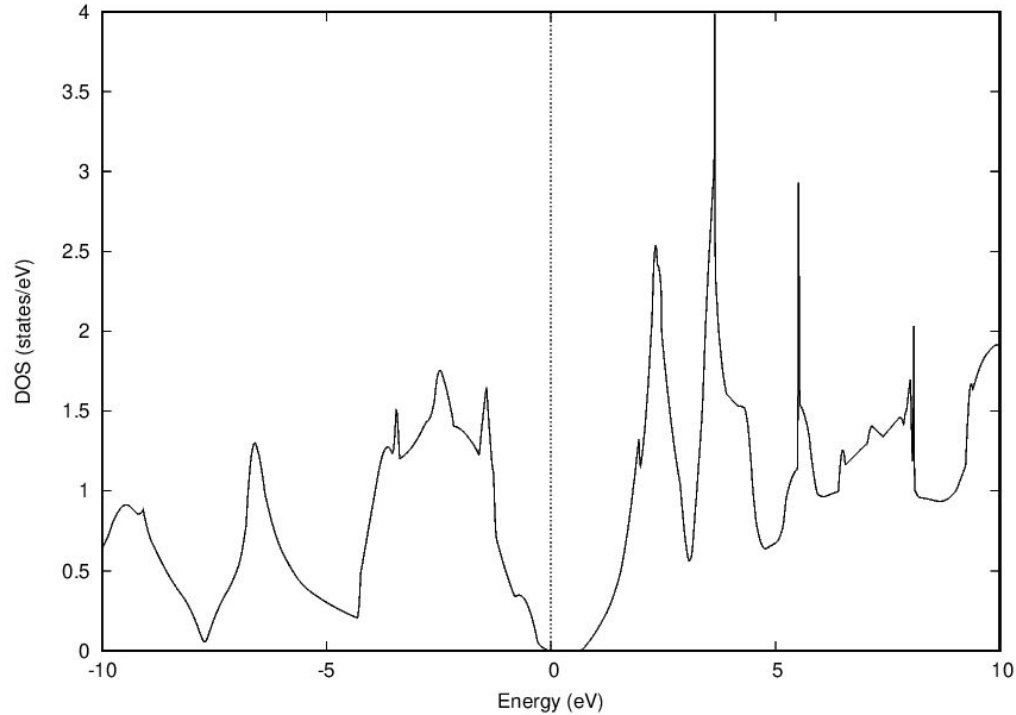
Kalkulasi telah selesai
dengan waktu 10 detik



nfefn.data				
~/1_Research/0_UNSOED...				
1	iter_ion,	iter_total,	etotal,	forcmx
2	1	19	-11.3996286317	0.0175865665
3	2	27	-11.3999608501	0.0011457512
4	3	31	-11.3999613550	0.0008409376

Energi Total -11.399 Hartree

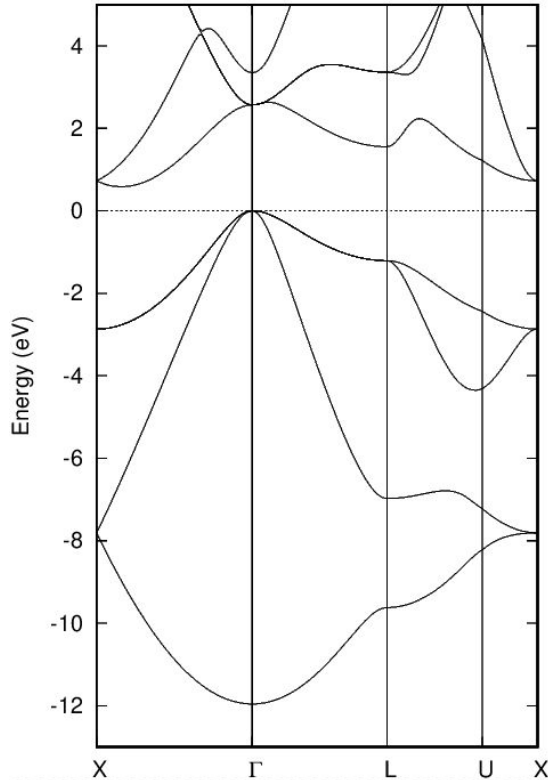
Silicon (3D) DOS



```
mpirun -np 2 ekcal
```

```
perl dos.pl dos.data -erange=-10,10 -color -with_fermi
```

Silicon (3D) Band Structure



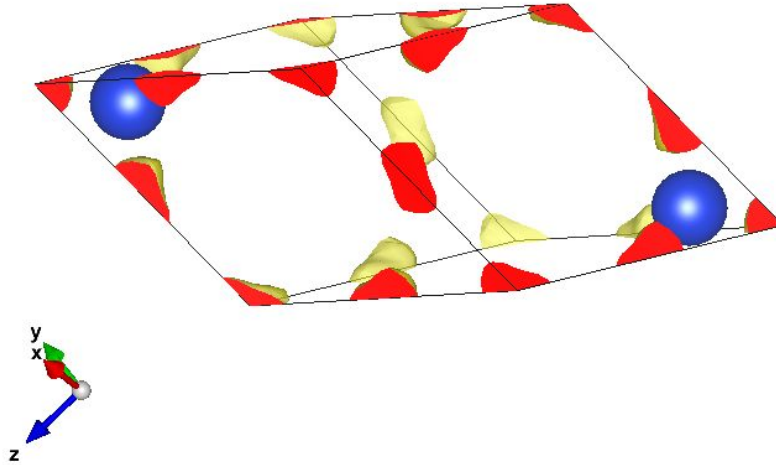
`mpirun -np 2 ekcal`

Berapa band gap dari silicene?

Material Silicene apakah termasuk konduktor atau semikonduktor?

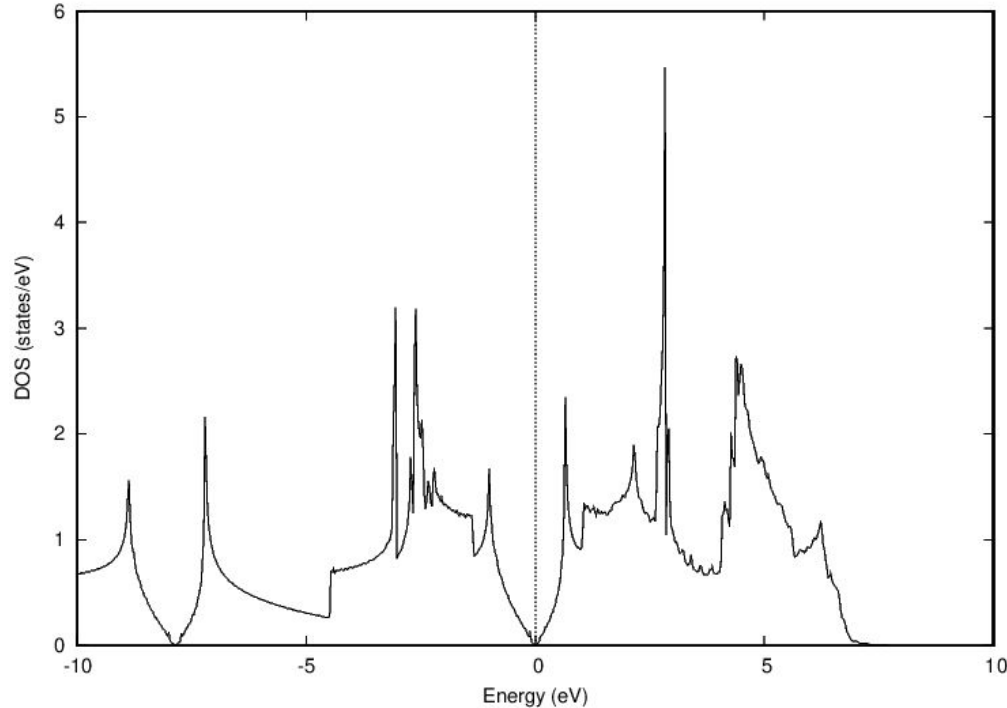
`perl band.pl nfenergy.data bandkpt.in -with_fermi -color`

Silicone (3D) Charge Density



1. Buka aplikasi Vesta
2. Masukkan nfchr.cube dengan drag

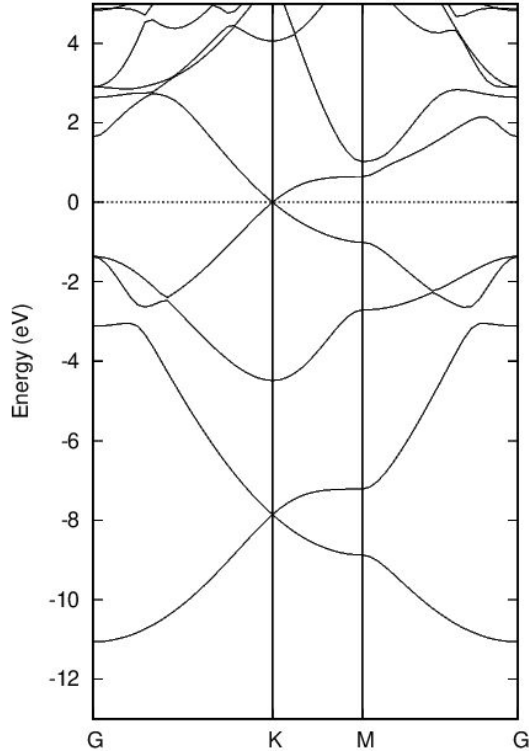
Silicene (2D) DOS



```
mpirun -np 2 ekcal
```

```
perl dos.pl dos.data -erange=-10,10 -color -with_fermi
```

Silicene (2D) Band Structure



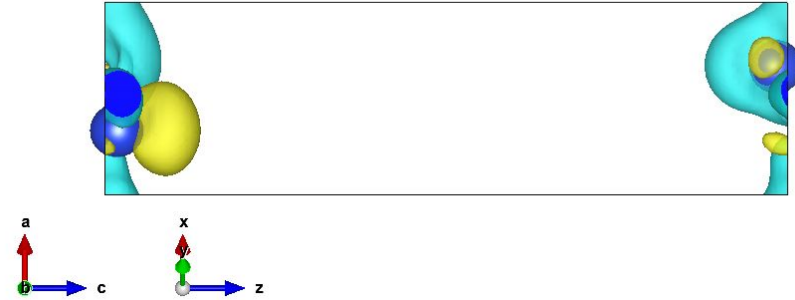
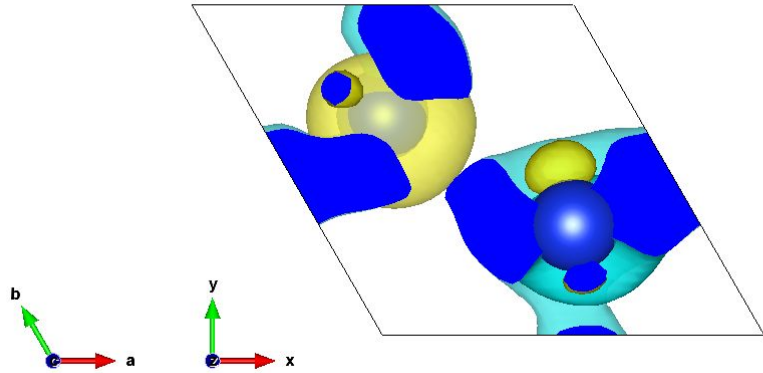
mpirun -np 2 ekcal

Berapa band gap dari silicene?

Material Silicene apakah termasuk konduktor atau semikonduktor?

perl band.pl nfenergy.data bandkpt.in -with_fermi -color

Silicene (2D) CDD



1. Buka aplikasi Vesta
2. Masukkan nfchr.down.cube dengan drag
3. Pilih edit -> volumetric data -> import -> subtract -> nfchr.down.cube

Tugas!

1. Install berikut di komputer Anda:

- Vesta
- Avogadro

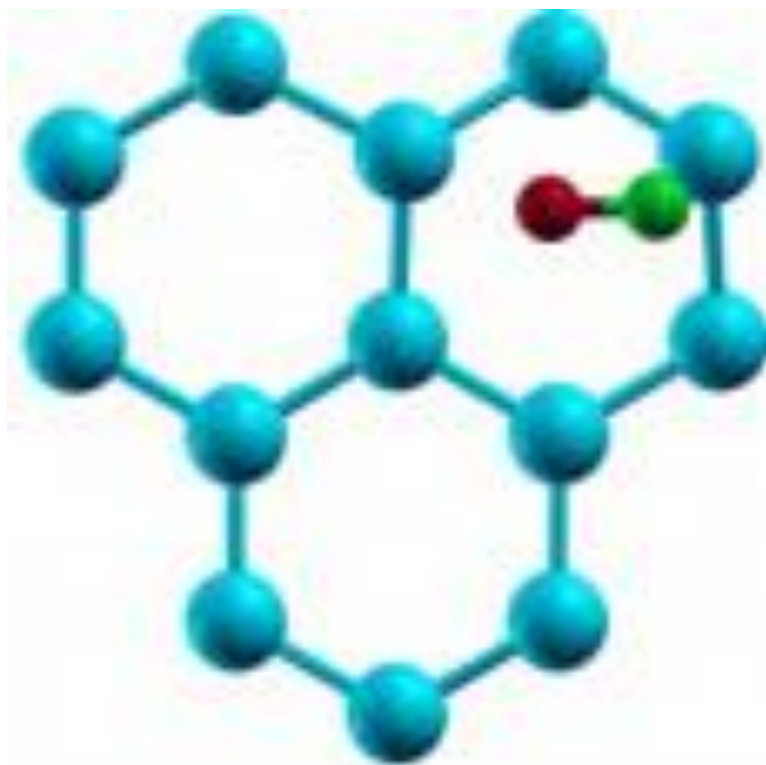
(Berikan bukti screenshoot)

2. Buatlah molekul **NO (Nitric Oxide)** dengan aplikasi webmo! (Hasil adalah POSCAR)
3. Buatlah supersel silicene (3x3x1) dengan menggunakan VESTA!
4. Letakan molekul NO di atas supersel silicene!

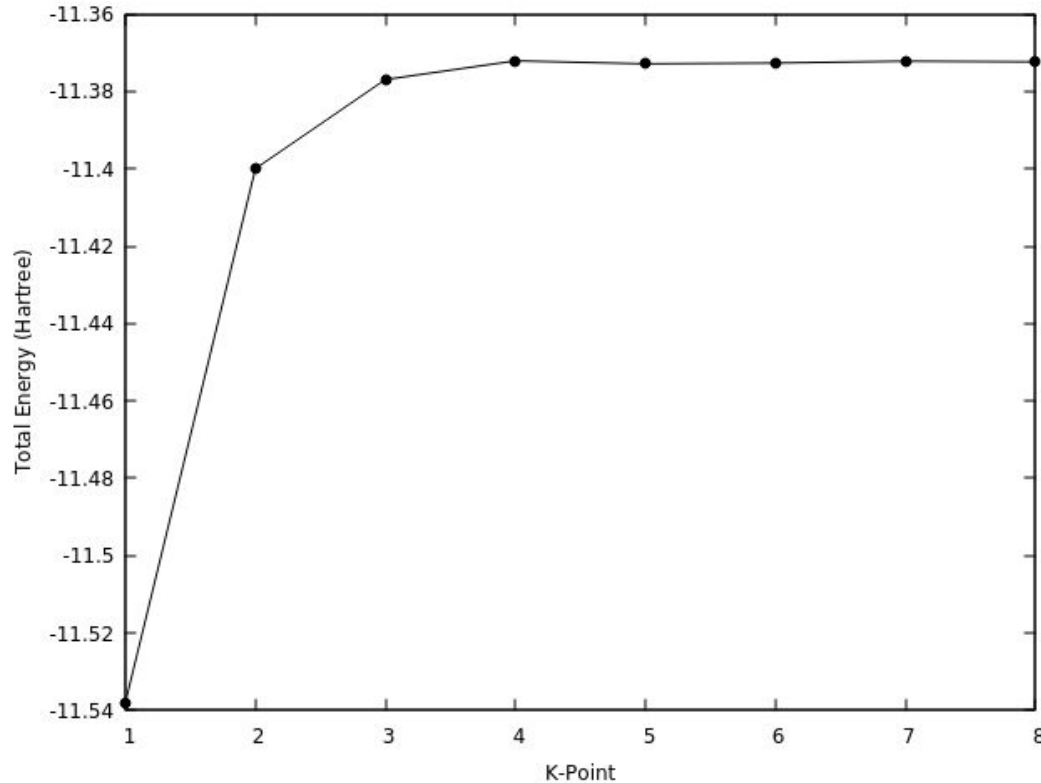
Tugas dikumpulkan sebelum kuliah minggu depan di mulai! (Max 23 Mei 2023)

Kumpulkan lewat email:

zohansyahfatom@mail.ugm.ac.id



Konvergensi Kpoint



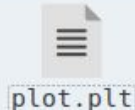
Buatlah diagram konvergensi
akurasi kpoint-mesh.

Dari 1x1x1, 2x2x1 ... s.d. 10x10x1!

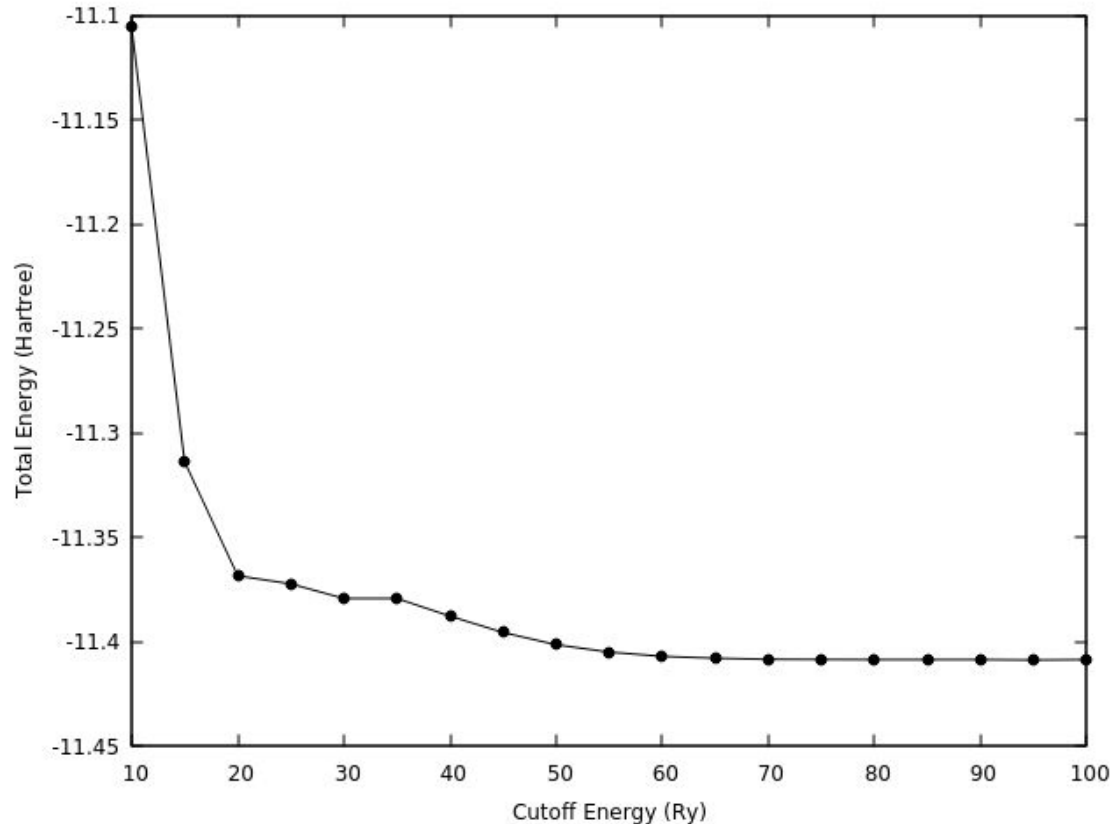
Visualisasi data (GNUPlot)

```
1 unset label
2 set title ""
3 set encoding iso_8859_1
4 set ylabel "Total Energy (Hartree)"
5 set xlabel "K-Point"
6 set style line 1 lt rgb "black" lw 1 pt 1
7 set style line 2 lc rgb 'black' pt 7
8 plot "dataK" using 1:2 title "" with lines ls 1 , \
9  "dataK" using 1:2 title "" with points ls 2
```

Plotting grafik dapat dilakukan dengan GnuPlot.

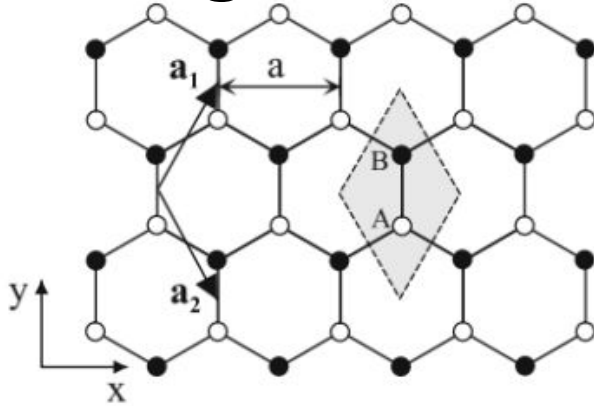


Konvergensi Energi Cutoff



**Buatlah diagram konvergensi
akurasi energi cutoff
wavefunction dari 25 Ry, 30 Ry,
..., s.d. 100 Ry!**

Hexagonal Lattice Structure



Primitive Lattice Vector I

$$\vec{a}_1 = a_0 \left(\frac{1}{2} \vec{x} + \frac{\sqrt{3}}{2} \vec{y} \right)$$

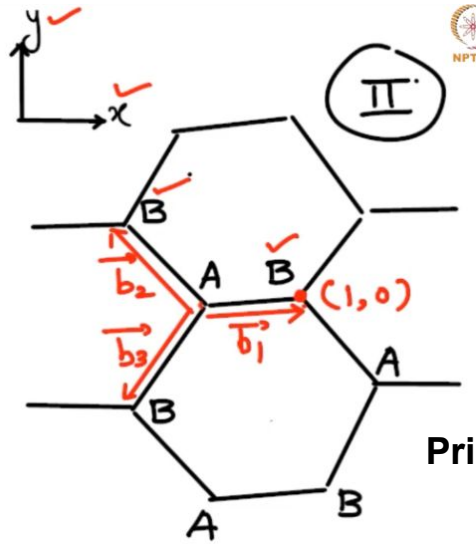
$$\vec{a}_2 = a_0 \left(\frac{1}{2} \vec{x} - \frac{\sqrt{3}}{2} \vec{y} \right)$$

a_0 = konstanta kisi graphene

Primitive Lattice Vector II

$$\vec{b}_1 = a_0 (1 \cdot \vec{x} + 0 \cdot \vec{y})$$

$$\vec{b}_2 = a_0 \left(-\frac{1}{2} \vec{x} + \frac{\sqrt{3}}{2} \vec{y} \right)$$



Primitive Unit Cell Graphene