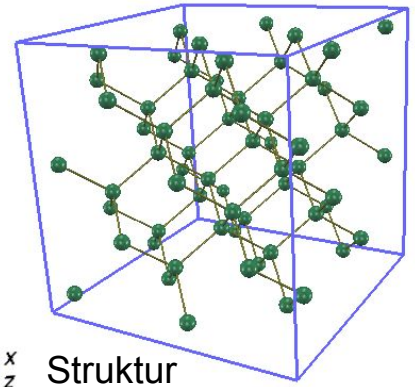
Selasa, 23 Maret 2023

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

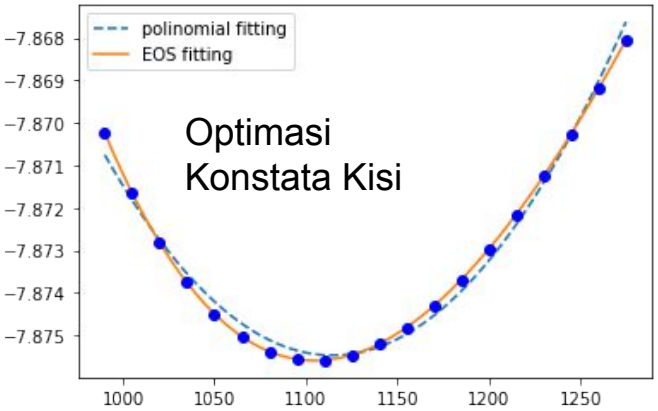
Zohan Syah Fatomi

Jurusan Fisika
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Jenderal Soedirman

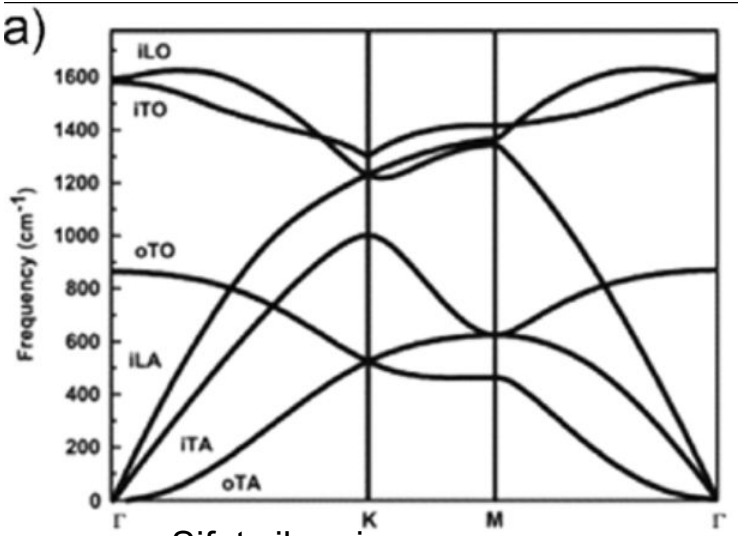
# Rekayasa Komputasi Material



Struktur kristal




Optimasi Konstata Kisi

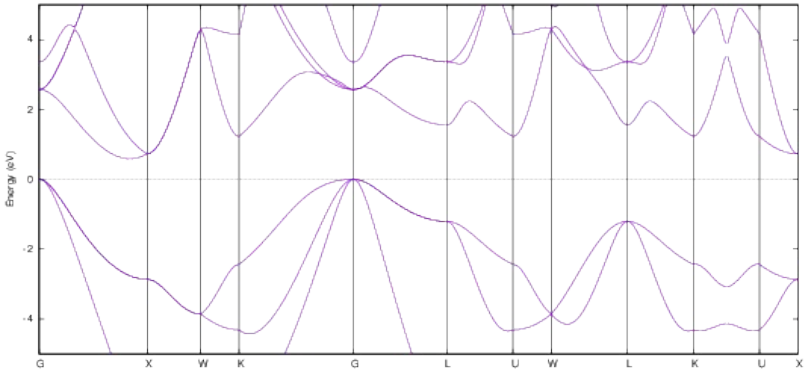



Sifat vibrasi (phonon dispersion)

- **Input:** Koordinat atomik

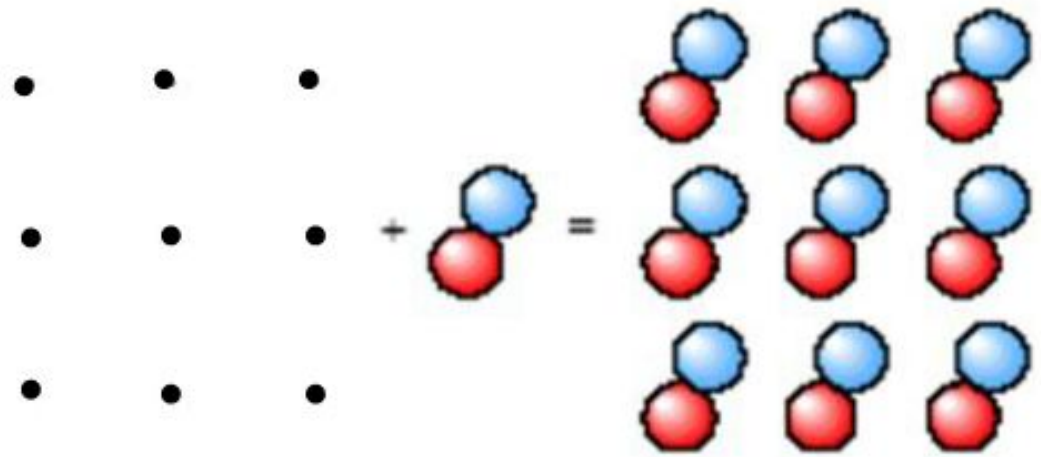
**Density Functional Theory (DFT) + Komputasi Numerik + Komputer**

- **Output:** **Sifat elektronik**, Optik, Magnetik, dlsb



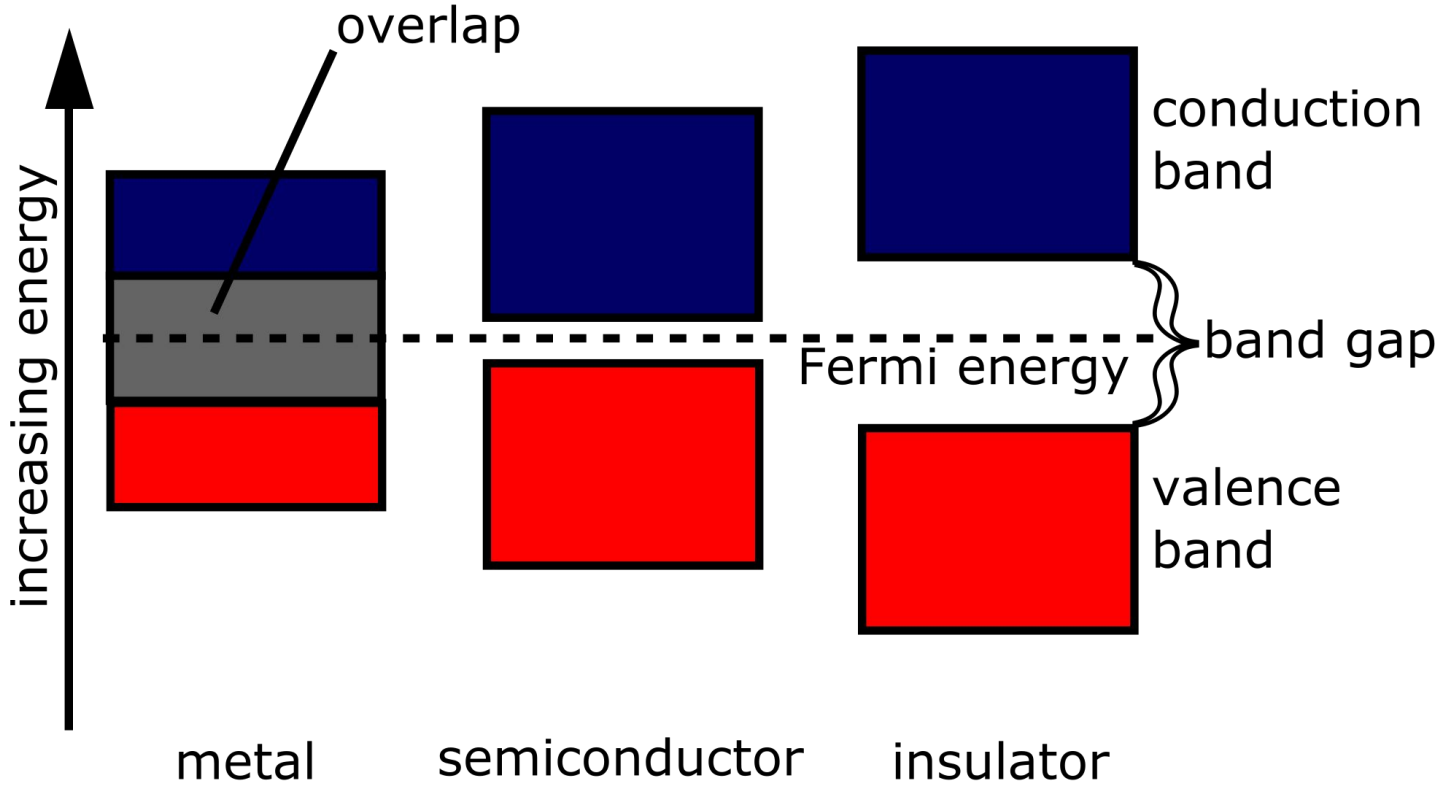

**Struktur elektronik**

# Sistem Kristal



Kisi + Basis = Struktur Kristal

# Struktur Band



# Sifat Elektronik pada Material

Berdasarkan kemagnetannya material dibedakan menjadi 3:

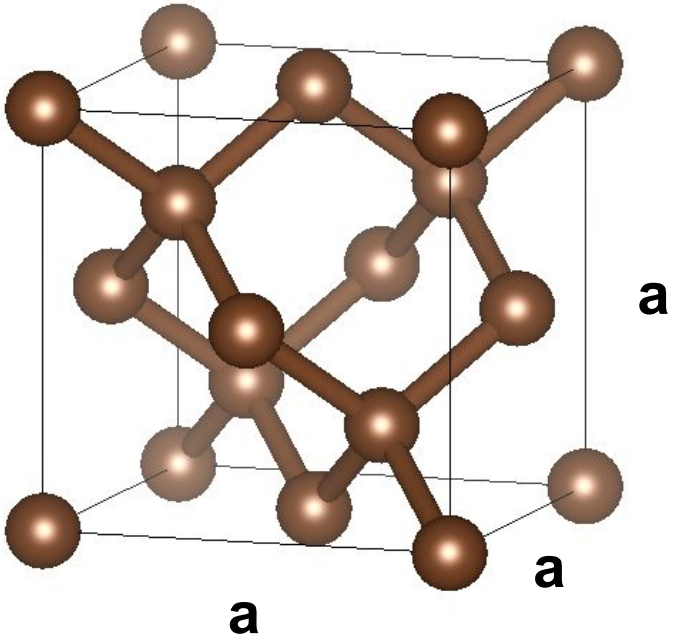
1. **Konduktor** : *conduction band* & *valence band* timpang tindih (*overlap*).
   Contoh: besi (Fe), tembaga (Cu) dll.
2. **Semikonduktor** : memiliki band gap sedang (0.1 - 4.0 eV).
   Contoh: Silicon, Germanium dll.
3. **Isolator** : memiliki band gap besar ( > 4.0 eV)
   Contoh: Diamond, kaca

# Diamond (3D)

**Apa jenis struktur kristal pada FCC pada diamond?**

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

**Apa itu hibridisasi orbital $sp_3$?**

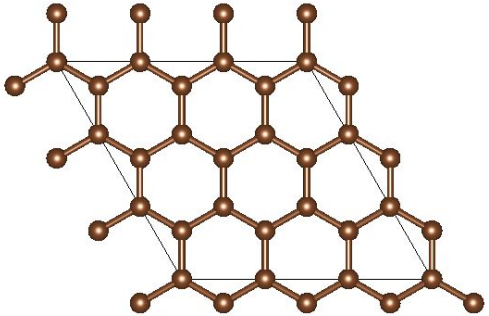


# Graphene (2D)

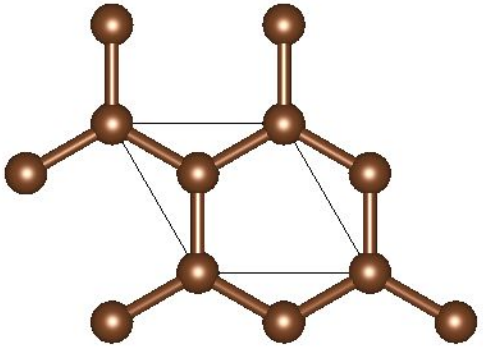
**Berapa atom Atom C di unit sel primitive?**

**Berapa lattice constant pada Graphene?**

**Apa itu hibridisasi orbital $sp_3$?**



Super sel 3x3x1 graphene

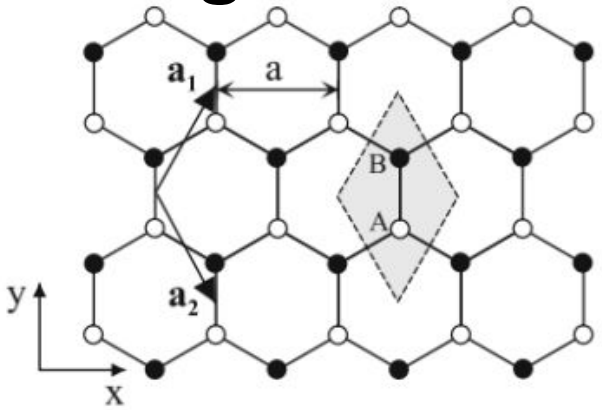


Struktur kristal primitif graphene

$$\vec{b_1} = a_0(1.\vec{x} + 0.\vec{y})$$

$$\vec{b_2} = a_0(-\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y})$$

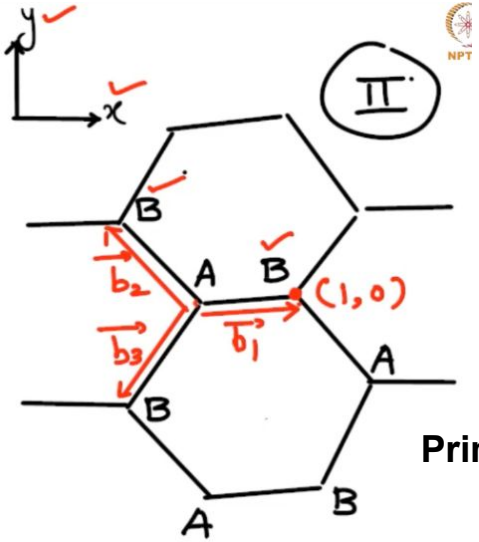
# Hexagonal Lattice Structure




Primitive Lattice Vector I

$$\vec{a_1} = a_0(\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y})$$

$$\vec{a_2} = a_0(\frac{1}{2}\vec{x} - \frac{\sqrt{3}}{2}\vec{y})$$




$a_0$= konstanta kisi graphene

Primitive Lattice Vector II

$$\vec{b_1} = a_0(1.\vec{x} + 0.\vec{y})$$

$$\vec{b_2} = a_0(-\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y})$$

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_Researc

```
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**)

# nfinp.data

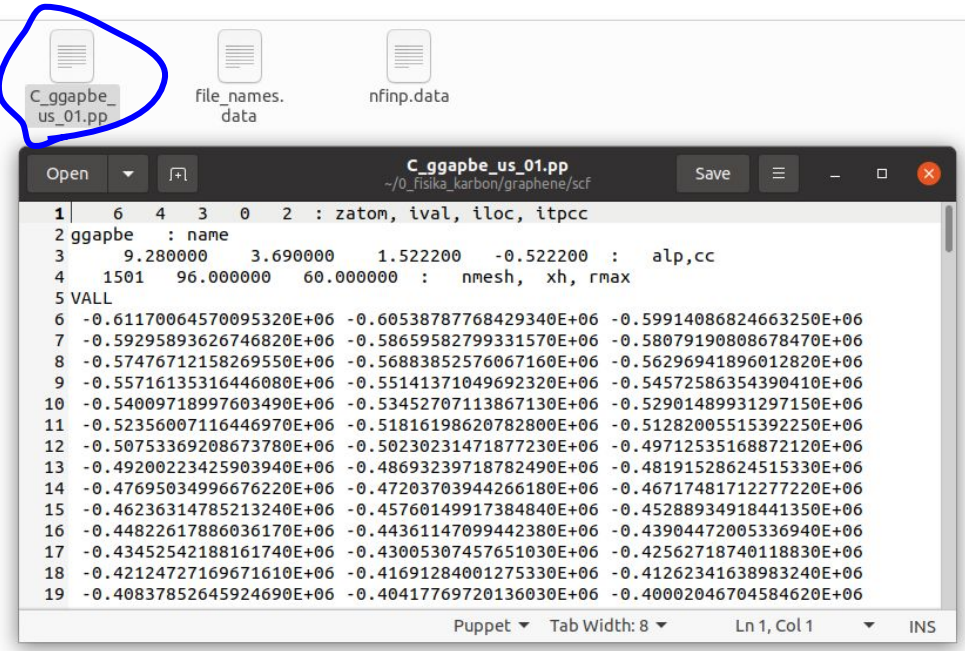
```
Control{
    cpumax = 3600 sec
    condition = Initial
}
accuracy{
    cutoff_wf = 25.00 rydberg
    cutoff_cd = 225.00 rydberg
    num_bands = 16
    ksampling{
        mesh{
            nx = 2
            ny = 2
            nz = 1
        }
    }
}
structure{
    unit_cell_type = primitive
    unit_cell{
        a_vector = 4.6646320985 0.00 0.00
        b_vector = -2.3323160493 4.0396898966 0.00
        c_vector = 0.00 0.00 18.895488655
    }
    atom_list{
        atoms{
            #tag element rx ry rz mobile
             C 0.66666667 0.33333333 0.0 1
             C 0.33333333 0.66666667 0.0 1
        }
    }
    element_list{
        #tag element atomicnumber mass zeta deviation
         C 6 21894.5796 0.0 1.83
    }
}
```

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.

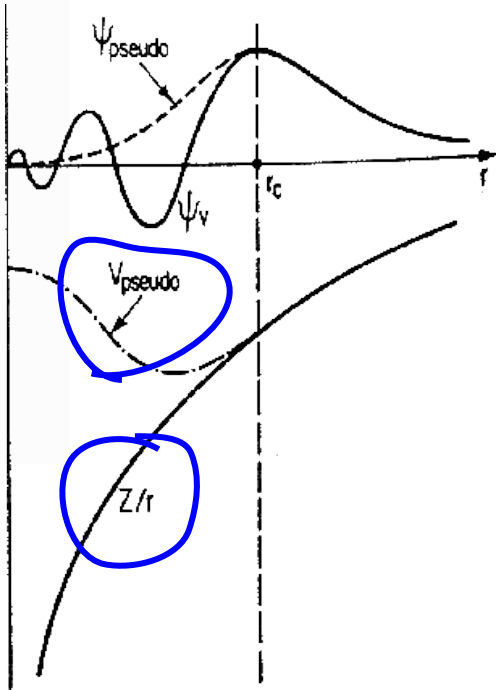
# File pseudopotential



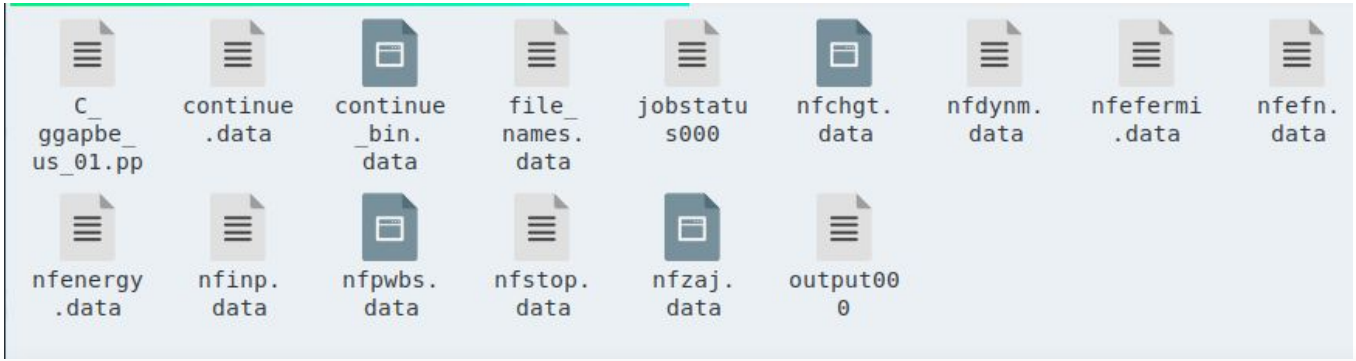

File pseudopotential ada di **phase/samples**

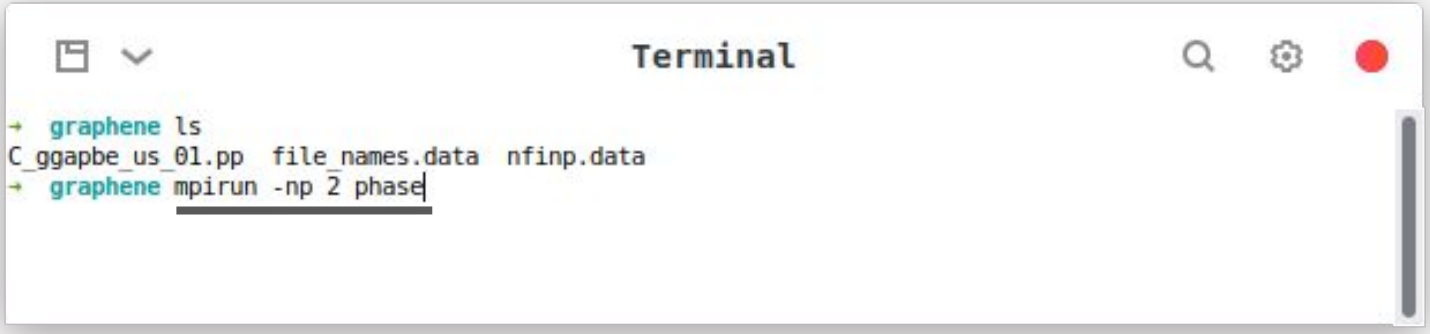
**Pseudopotential** digunakan untuk mengaproksimasi bentuk potential yang ekstrim.

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



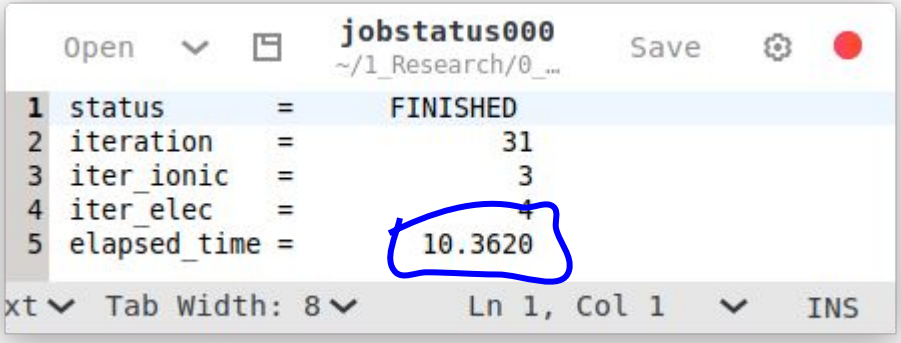
# SCF



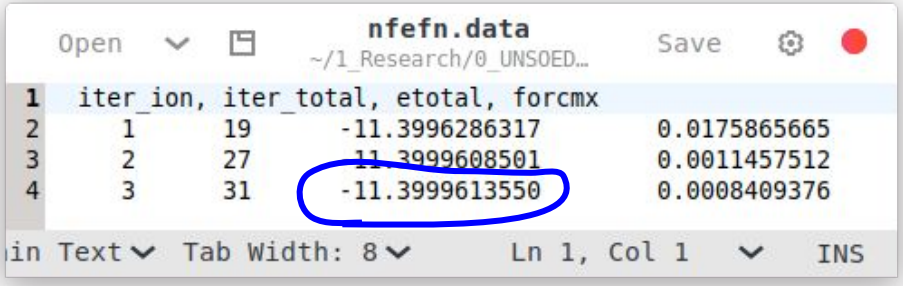

**mpirun -np 2 phase**

# Kalkulasi SCF



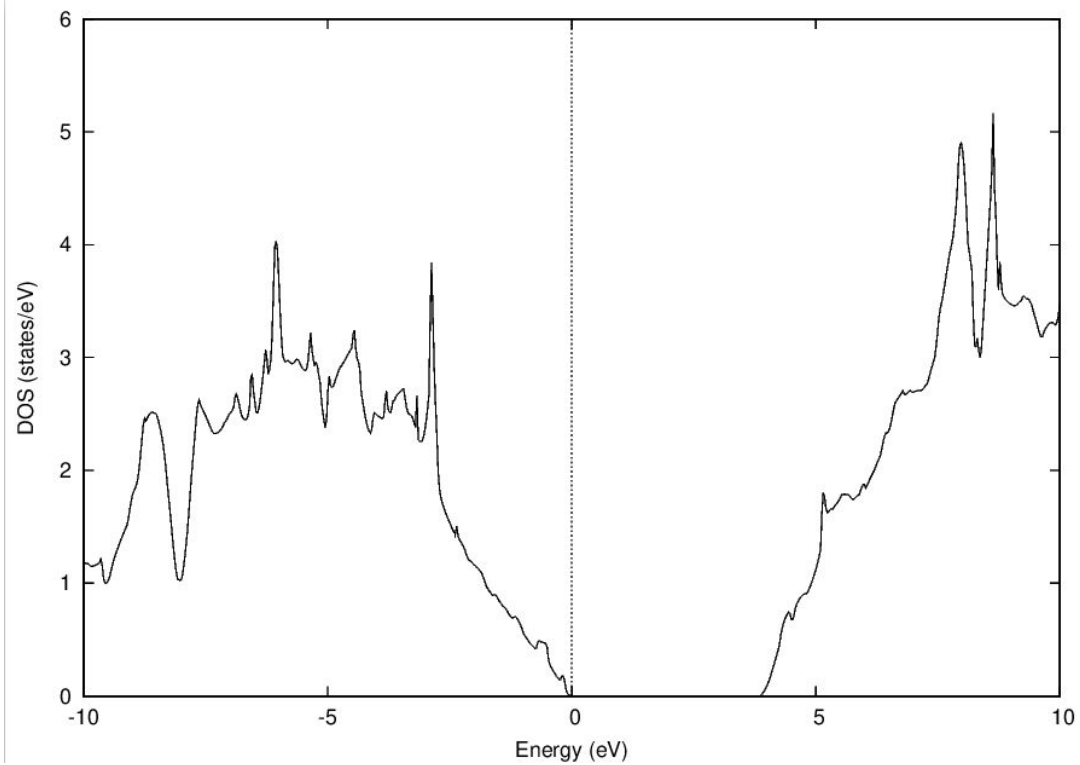

Kalkulasi telah selesai

dengan waktu 10 detik




Energi Total -11.399 Hartree

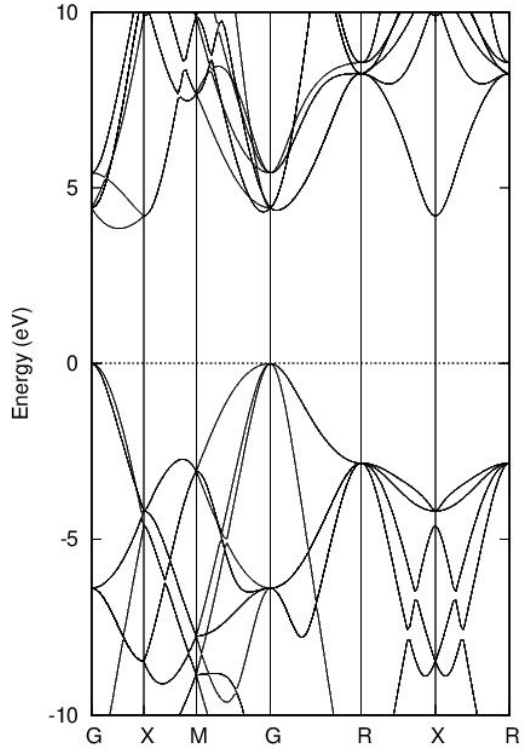
# Diamond (3D) DOS




```
mpirun -np 2 ekcal
```

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

# Diamond (3D) Band Structure



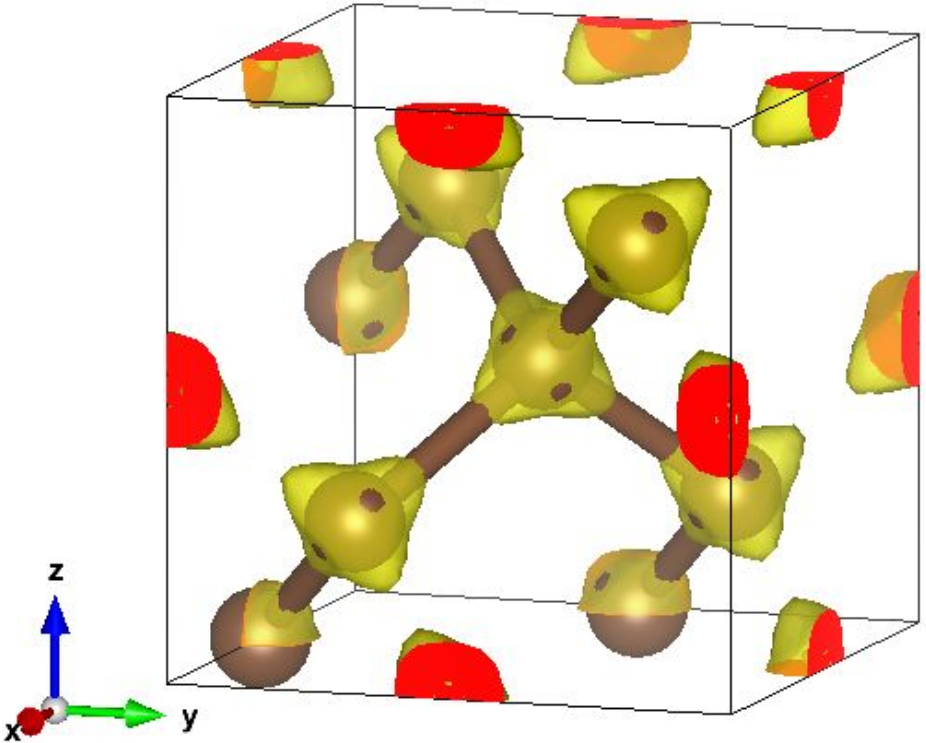

```
mpirun -np 2 ekcal
```

**Berapa band gap dari diamond?**

**Material Diamond apakah termasuk konduktor atau semikonduktor atau isolator?**

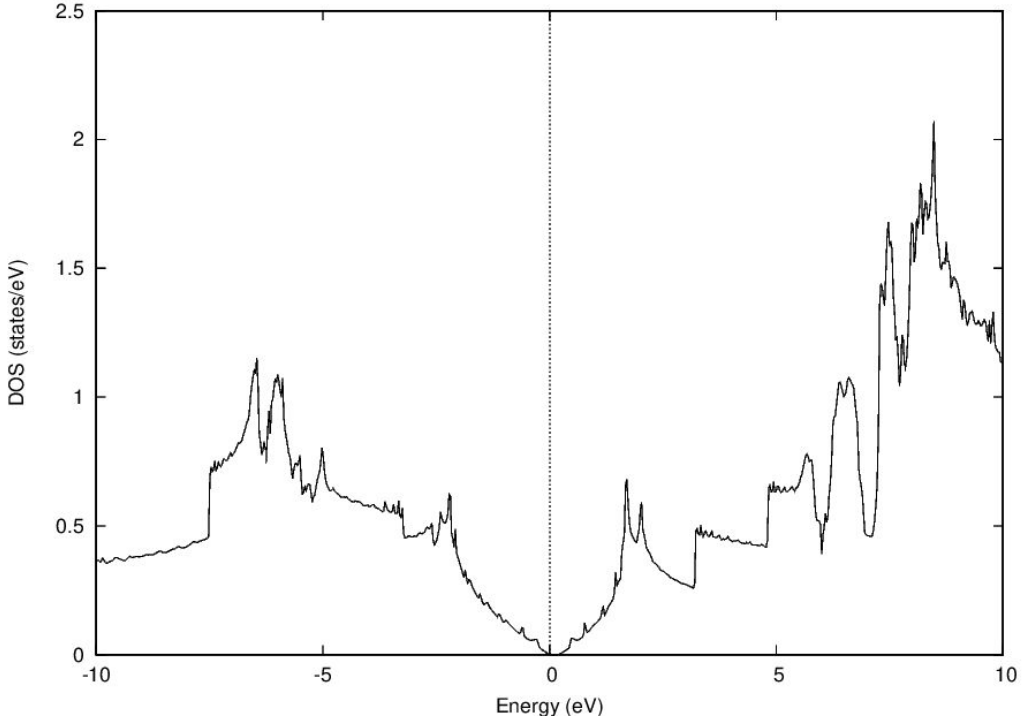
```
perl band.pl nfenergy.data bandkpt.in -with_fermi -color
```

# Diamond (3D) Charge Density




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

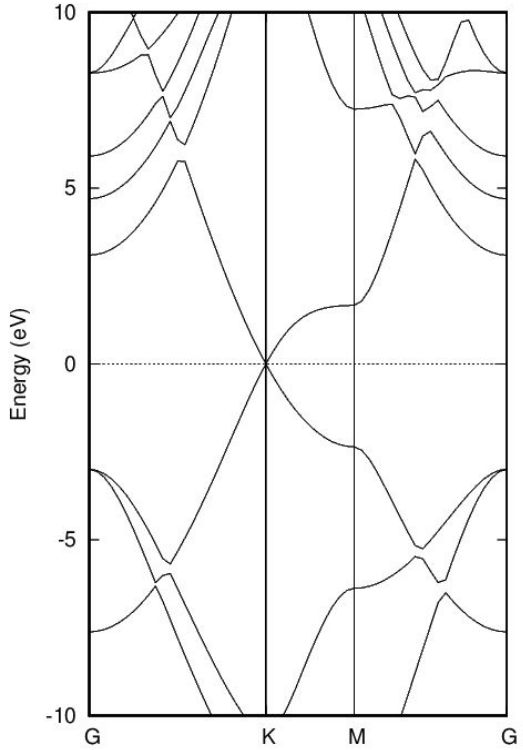
# Graphene (2D) DOS




**mpirun -np 2 ekcal**

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

# Graphene (2D) Band Structure



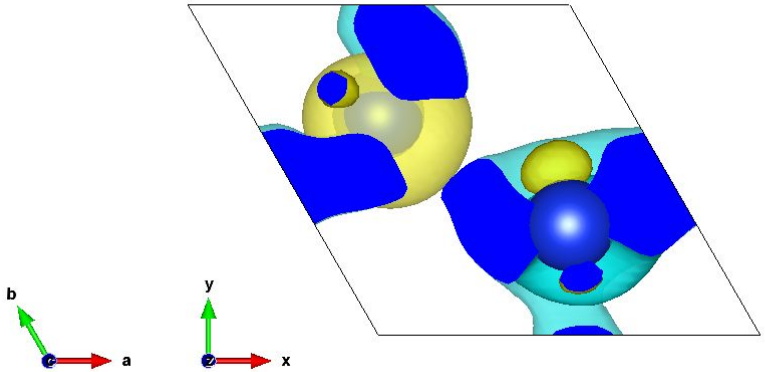

```
mpirun -np 2 ekcal
```

**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. Masukan 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

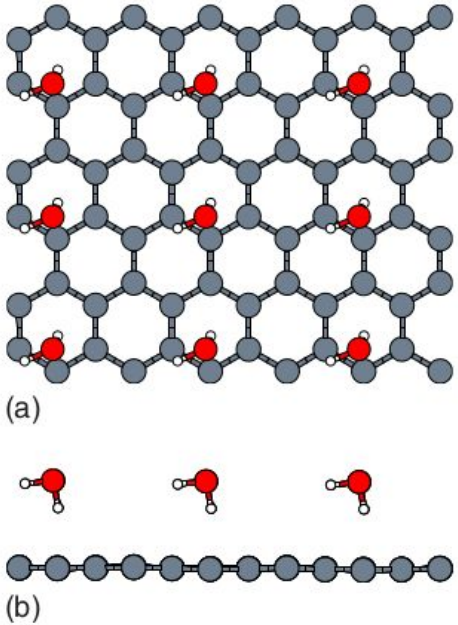
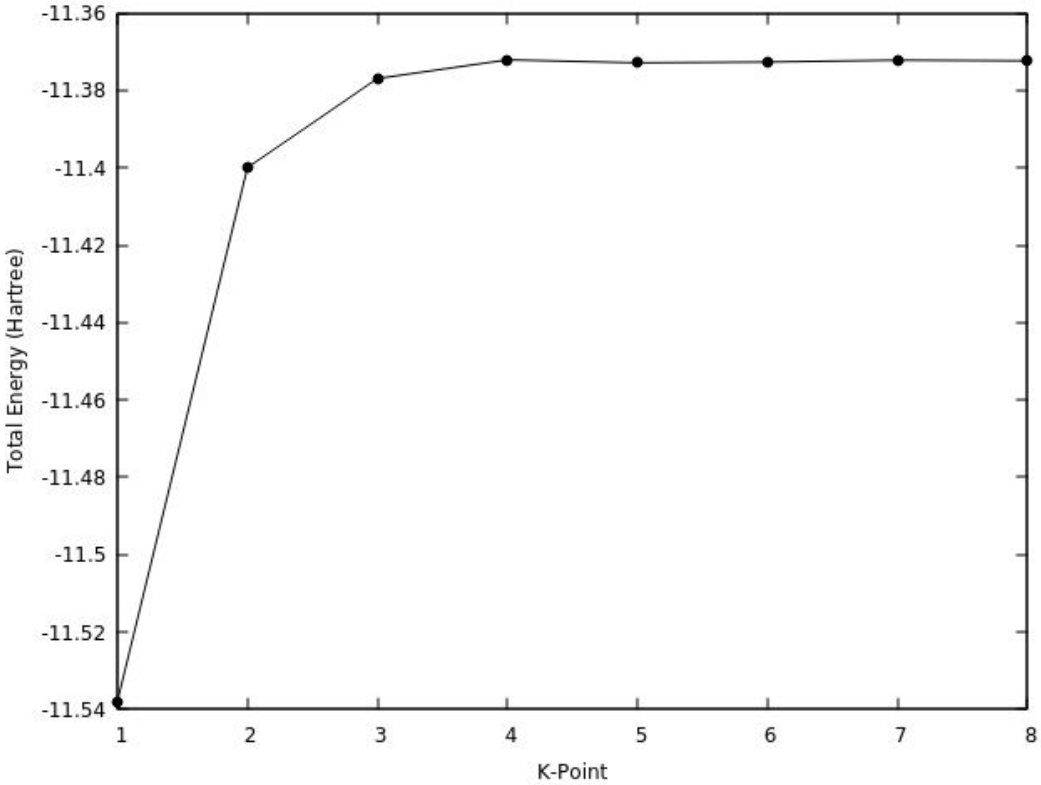



FIG. 1. (Color online) Water on the top of graphene: top and side views.

# Konvergensi Kpoint




Buatlah diagram konvergensi akurasi kpoint-mesh.

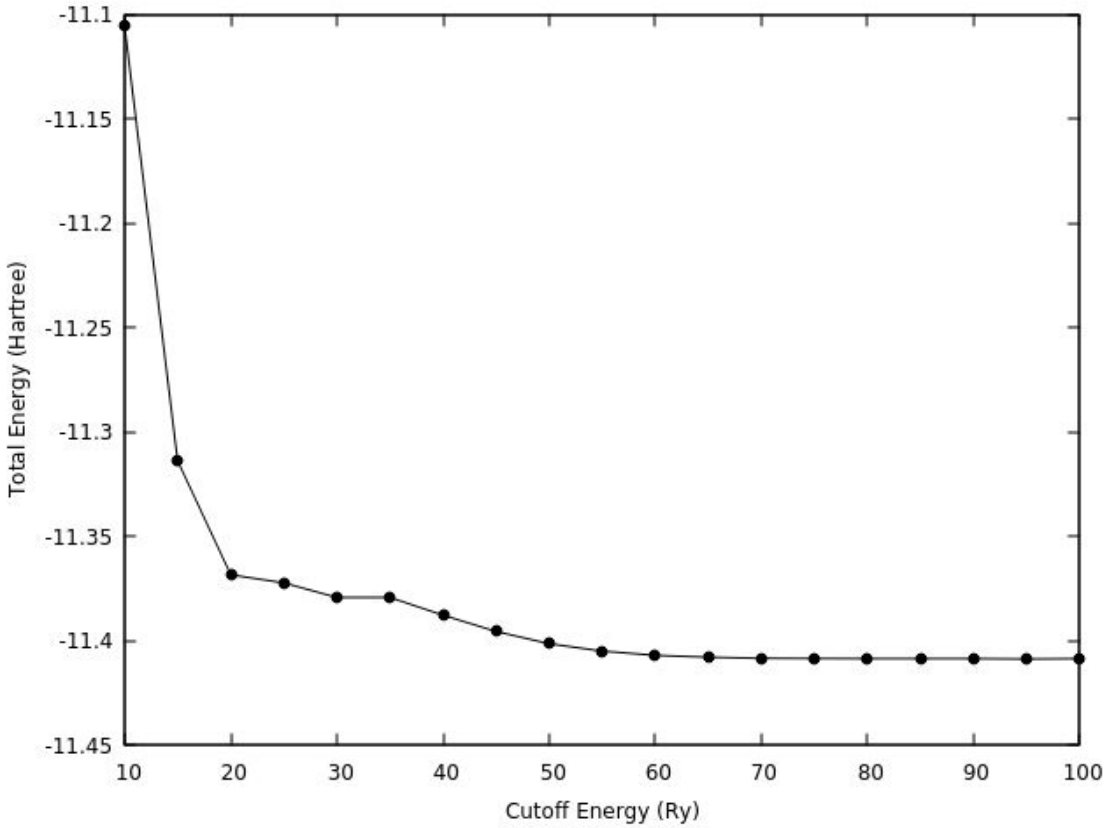
Dari 1x1x1, 2x2x1 … s.d. 10x10x1!

# 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
```

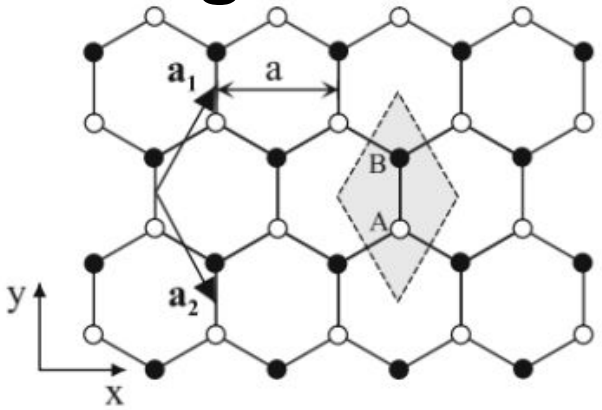
Plotting grafik dapat dilakukan dengan GnuPlot.

# Konvergensi Energi Cutoff




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

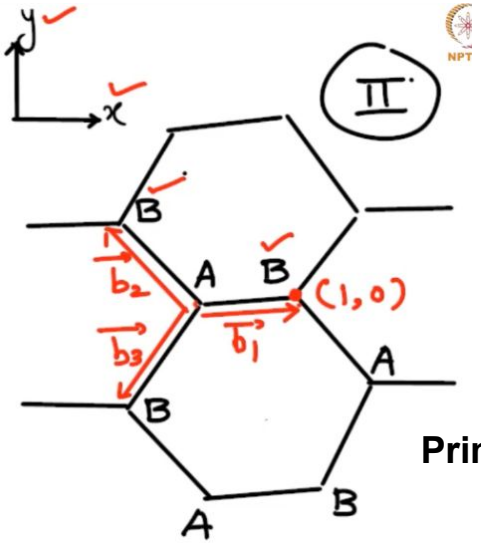
# Hexagonal Lattice Structure




Primitive Lattice Vector I

$$\vec{a_1} = a_0(\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y})$$

$$\vec{a_2} = a_0(\frac{1}{2}\vec{x} - \frac{\sqrt{3}}{2}\vec{y})$$




$a_0$= konstanta kisi graphene

Primitive Lattice Vector II

$$\vec{b_1} = a_0(1.\vec{x} + 0.\vec{y})$$

$$\vec{b_2} = a_0(-\frac{1}{2}\vec{x} + \frac{\sqrt{3}}{2}\vec{y})$$

Primitive Unit Cell Graphene