

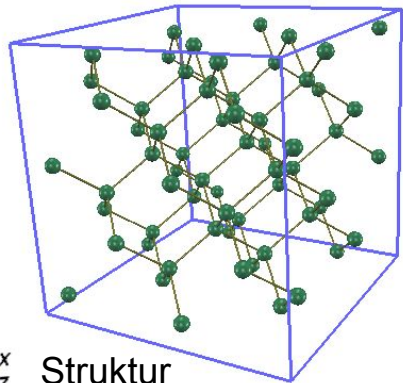
Struktur Elektronik: Diamond (3D) & Graphene (2D)

Zohan Syah Fatomi

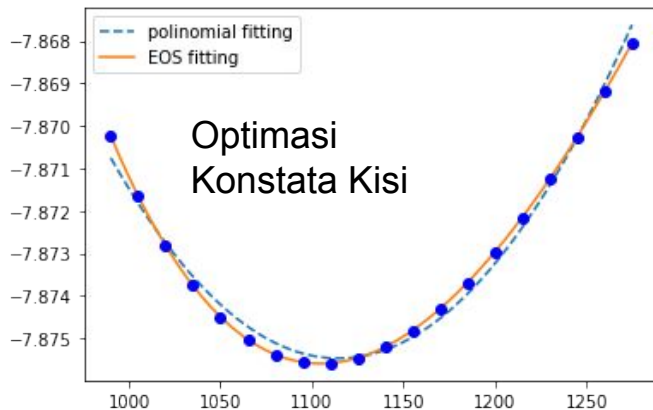


Jurusan Fisika
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Jenderal Soedirman

Rekayasa Komputasi Material

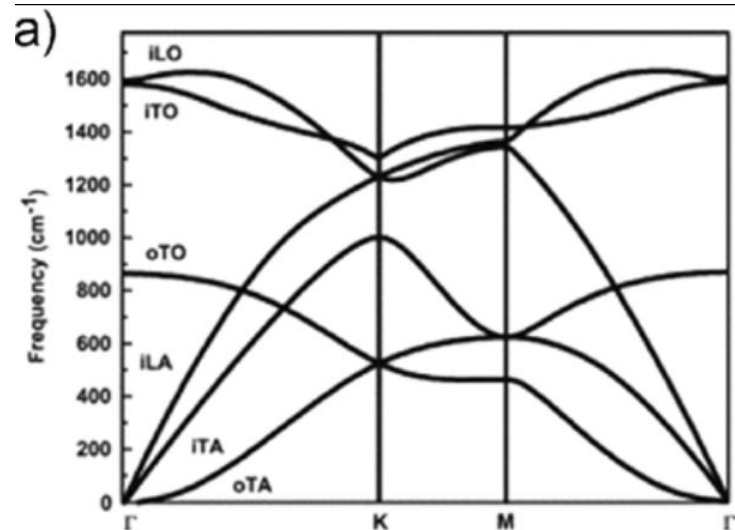


Struktur kristal

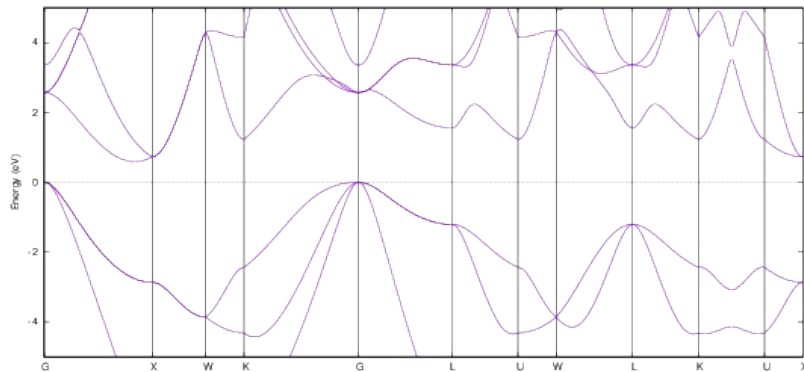


**Density Functional
Theory (DFT) +
Komputasi Numerik
+ Komputer**

Output:
Sifat elektronik,
Optik, Magnetik,
dlsb

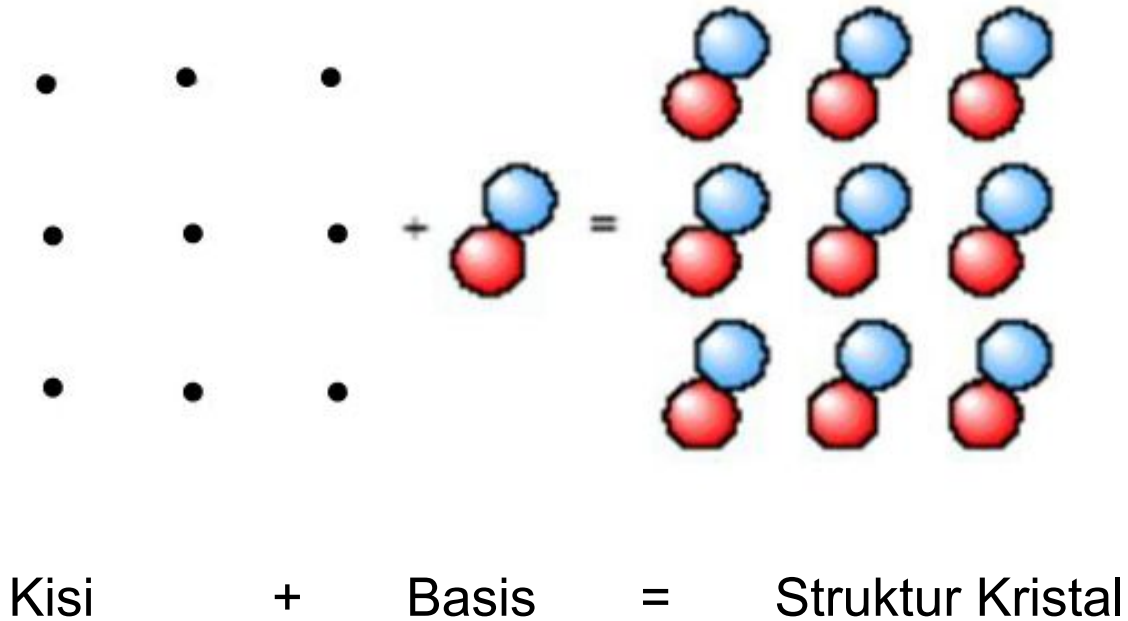


Sifat vibrasi
(phonon dispersion)

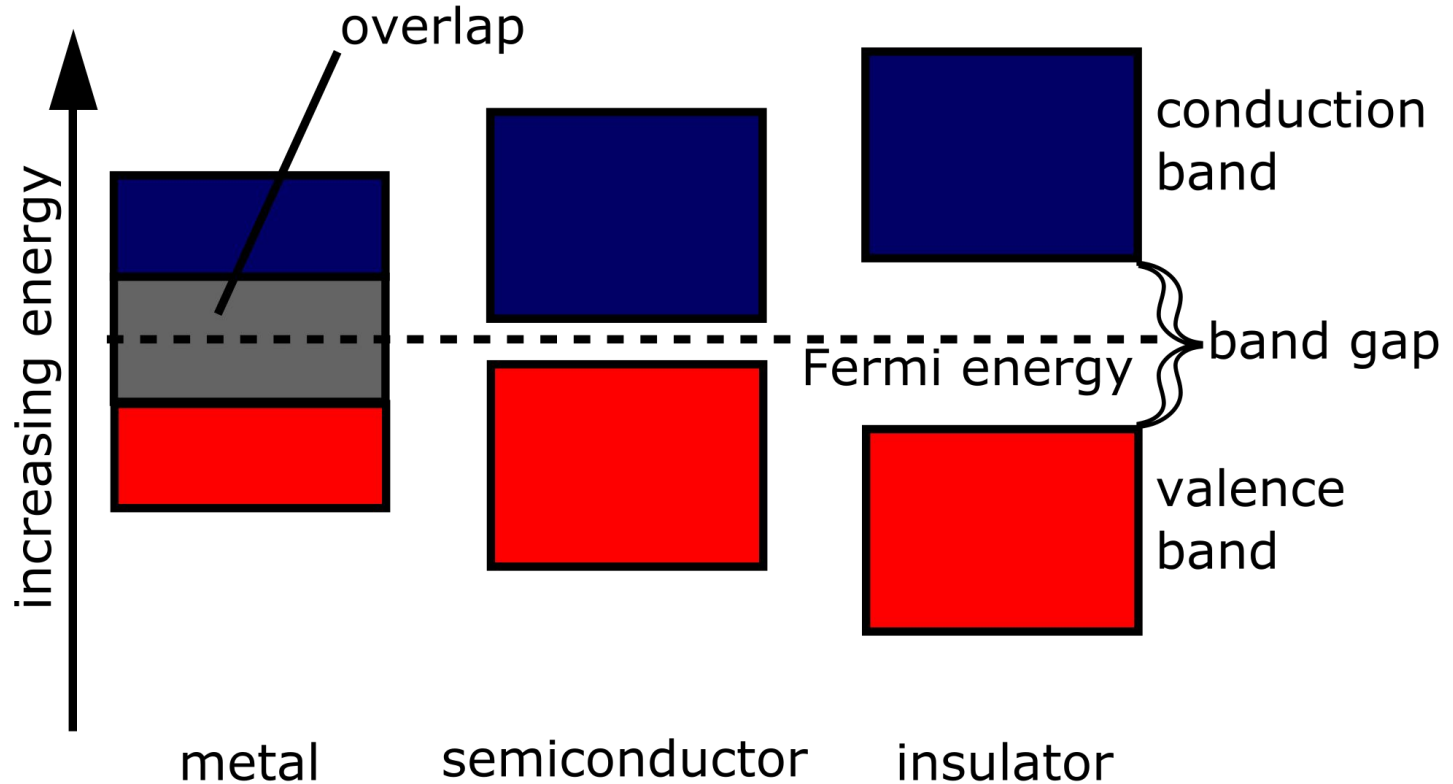


Struktur elektronik

Sistem Kristal



Struktur Band



Sifat Elektronik pada Material

Berdasarkan kemagnetannya material dibedakan menjadi 3:

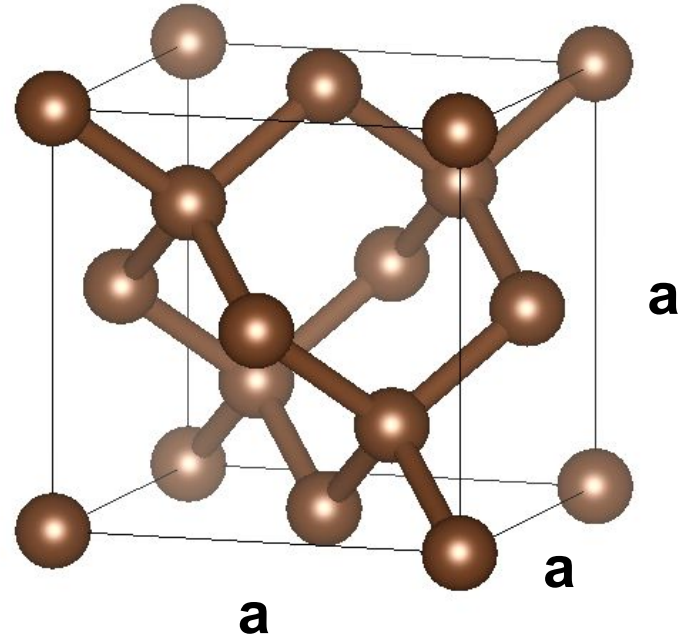
1. **Konduktor** : *conduction band & valence band* timpang tindih (*overlap*).
Contoh: besi (Fe), tembaga (Cu) dll.
2. **Semikonduktor** : memiliki band gap sedang (0.1 - 4.0 eV).
Contoh: Silicon, Germanium dll.
3. **Isolator** : memiliki band gap besar (> 4.0 eV)
Contoh: Diamond, kaca

Diamond (3D)

Apa jenis struktur kristal pada FCC pada diamond?

Berapa atom Atom Si di unit sel?

Apa itu hibridisasi orbital sp_3 ?

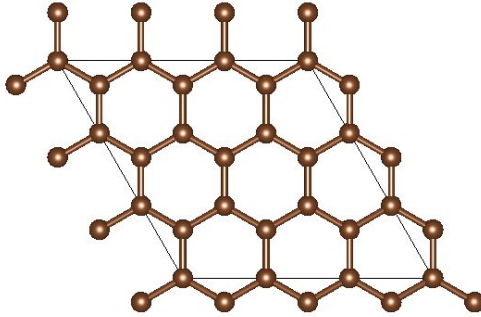


Graphene (2D)

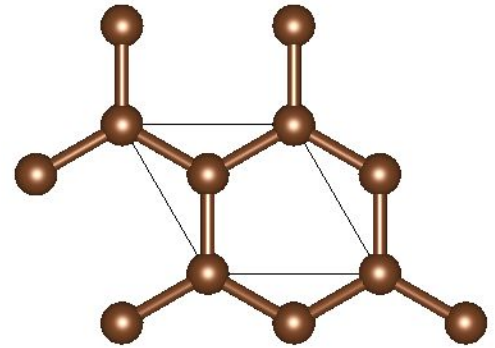
Berapa atom
Atom C di unit sel
primitive?

Berapa lattice
constant pada
Graphene?

Apa itu hibridisasi
orbital sp_3 ?



Super sel 3x3x1
graphene

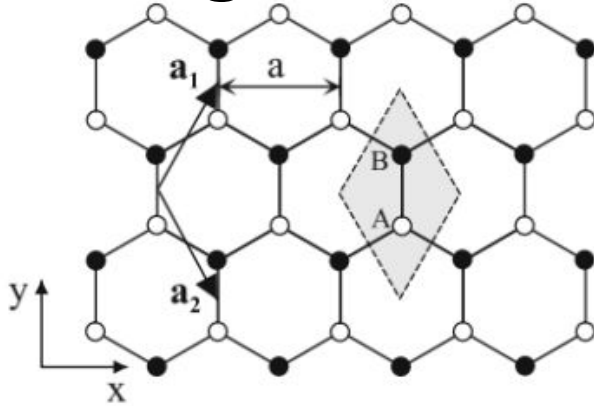


Struktur kristal
primitif graphene

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

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

Hexagonal Lattice Structure



Primitive Lattice Vector I

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

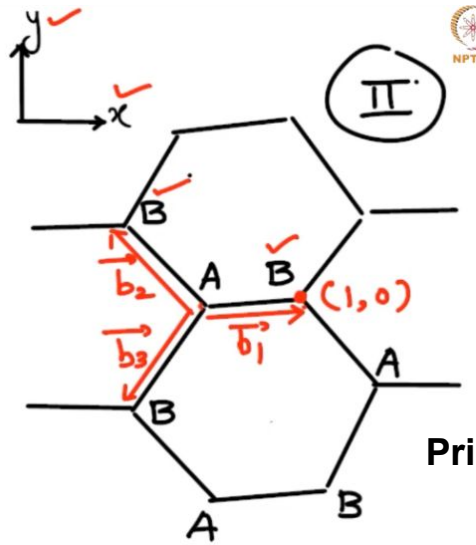
$$\vec{a}_2 = a_0 \left(\frac{1}{2} \vec{x} - \frac{\sqrt{3}}{2} \vec{y} \right)$$

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

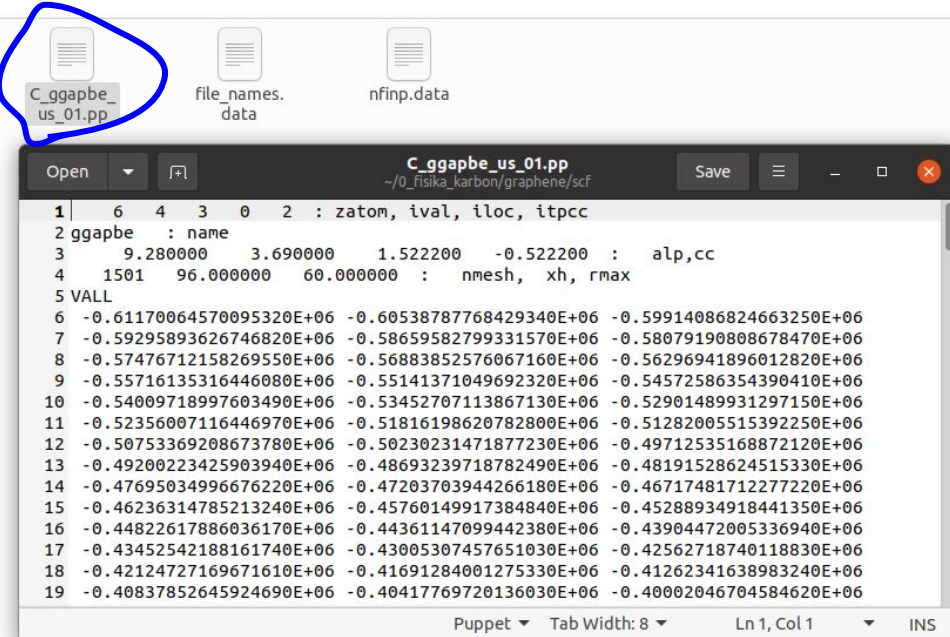
```
1 Control{
2     cpumax = 3600 sec
3     condition = Initial
4 }
5 accuracy{
6     cutoff_wf = 25.00 rydberg
7     cutoff_cd = 225.00 rydberg
8     num_bands = 16
9     ksampling{
10         mesh{
11             nx = 2
12             ny = 2
13             nz = 1
14         }
15     }
16 }
17 structure{
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



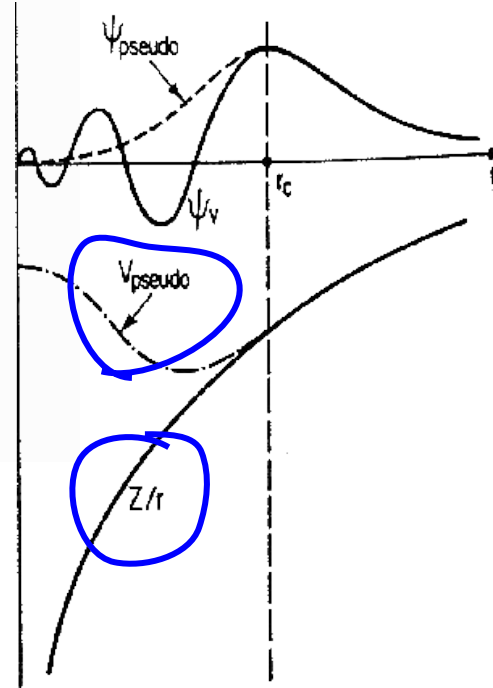
The image shows a file manager window with three files: 'C_ggapbe_us_01.pp' (circled in blue), 'file_names.data', and 'nfinp.data'. Below it is a text editor window titled 'C_ggapbe_us_01.pp' showing the contents of the pseudopotential file. The file contains a header section with parameters like 'name', '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 coefficients.

```
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
```

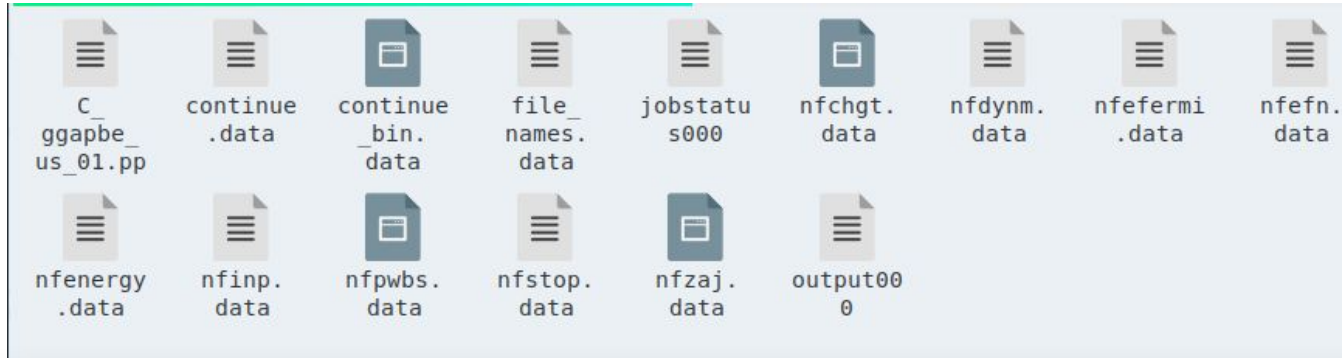
File pseudopotential ada di **phase/samples**

Pseudopotential digunakan untuk mengaproksimasi bentuk potensial yang ekstrim.

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



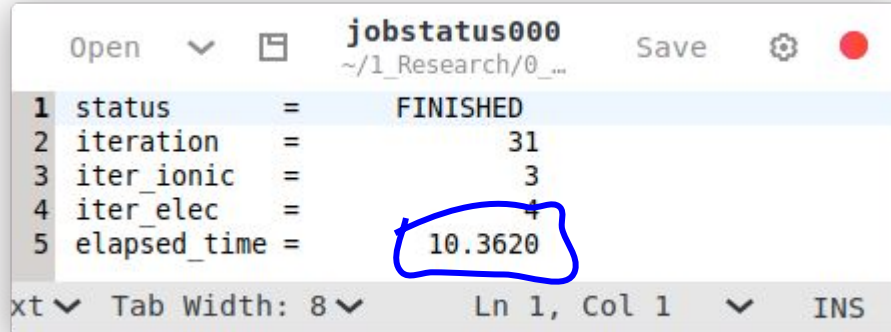
SCF



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

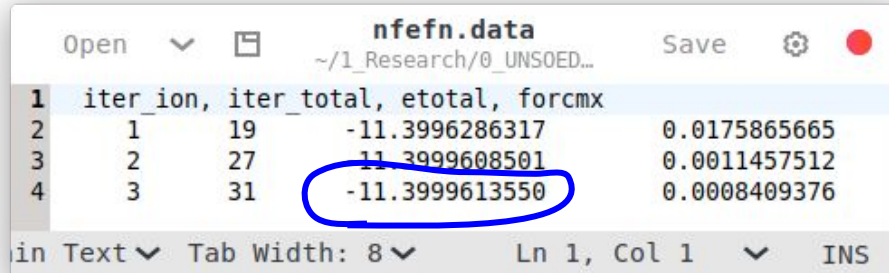
mpirun -np 2 phase

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

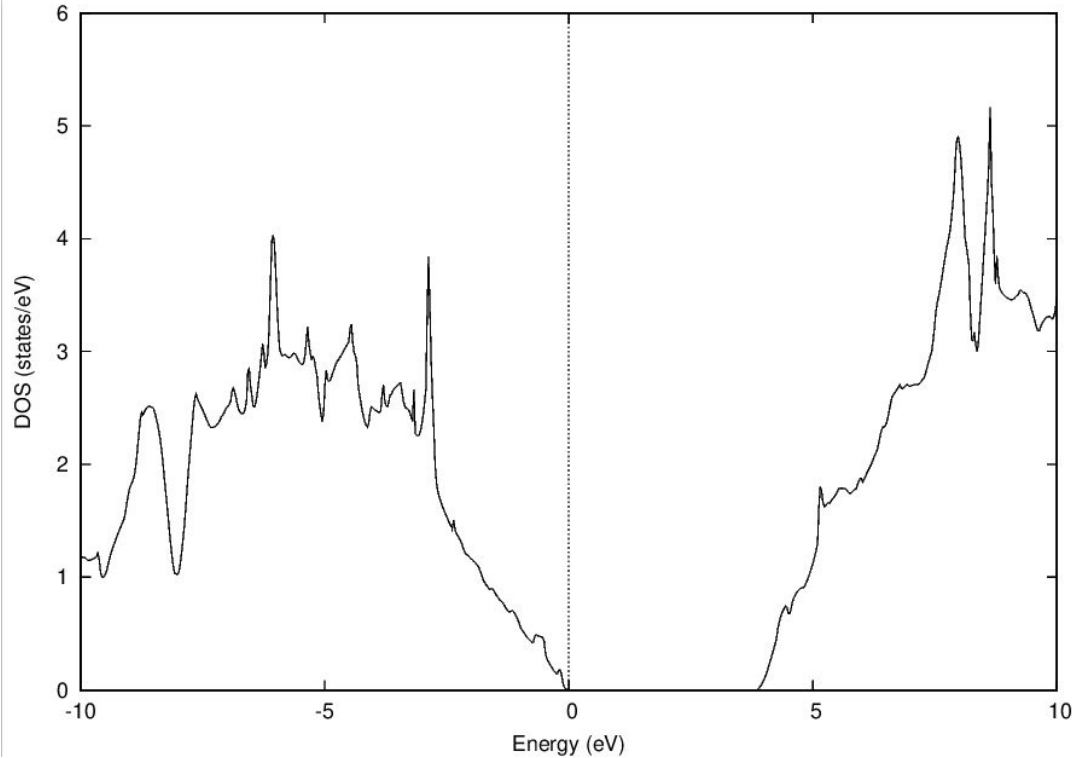
Kalkulasi telah selesai
dengan waktu 10 detik



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

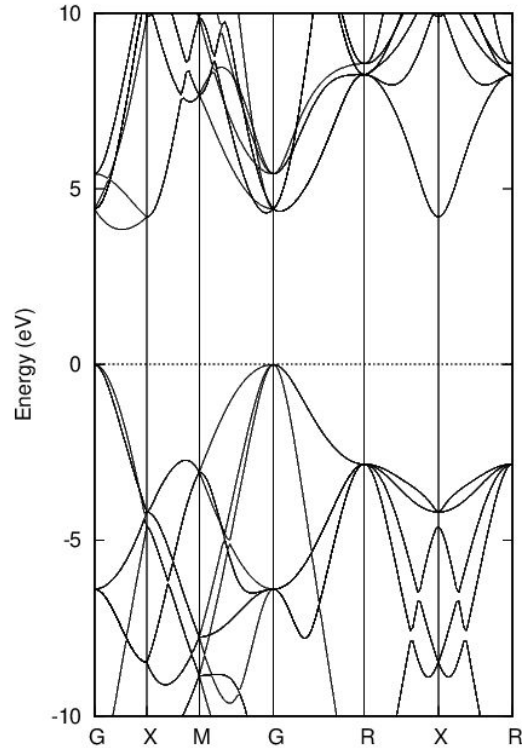
Diamond (3D) DOS



`mpirun -np 2 ekcal`

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

Diamond (3D) Band Structure



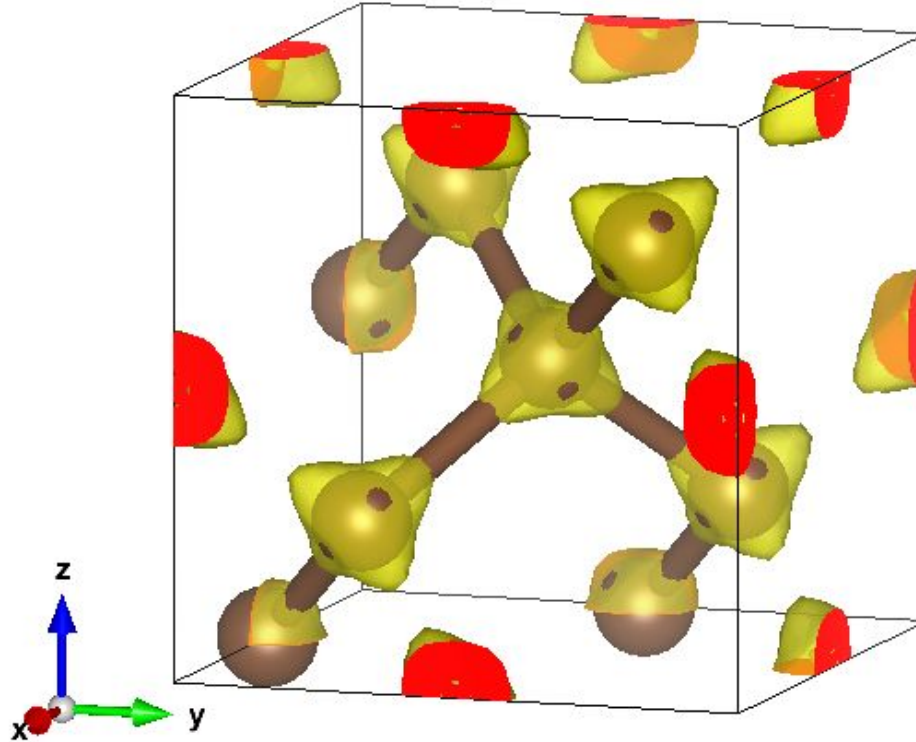
`mpirun -np 2 ekcal`

Berapa band gap dari diamond?

Material Diamond apakah termasuk konduktor atau semikonduktor atau isolator?

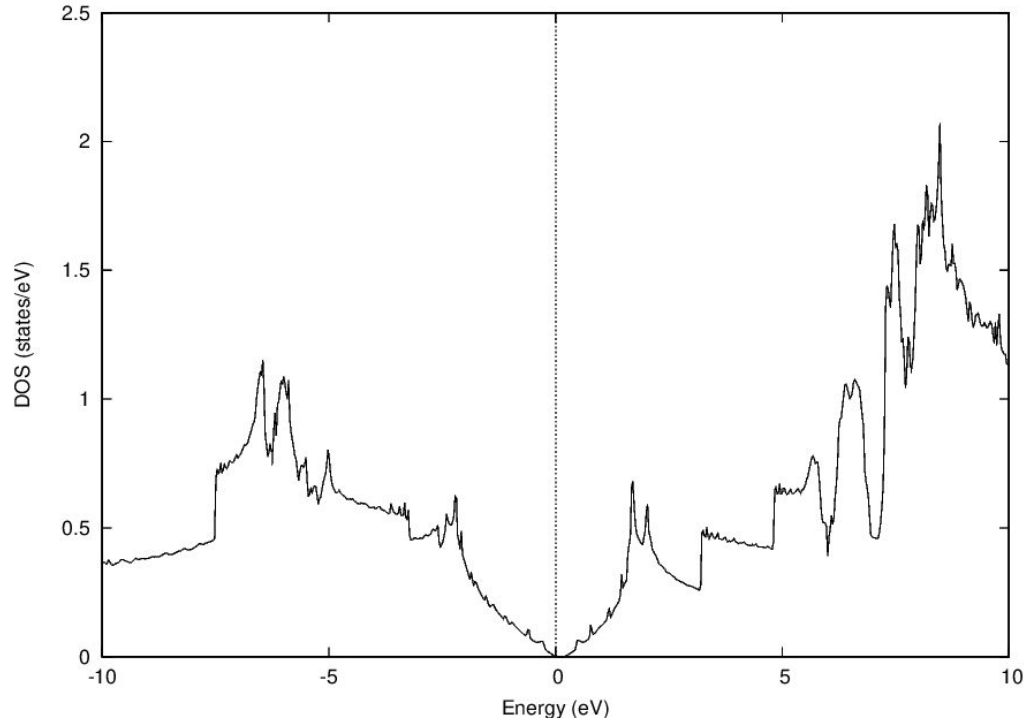
`perl band.pl nfenergy.data bandkpt.in -with_fermi -color`

Diamond (3D) Charge Density



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

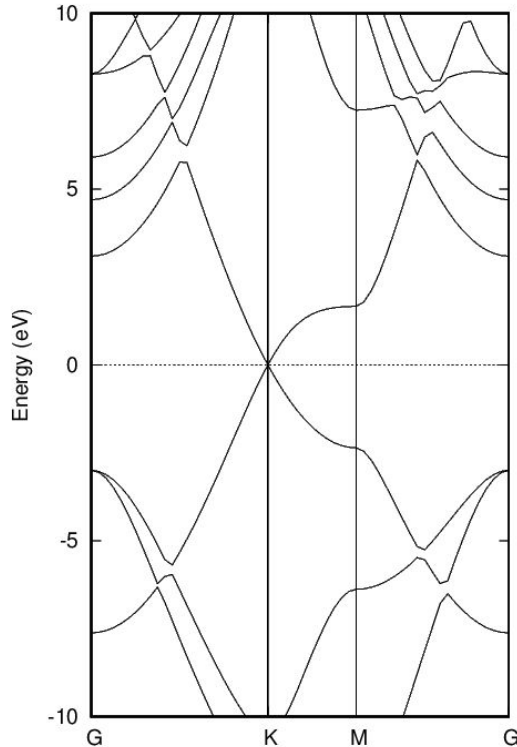
Graphene (2D) DOS



```
mpirun -np 2 ekcal
```

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

Graphene (2D) Band Structure



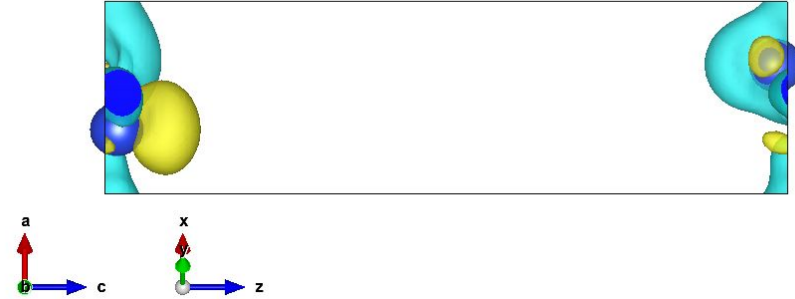
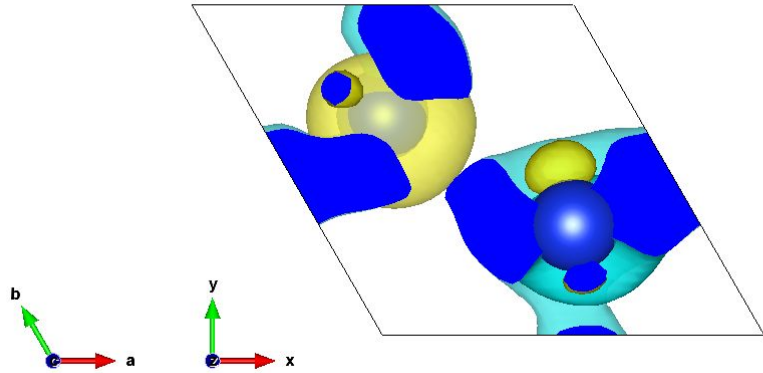
`mpirun -np 2 ekcal`

Berapa band gap dari graphene?

Material Graphene apakah termasuk konduktor atau semikonduktor?

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

Graphene (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 H_2O (**Water**) dengan aplikasi webmo!
(Hasil adalah POSCAR)

3. Buatlah supersel graphene (3x3x1) dengan menggunakan VESTA!

4. Letakan molekul H_2O di atas supersel graphene!

Tugas dikumpulkan sebelum kuliah minggu depan di mulai! (Max 30 Mei 2023)

Kumpulkan lewat email:

zohansyahfatomi@mail.ugm.ac.id

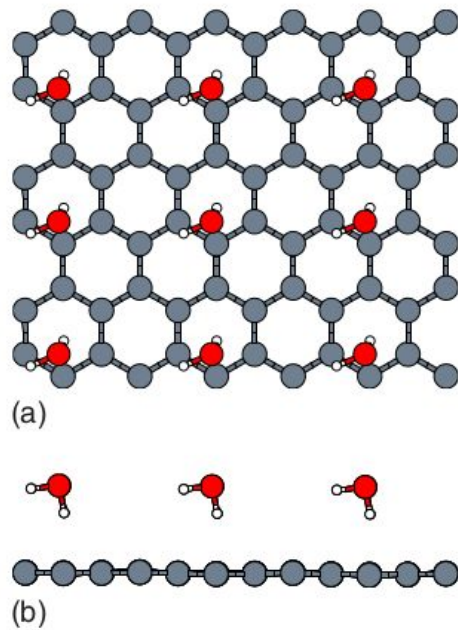
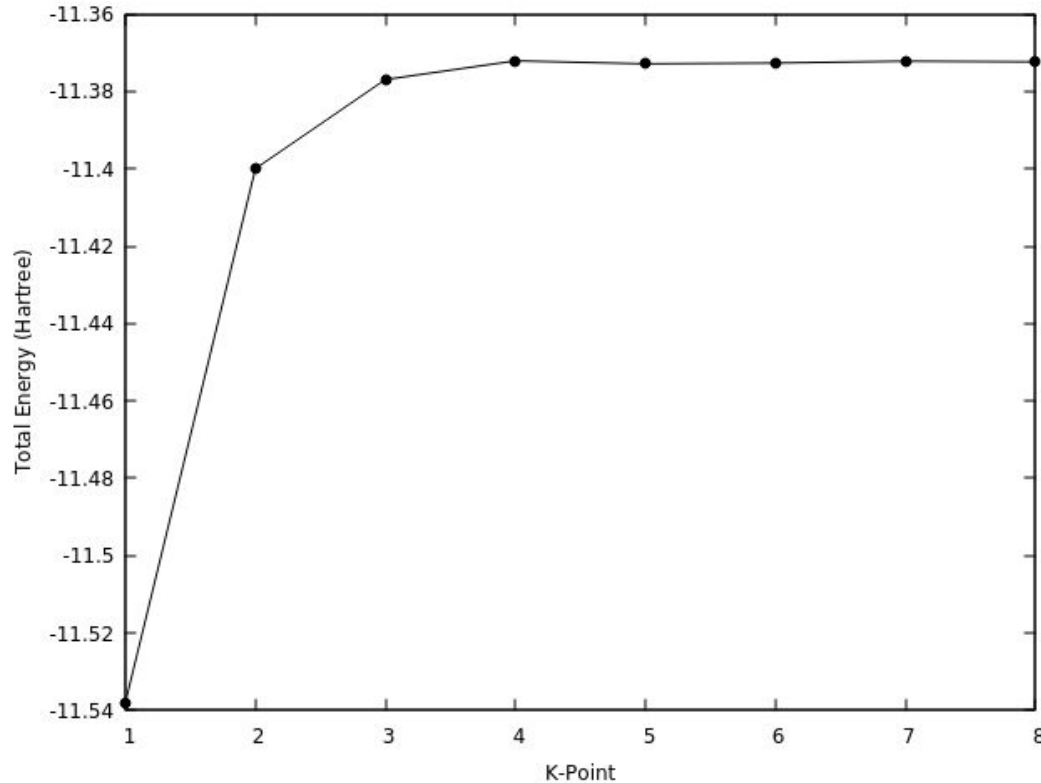


FIG. 1. (Color online) Water on the top of graphene: top and side views.

Konvergensi Kpoint



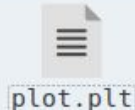
Buatlah diagram konvergensi
akurasi kpoint-mesh.

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

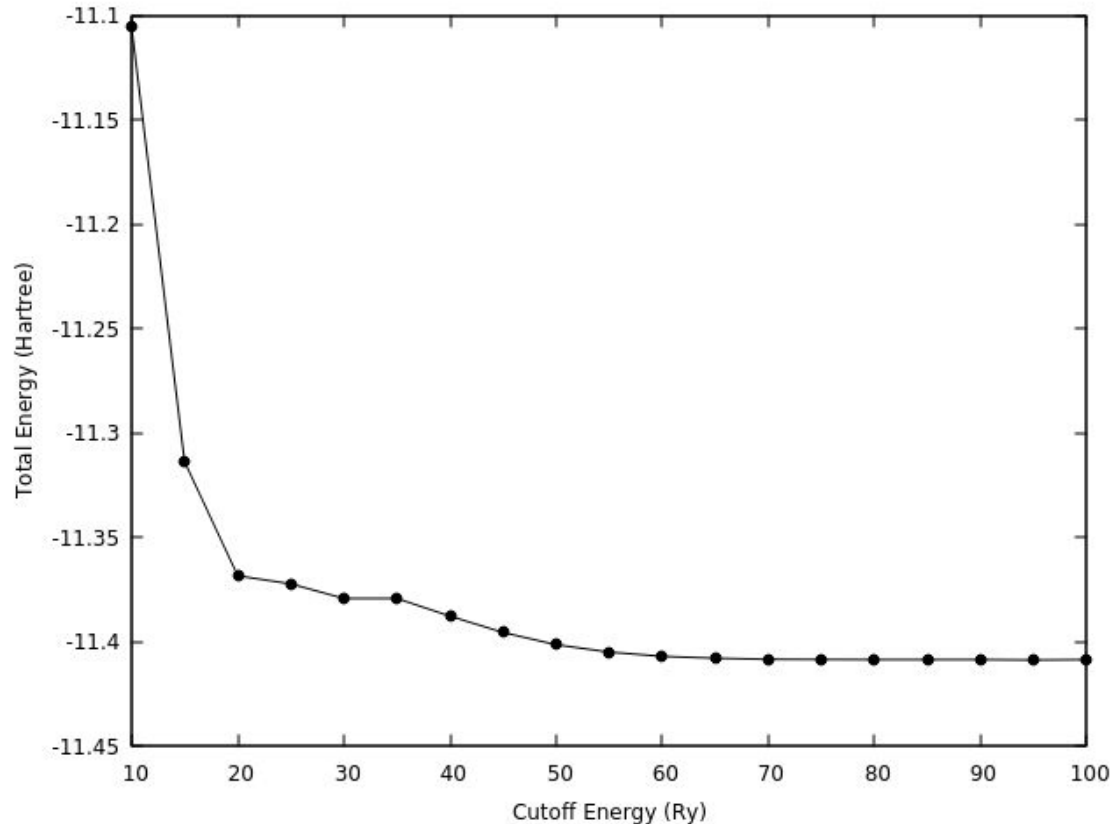
Visualisasi data (GNUPlot)

```
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.

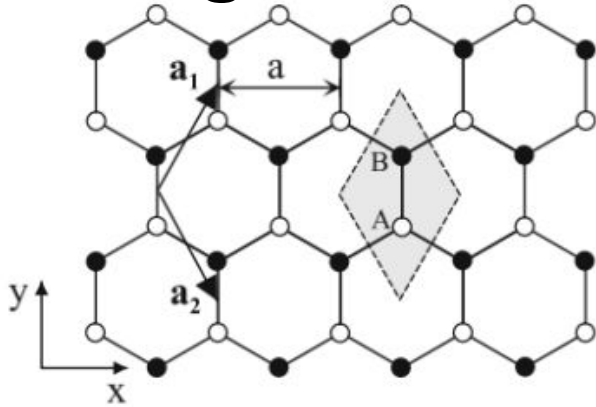


Konvergensi Energi Cutoff



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

Hexagonal Lattice Structure



Primitive Lattice Vector I

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

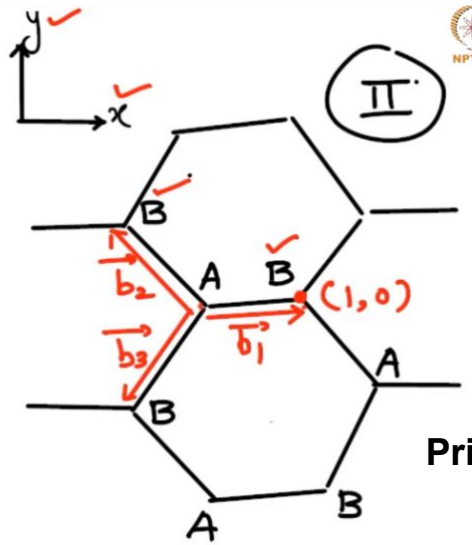
$$\vec{a}_2 = a_0 \left(\frac{1}{2} \vec{x} - \frac{\sqrt{3}}{2} \vec{y} \right)$$

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