Selasa, 16 Maret 2023

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

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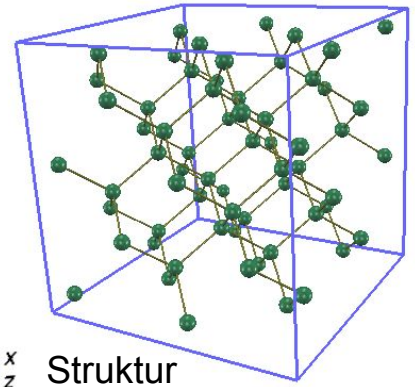
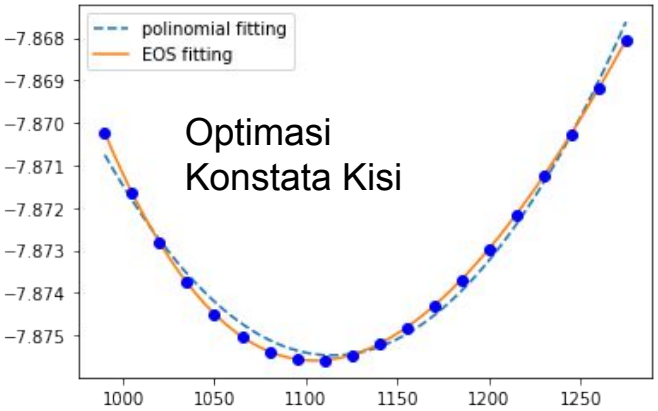
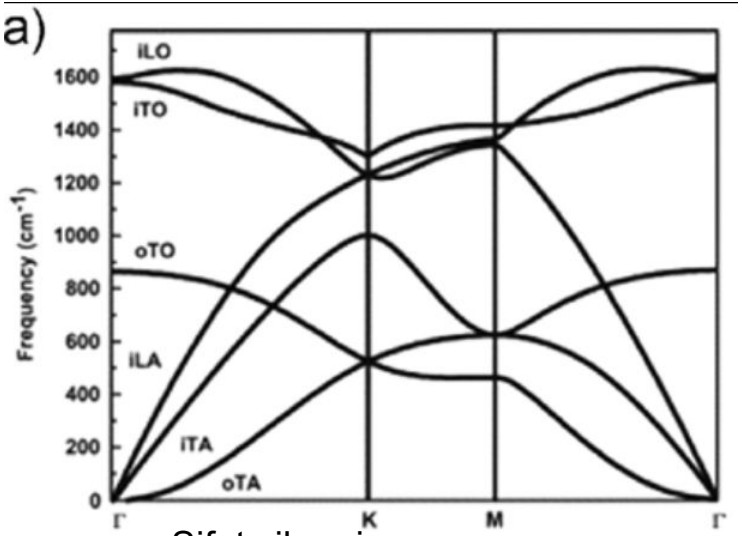
Rekayasa Komputasi Material



Struktur kristal



Optimasi Konstata Kisi

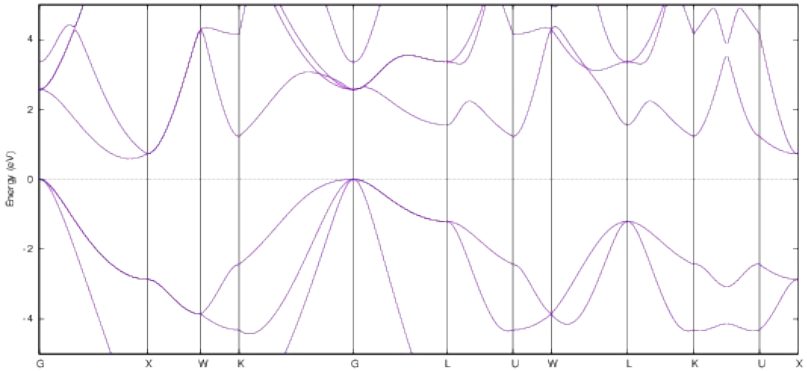


Sifat vibrasi (phonon dispersion)

- **Input:** Koordinat atomik

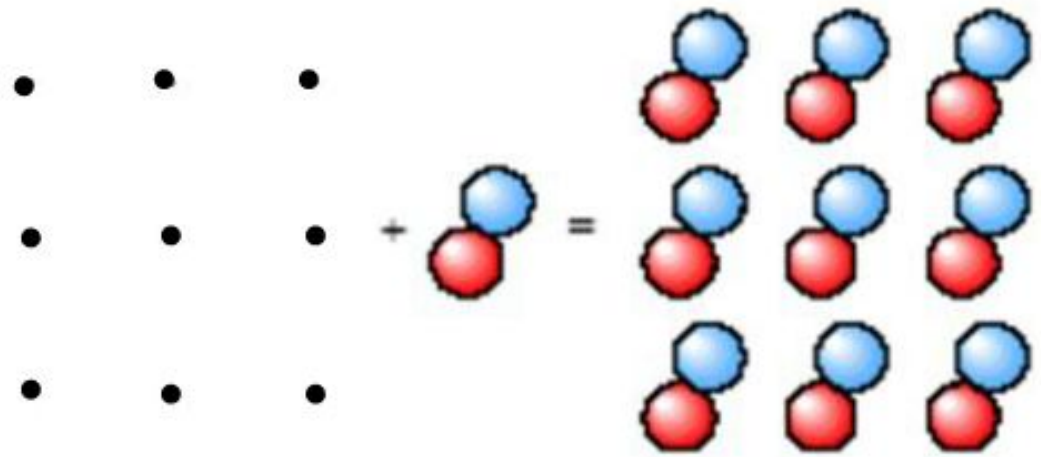
Density Functional Theory (DFT) + Komputasi Numerik + Komputer

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



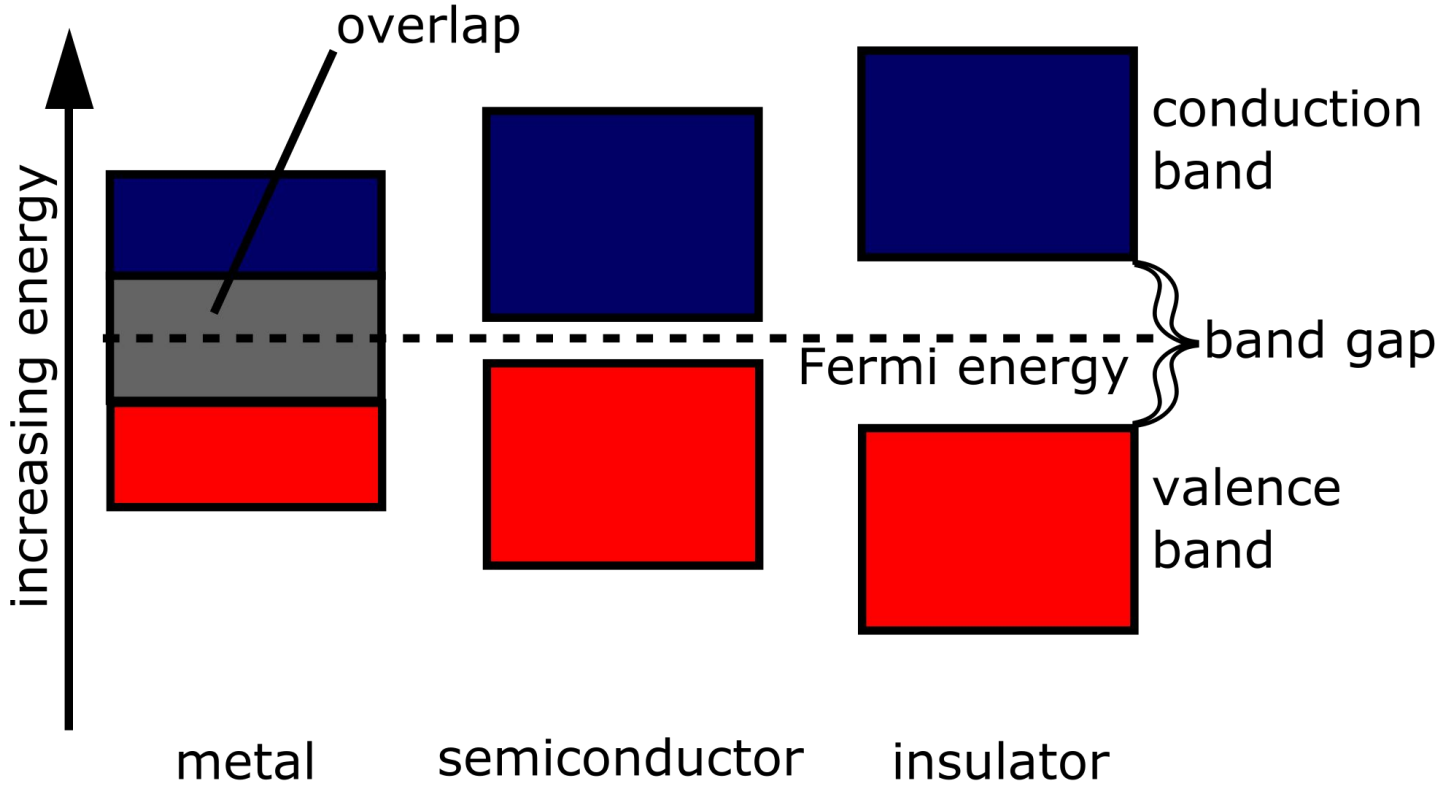
Struktur elektronik

Sistem Kristal



Kisi + Basis = Struktur Kristal

Struktur Band



Sifat Elektronik pada Material

Berdasarkan kemagnetannya material dibedakan menjadi 3:

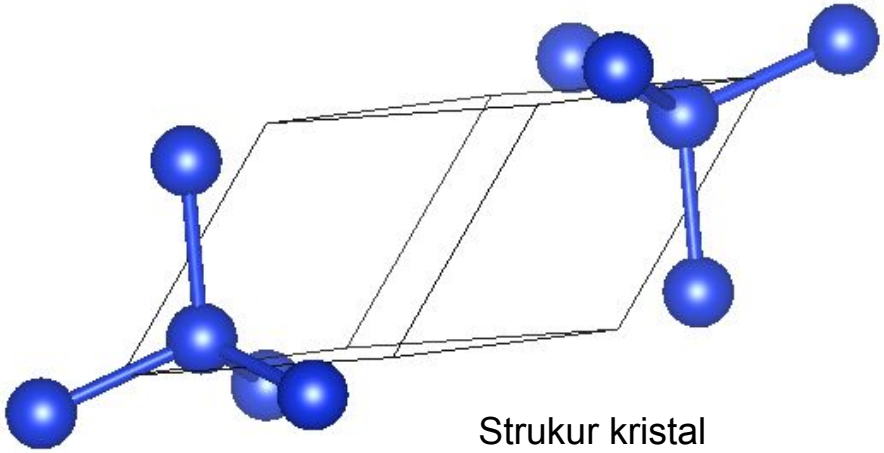
1. **Konduktor** : *conduction band* & *valence band* timpang tindih (*overlap*).
   Contoh: besi (Fe), tembaga (Cu) dll.
2. **Semikonduktor** : memiliki band gap sedang (0.1 - 4.0 eV).
   Contoh: Silicon, Germanium dll.
3. **Isolator** : memiliki band gap besar (> 4.0 eV)
   Contoh: Diamond, kaca

Silicone (3D)

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

Berapa atom Atom Si di unit sel?

Berapa lattice constant pada Si?



Strukur kristal primitiv Silicon

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

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

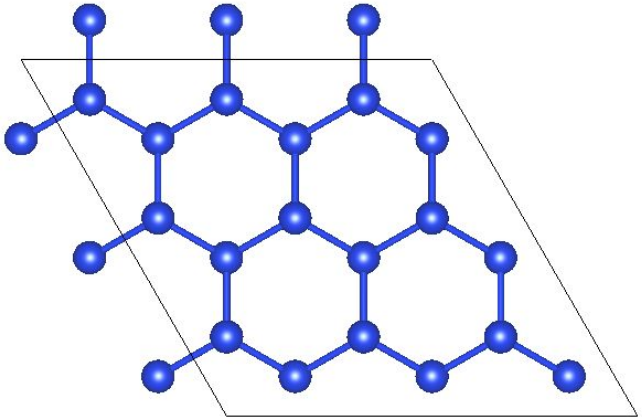
$$a_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

Silicene (2D)

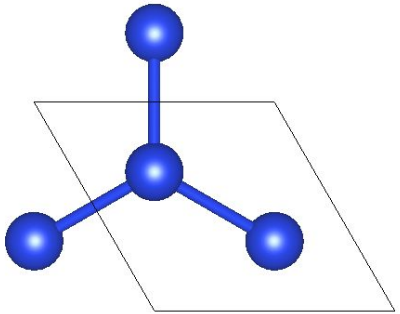
Struktur kristal unit sel Si (3D) adalah diamond FCC.

Berapa atom Atom Si di unit sel?

Berapa lattice constant pada Silicene?



Super sel 3x3x1 silicene

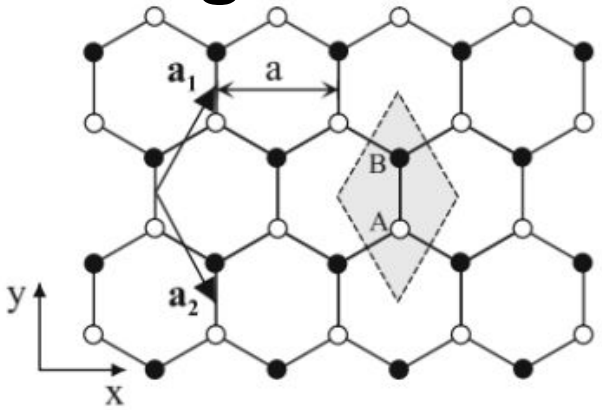


Strukur kristal primitif silicene

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

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

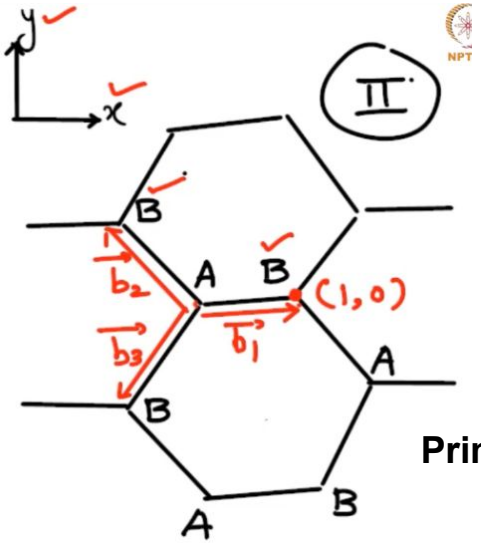
Hexagonal Lattice Structure



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

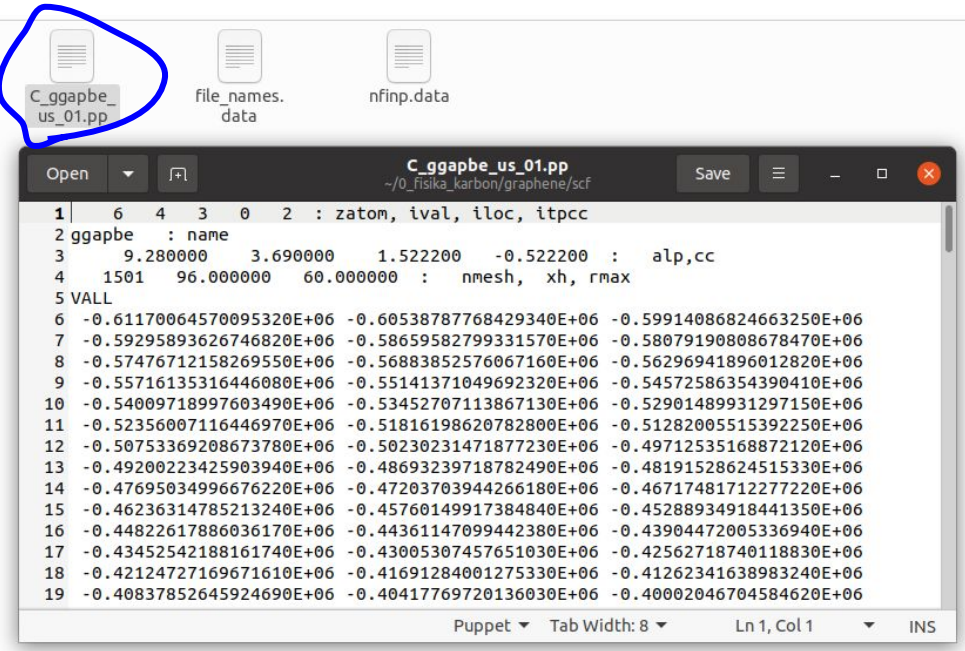
```
Control{
    cpumax = 3600 sec
    condition = Initial
}
accuracy{
    cutoff_wf = 25.00 rydberg
    cutoff_cd = 225.00 rydberg
    num_bands = 16
    ksampling{
        mesh{
            nx = 2
            ny = 2
            nz = 1
        }
    }
}
structure{
    unit_cell_type = primitive
    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.

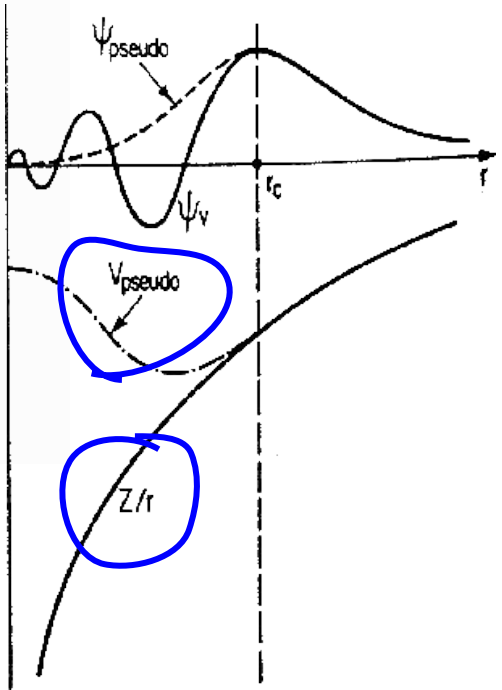
File pseudopotential



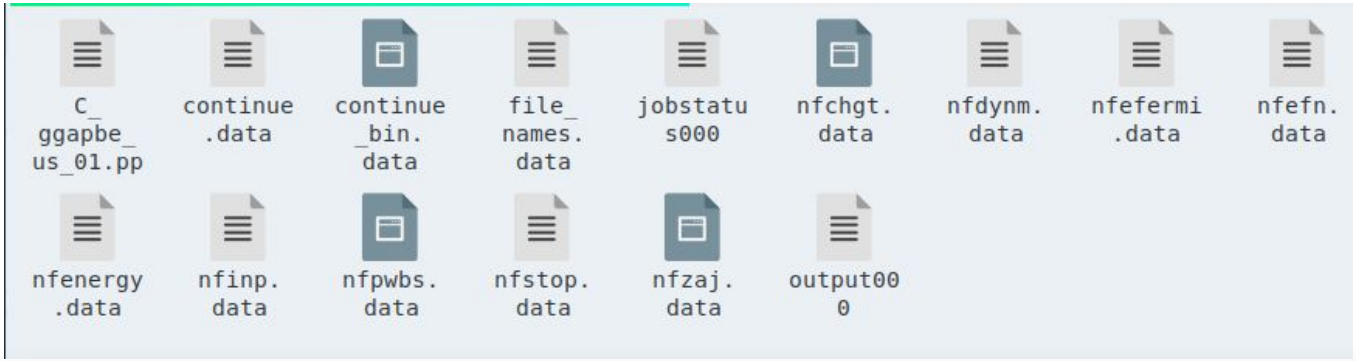
File pseudopotential ada di **phase/samples**

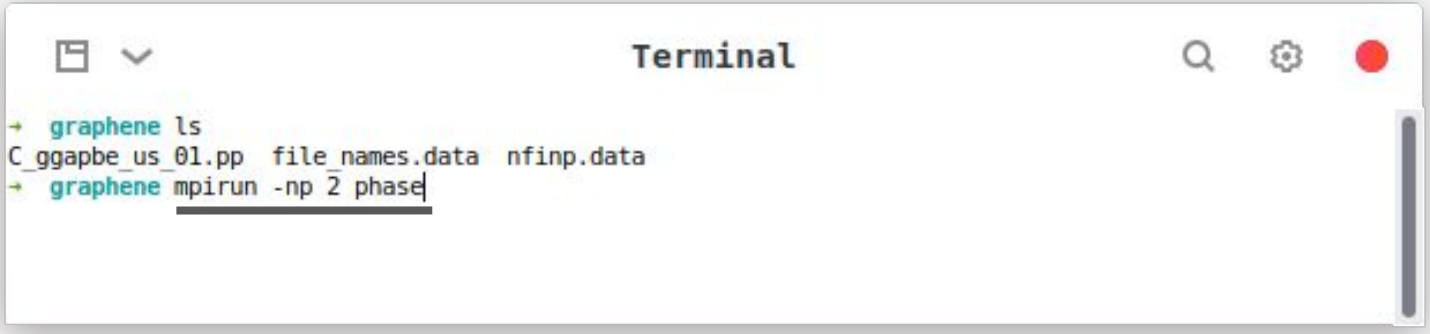
Pseudopotential digunakan untuk mengaproksimasi bentuk potential yang ekstrim.

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



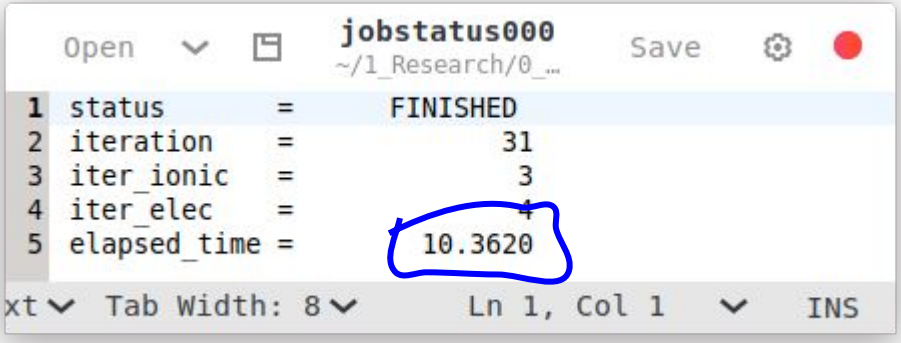
SCF





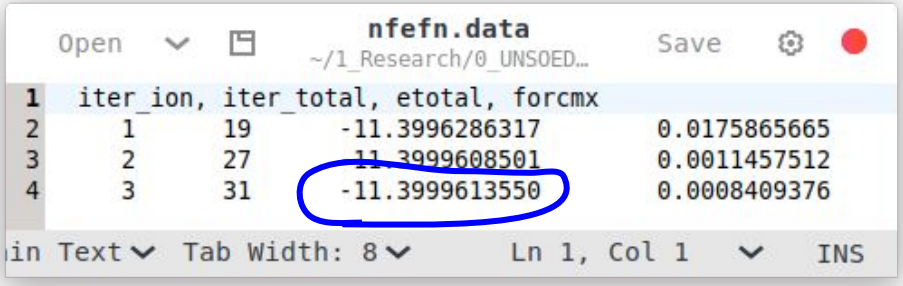
mpirun -np 2 phase

Kalkulasi SCF



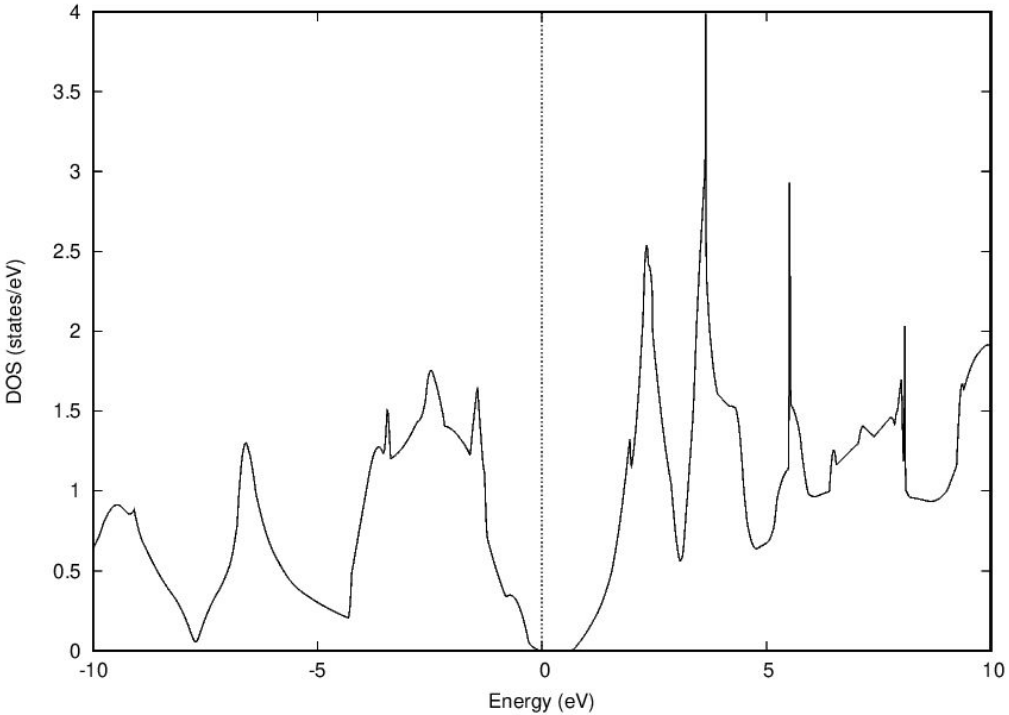
Kalkulasi telah selesai

dengan waktu 10 detik



Energi Total -11.399 Hartree

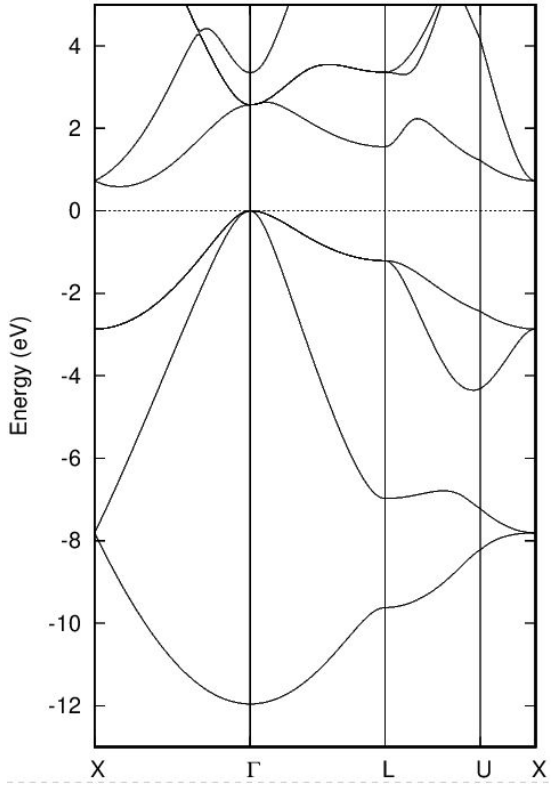
Silicon (3D) DOS




```
mpirun -np 2 ekcal
```

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

Silicon (3D) Band Structure



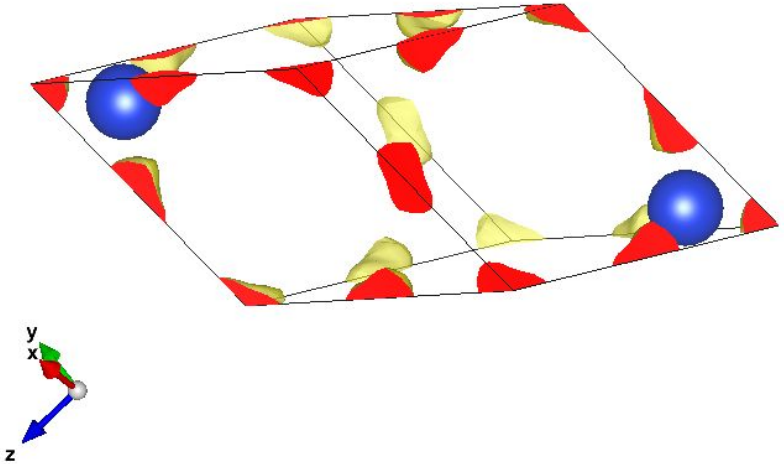

```
mpirun -np 2 ekcal
```

Berapa band gap dari silicene?

Material Silicene apakah termasuk konduktor atau semikonduktor?

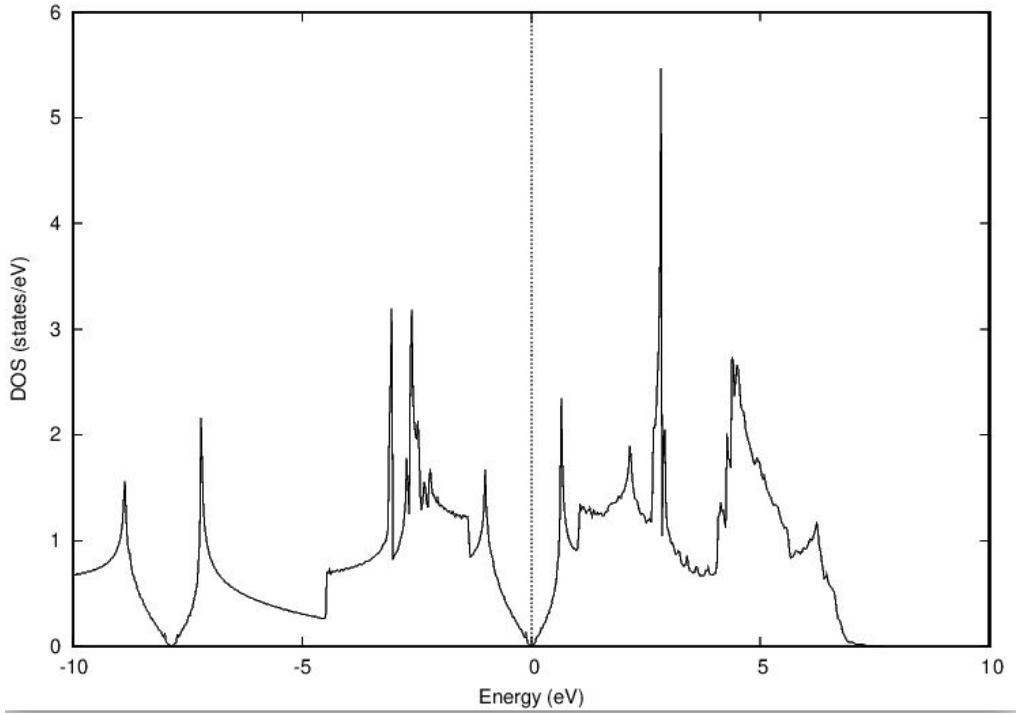
```
perl band.pl nfenergy.data bandkpt.in -with_fermi -color
```

Silicone (3D) Charge Density



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

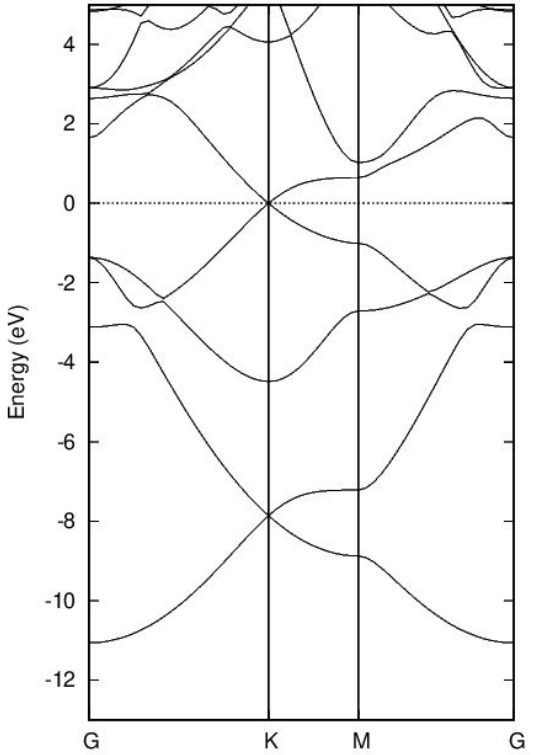
Silicene (2D) DOS




```
mpirun -np 2 ekcal
```

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

Silicene (2D) Band Structure



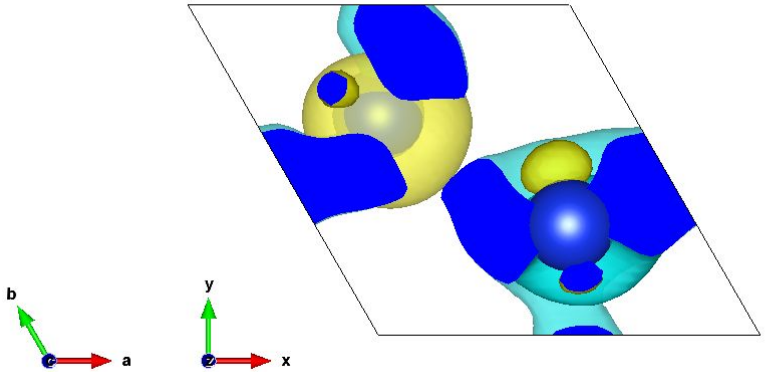

```
mpirun -np 2 ekcal
```

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

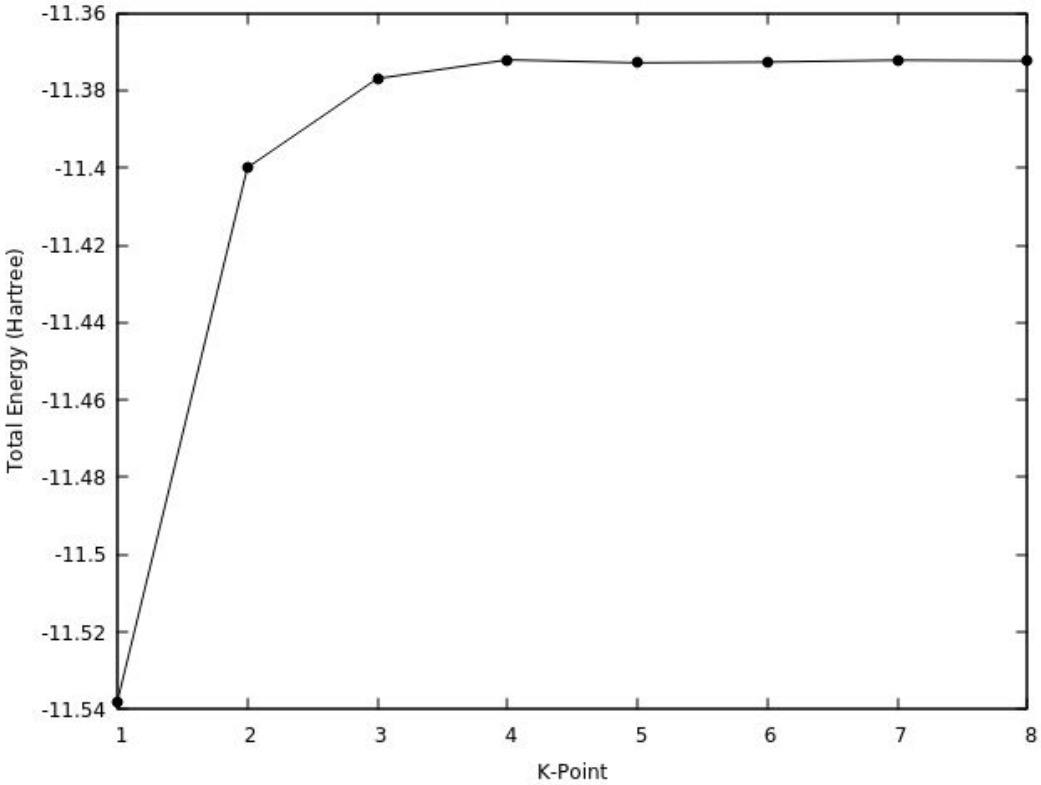


1. Buka aplikasi Vesta
2. Masukan nfchr.down.cube dengan drag
3. Pilih edit -> volumetric data -> import -> subtract -> nfchr.down.cube

Tugas!

1. Pelajarilah aplikasi webmo!
2. Buatlah struktur molekul NO dengan webmo!
   Hasil adalah file POSCAR

Konvergensi Kpoint



Buatlah diagram konvergensi akurasi kpoint-mesh.

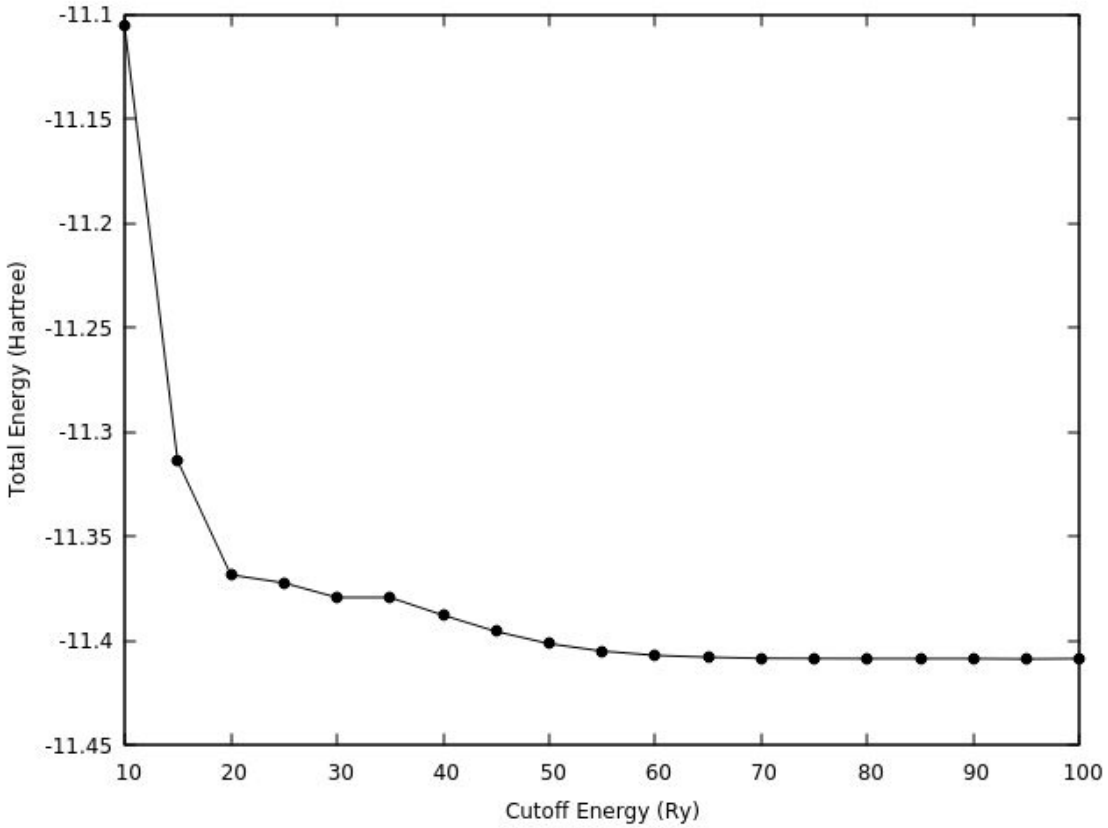
Dari 1x1x1, 2x2x1 … s.d. 10x10x1!

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
```

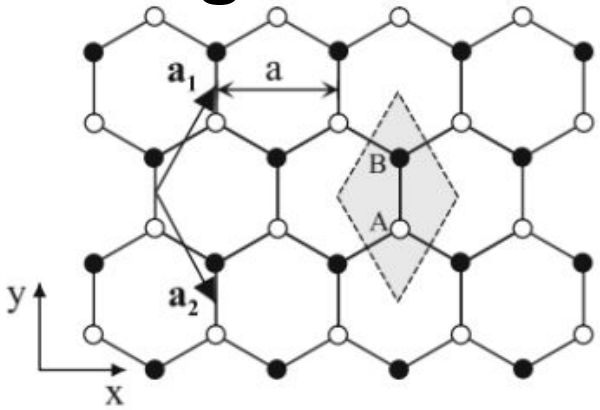
Plotting grafik dapat dilakukan dengan GnuPlot.

Konvergensi Energi Cutoff



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

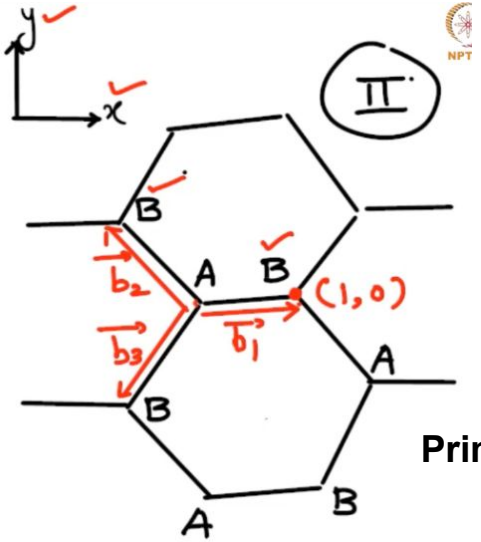
Hexagonal Lattice Structure



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