Selasa, 30 Mei 2023

Struktur Elektronik: Platinum

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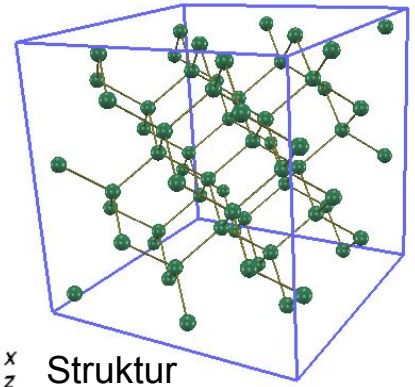
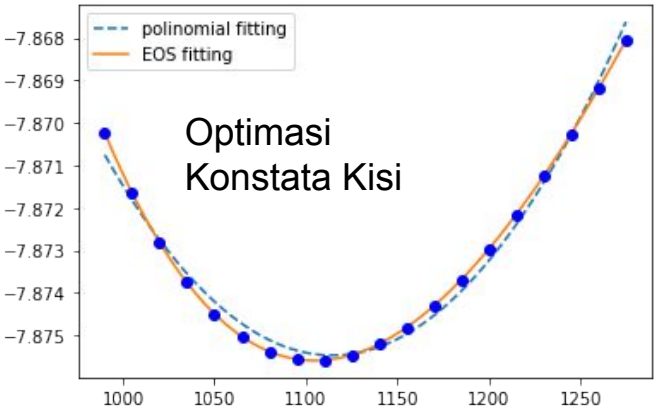
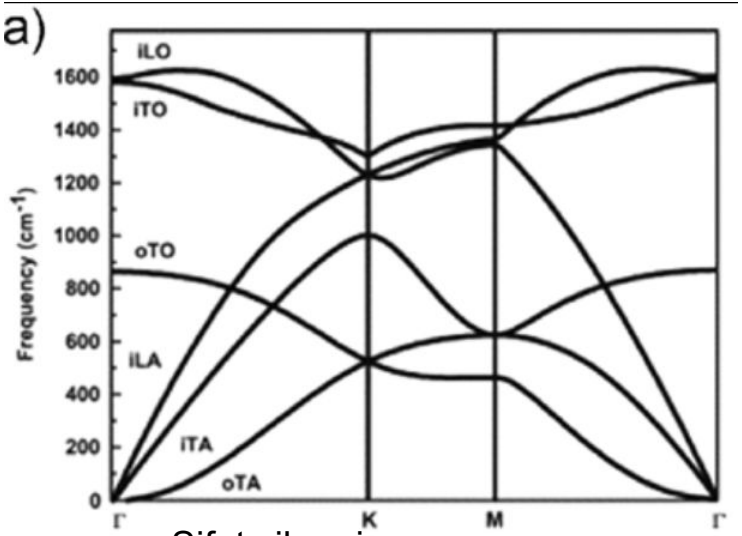
Rekayasa Komputasi Material



Struktur kristal



Optimasi Konstata Kisi

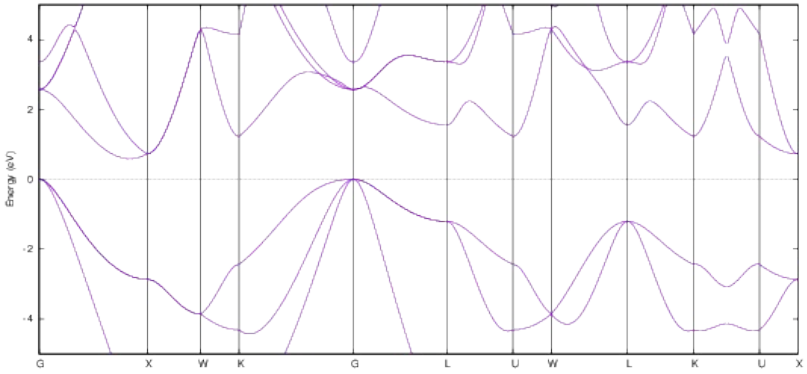


Sifat vibrasi (phonon dispersion)

- **Input:**
  Koordinat atomik

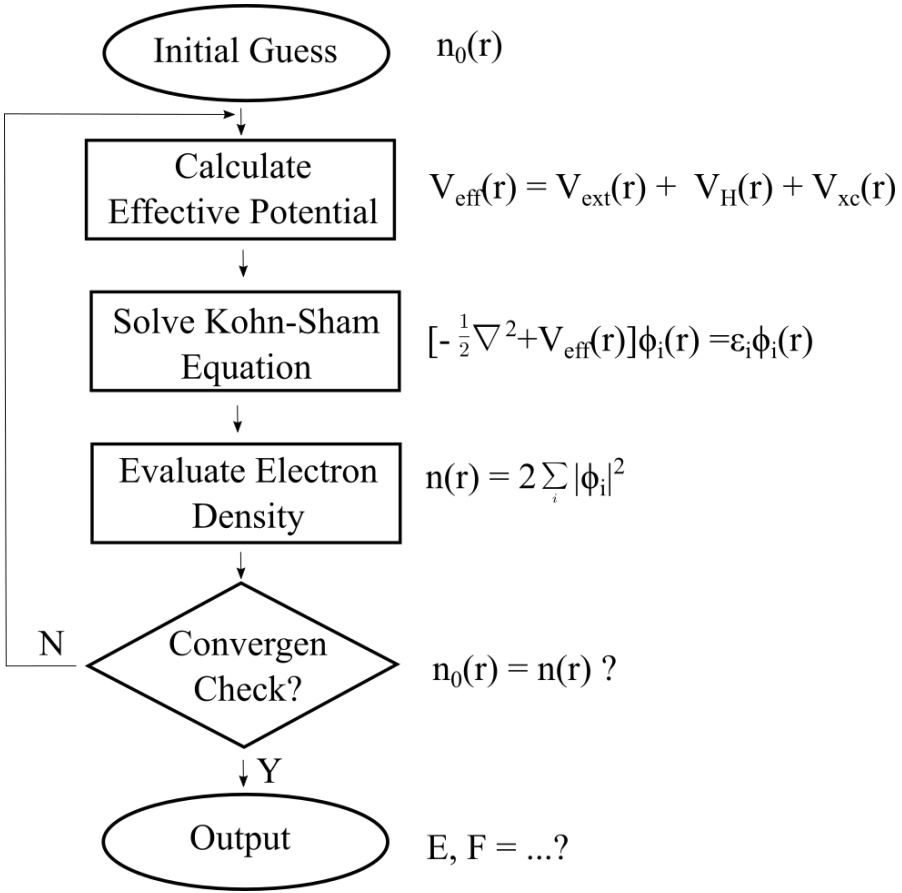
Density Functional Theory (DFT) + Komputasi Numerik + Komputer

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



Struktur elektronik

Density Functional Theory (Kohn-Sham Equation)



- $n_0(r)$: Initial electron density

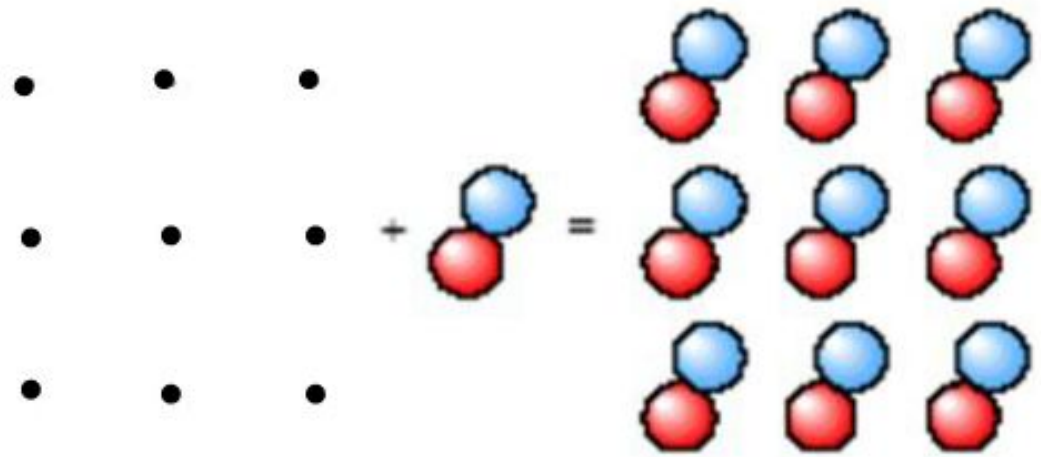
- V_{eff} : Effective potential
- V_{ext} : External potential
- V_h : Hartree potential
- V_{xc} : Exchange-Correlation potential

- $-½\nabla^2$: Kinetic Energy
- Φ_i : Kohn-Sham Orbitals

- E : Total Energy
- F : Total Force

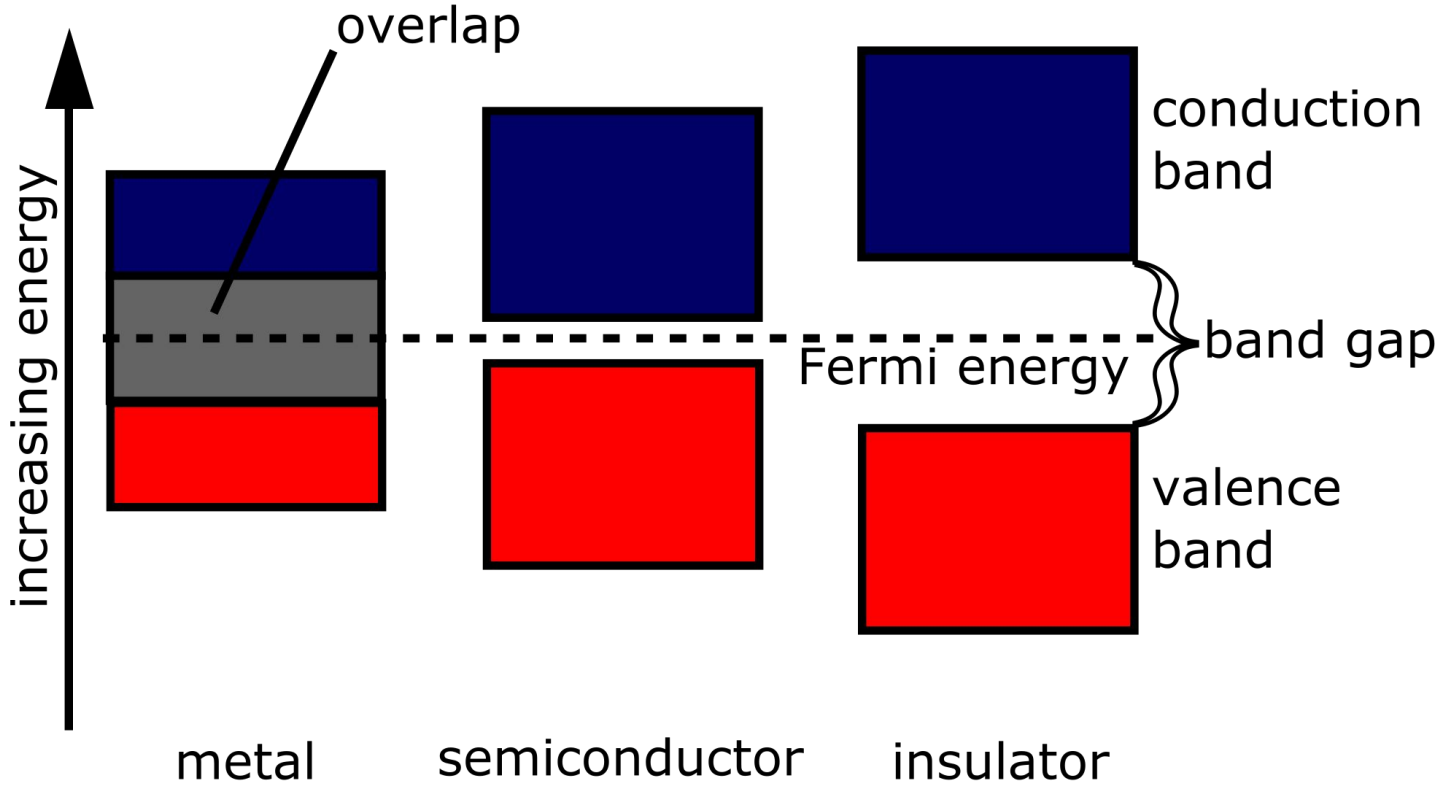
SCF Iteration method for DFT calculation

Sistem Kristal



Kisi + Basis = Struktur Kristal

Struktur Band

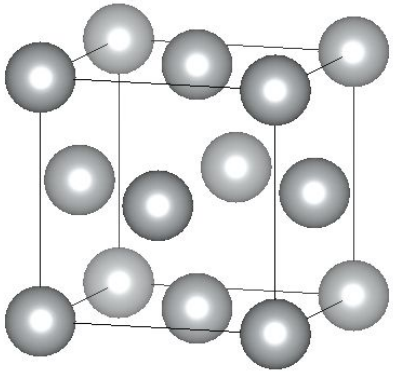


Sifat Elektronik pada Material

Berdasarkan kemagnetannya material dibedakan menjadi 3:

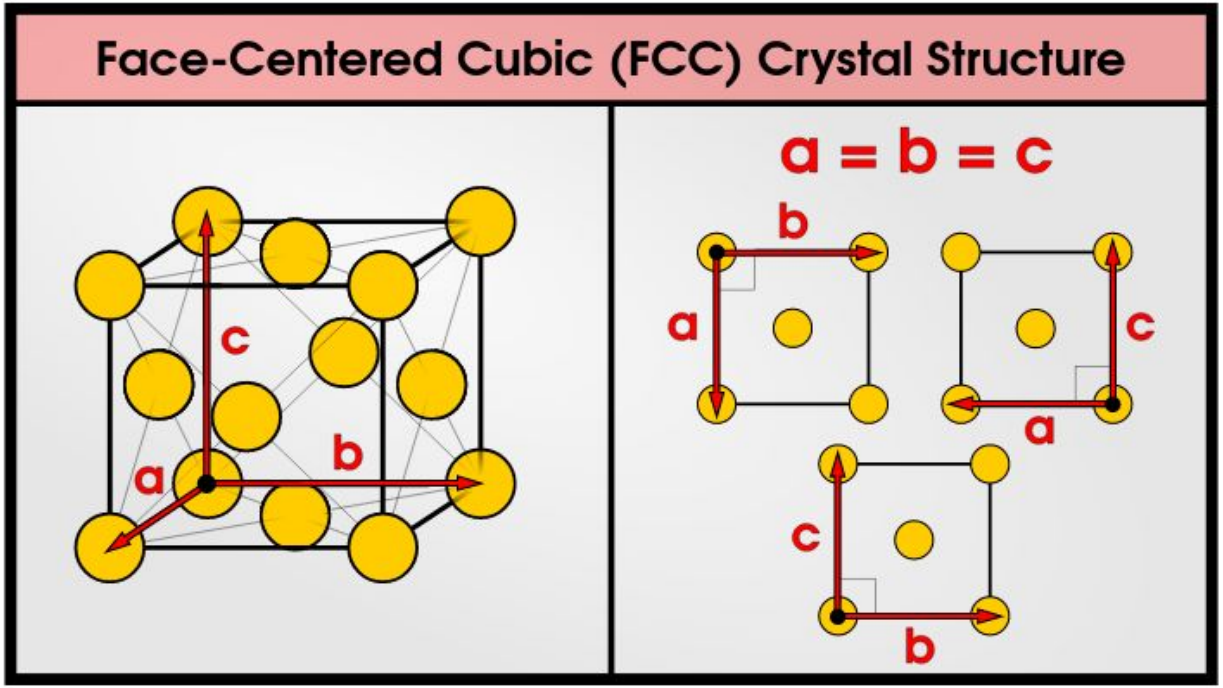
1. **Konduktor** : *conduction band* & *valence band* timpang tindih (*overlap*).
   Contoh: besi (Fe), tembaga (Cu) dll.
2. **Semikonduktor** : memiliki band gap sedang (0.1 - 4.0 eV).
   Contoh: Silicon, Germanium dll.
3. **Isolator** : memiliki band gap besar (> 4.0 eV)
   Contoh: Diamond, kaca

Platinum (Pt)

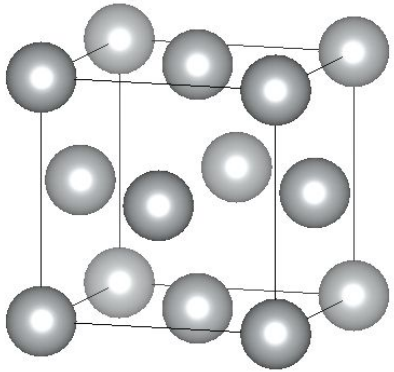


Struktur kristal unit sel Platinum (Pt) adalah Face Center Cubic (FCC).

Berapa atom Pt pada sebua unit sel Platinum?

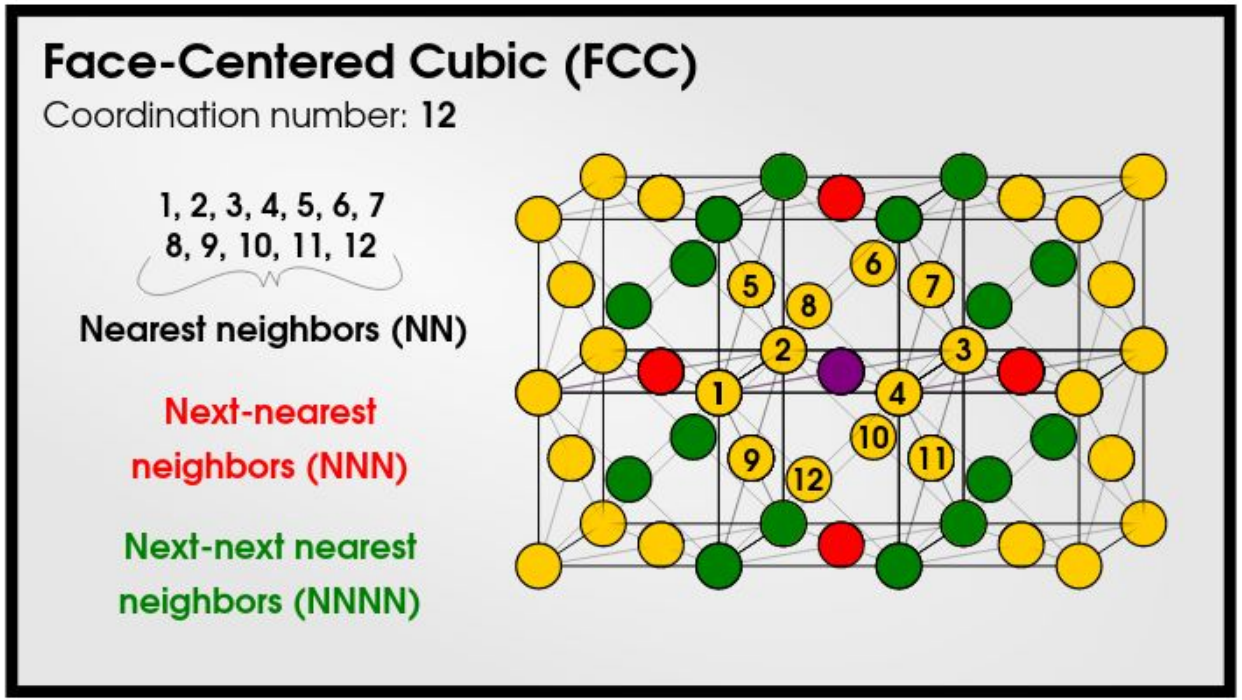


Platinum (Pt)

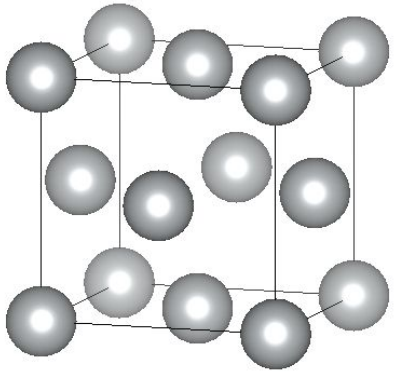


Struktur kristal unit sel Platinum (Pt) adalah Face Center Cubic (FCC).

Berapa atom tetangga pada sebuah atom Pt?



Platinum (Pt)



Struktur kristal unit sel Platinum (Pt) adalah Face Center Cubic (FCC).

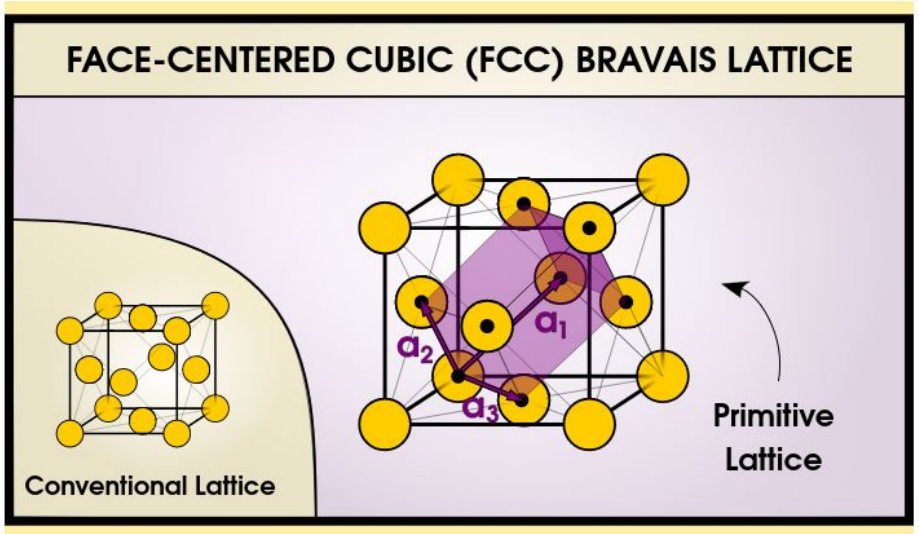
Vektor kisi Platinum

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

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

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

Unit sel Primitif Platinum (Pt)



Vektor unit sel primitif Platinum (Pt)

Berapa atom Pt pada sebuah unit sel primitif Platinum (Pt)?

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

file_names.data
~/1_Research/0_UNSOED_Research/3_FISIKA_CA…TURE/1_Fisi

```
&fnames
 F_INP    = './input_bcc_Fe.data'
 F_POT(1) = '../pp/Fe_ggapbe_paw_us_02.pp'
 F_ENERG  = './nfenergy.data'
 F_CHGT   = './nfcharge.data'
 F_ZAJ    = './zaj.data'
/

```

filenames.data digunakan untuk mengidentifikasi

file **input** dan **pseudopotential**.

Ubah nama file pada **F_POT(1)** dengan nama

Pseudopotential yang sesuai (**Fe_ggapbe_paw_us_02.pp**)

nfinp.data

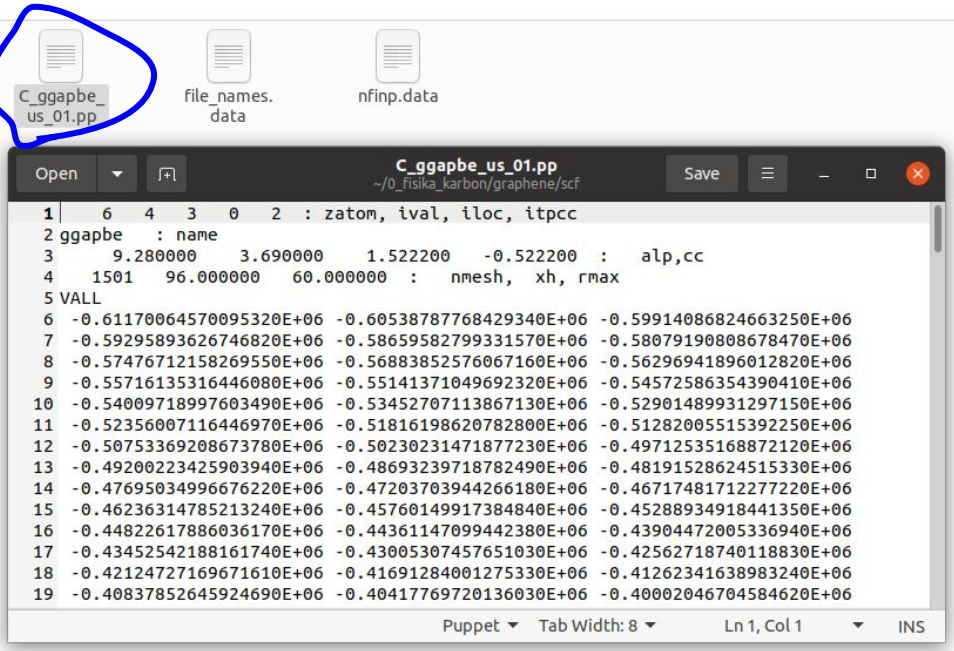
```
Control{
    cpumax = 3600 sec
    condition = Initial
}
accuracy{
    cutoff_wf = 25.00 rydberg
    cutoff_cd = 225.00 rydberg
    num_bands = 16
    ksampling{
        mesh{
            nx = 2
            ny = 2
            nz = 1
        }
    }
}
structure{
    unit_cell_type = primitive
    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 **Iron (Fe)**, **graphene**, **diamond**, **stanene**, **silicine** dlsb, tergantung konfigurasi pada block tsb.

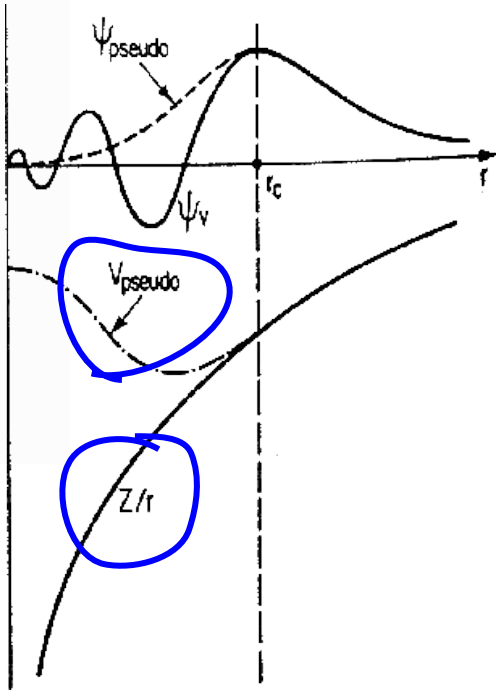
File pseudopotential



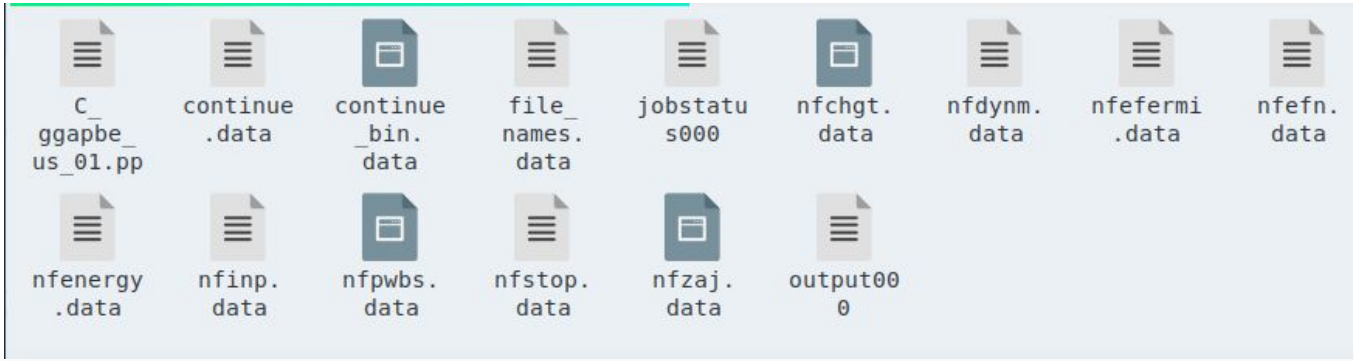
File pseudopotential ada di **phase/samples**

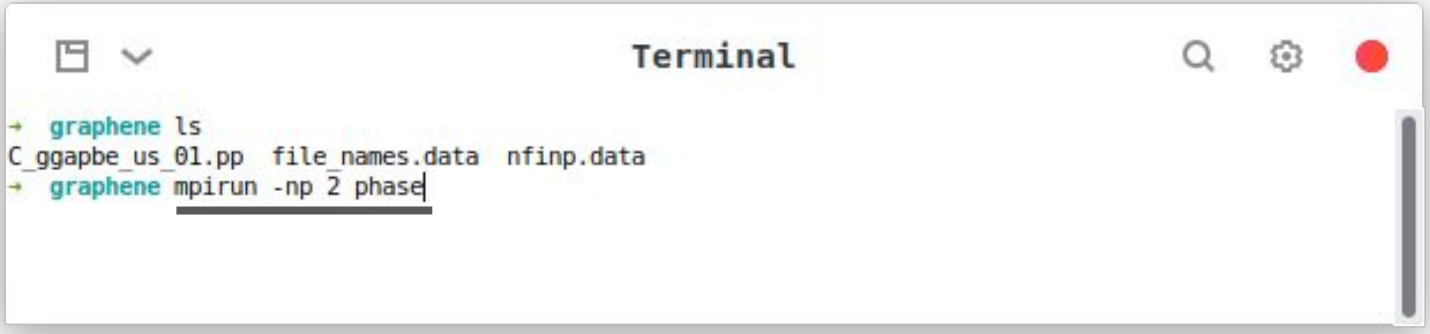
Pseudopotential digunakan untuk mengaproksimasi bentuk potential yang ekstrim.

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



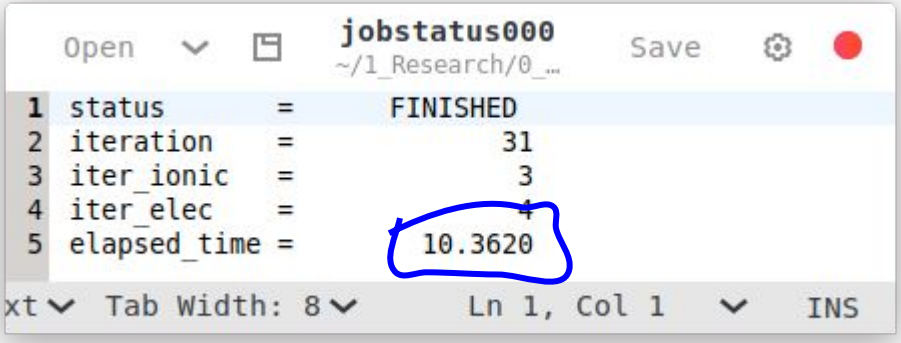
SCF





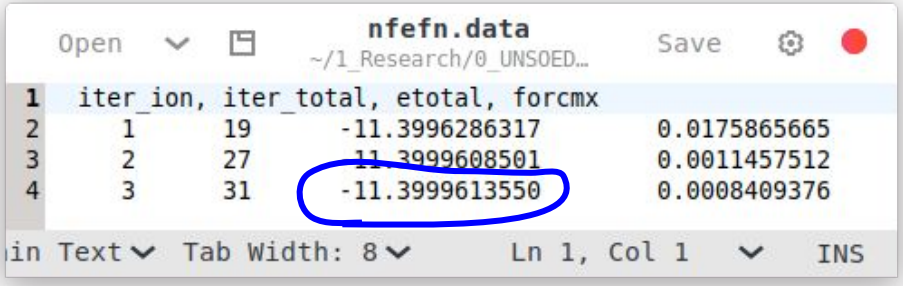
mpirun -np 2 phase

Kalkulasi SCF Platinum



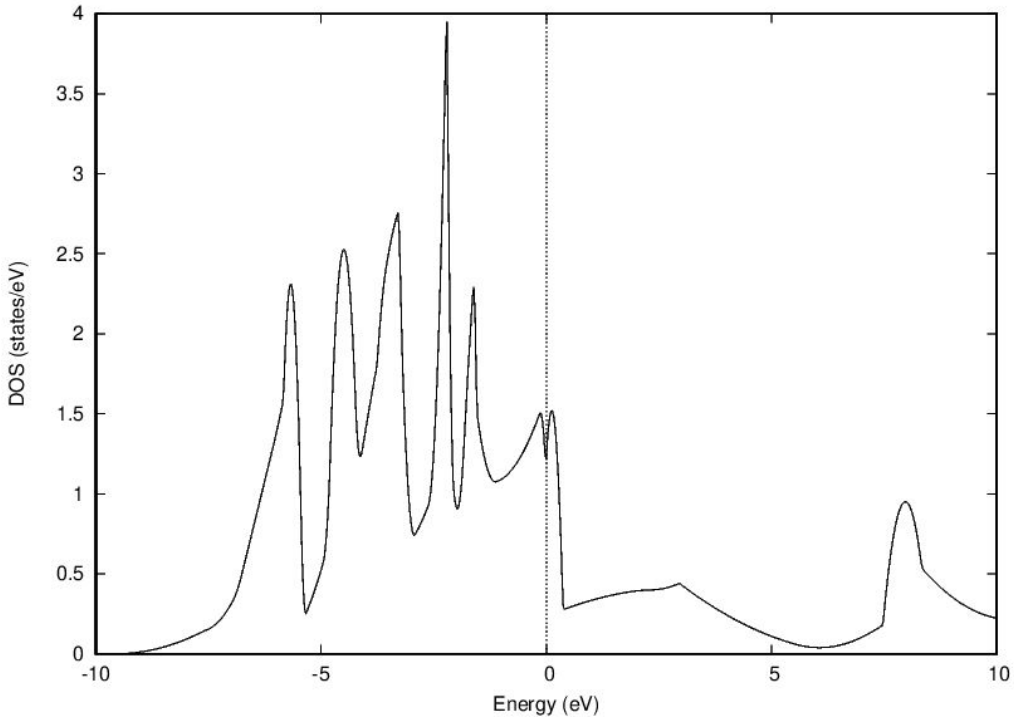
Kalkulasi telah selesai

dengan waktu 10 detik



Energi Total -11.399 Hartree

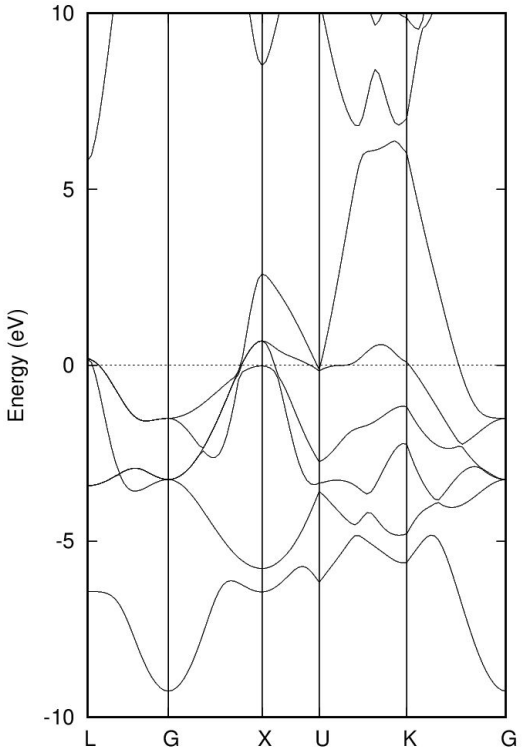
Platinum DOS




```
mpirun -np 2 ekcal
```

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

Platinum Band Structure



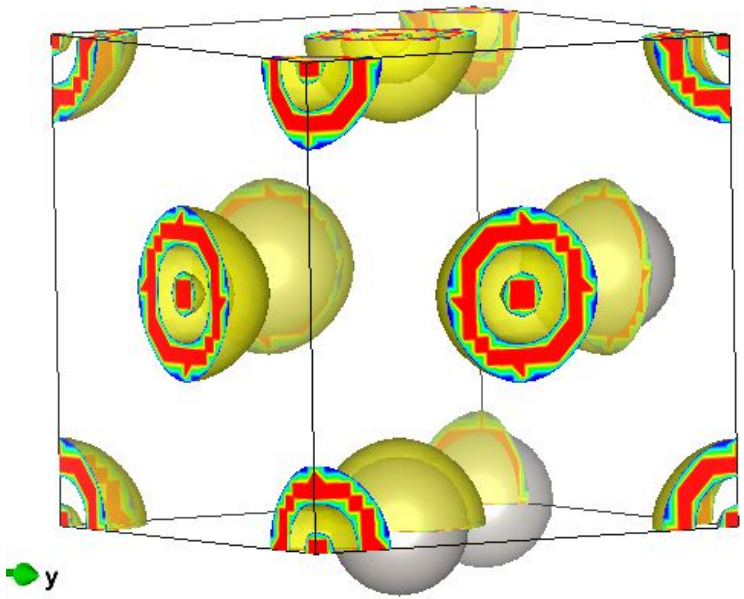
mpirun -np 2 ekcal

Berapa band gap dari platinum?

Material platinum apakah termasuk konduktor atau semikonduktor atau isolator?

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

Platinum (3D) Charge Density



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