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Fisika Magnet: Komputasi Material Iron (Fe)

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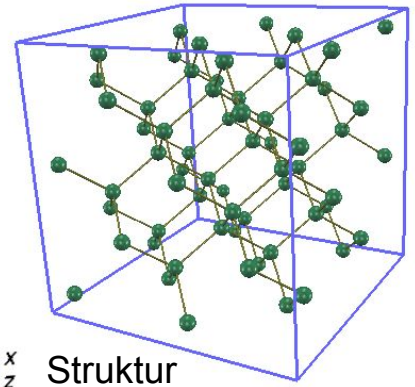
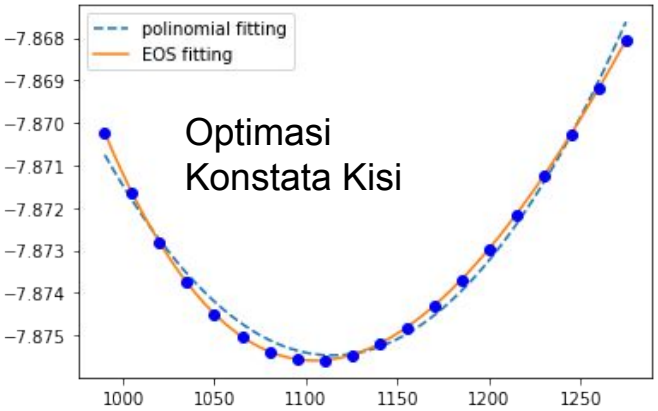
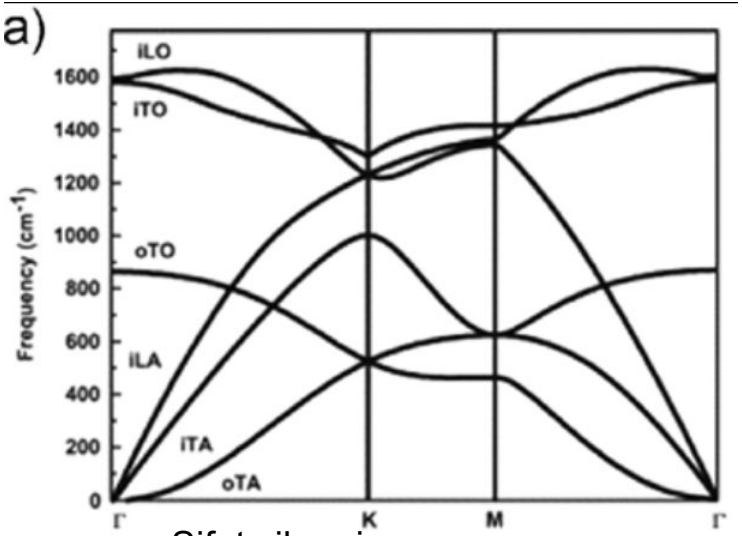
Rekayasa Komputasi Material



Struktur kristal



Optimasi Konstata Kisi

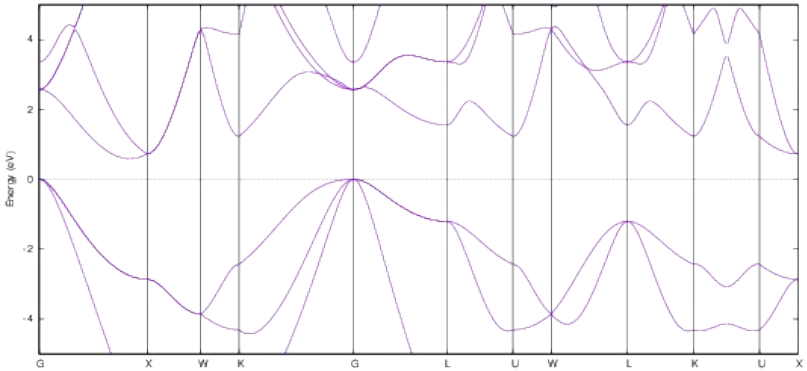


Sifat vibrasi (phonon dispersion)

Density Functional Theory (DFT) + Komputasi Numerik + Komputer

- **Input:**
  Koordinat atomik

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



Struktur elektronik

Sifat Magnet pada Material

Suseptibilitas Magnetik (χ) :
-> Ukuran Material untuk memiliki sifat kemagnetan saat berada di dalam medan magnet.

$$\chi = M/H$$

M = Momen magnetik per unit volume
H = Intensitas medan magnetik

Sifat Magnet pada Material

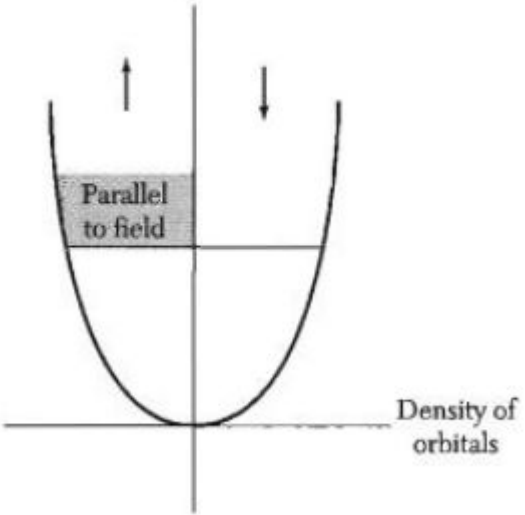
Berdasarkan kemagnetannya material dibedakan menjadi 3:

1. **Paramagnetik** : Suseptibilitas Magnetik **negatif** dan **kecil**, kemagnetan lemah.
   Contoh: magnesium, molybdenum, lithium, dan tantalum
2. **Diamagnetik** : Suseptibilitas Magnetik **positif** dan **kecil**, Kemagnetan lemah.
   Contoh: copper, silver, dan gold
3. **Feromagnetik** : Suseptibilitas Magnetik **positif** dan **tinggi**, kemagnetan kuat.
   Contoh: Iron, nickel, dan cobalt

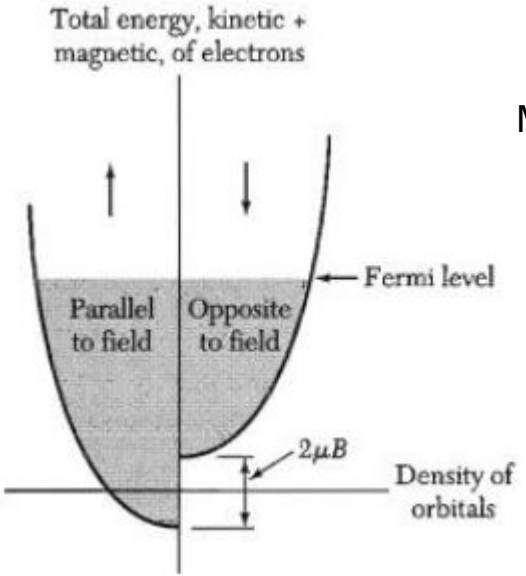
Sifat Magnet pada Material

Material bersifat **non-magnetik** jika kalkulasi DOS menunjukkan **tidak adanya perbedaan** DOS spin up dan spin down pada pada level-level energinya.

Sementara untuk material yang **memiliki perbedaan** keadaan spin up dan spin down pada level energinya, dapat dimaknai bahwa **resultan momen magnetik atomisnya bernilai tidak nol**, sehingga material **bersifat magnetik**.

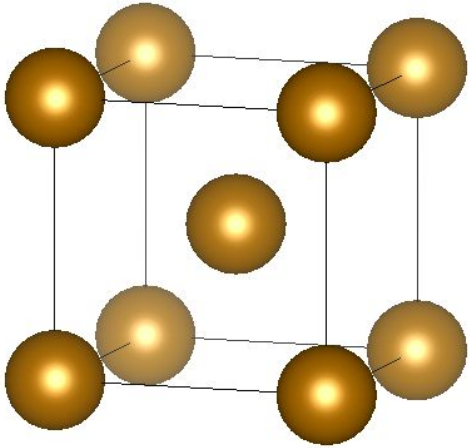


Non Magnetik



Magnetik

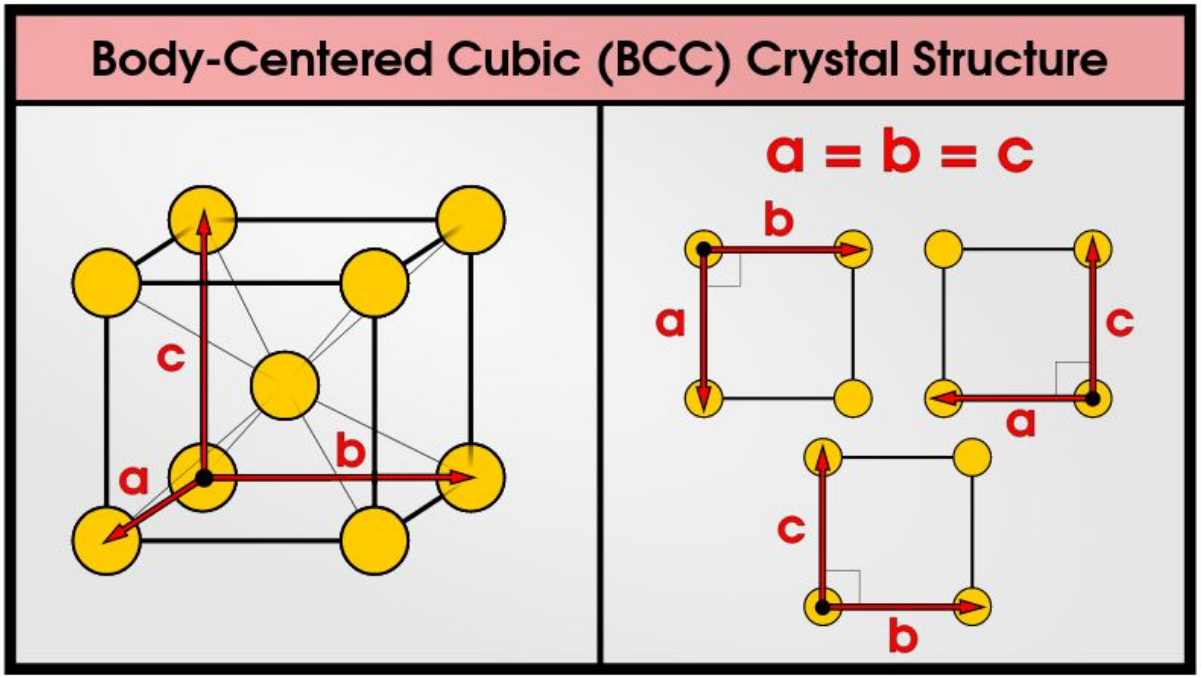
Iron (Fe)



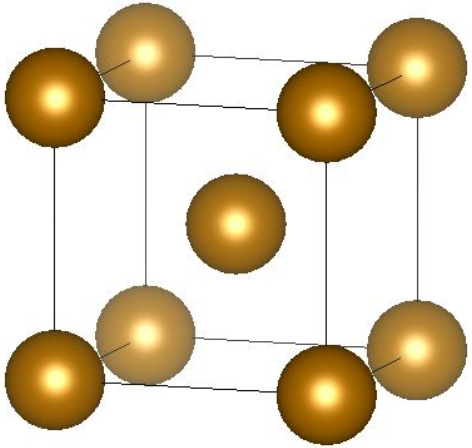
Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

Berapa atom Fe pada sebuah unit sel Iron?

Berapa atom tetangga terdekat pada sebuah atom Fe?

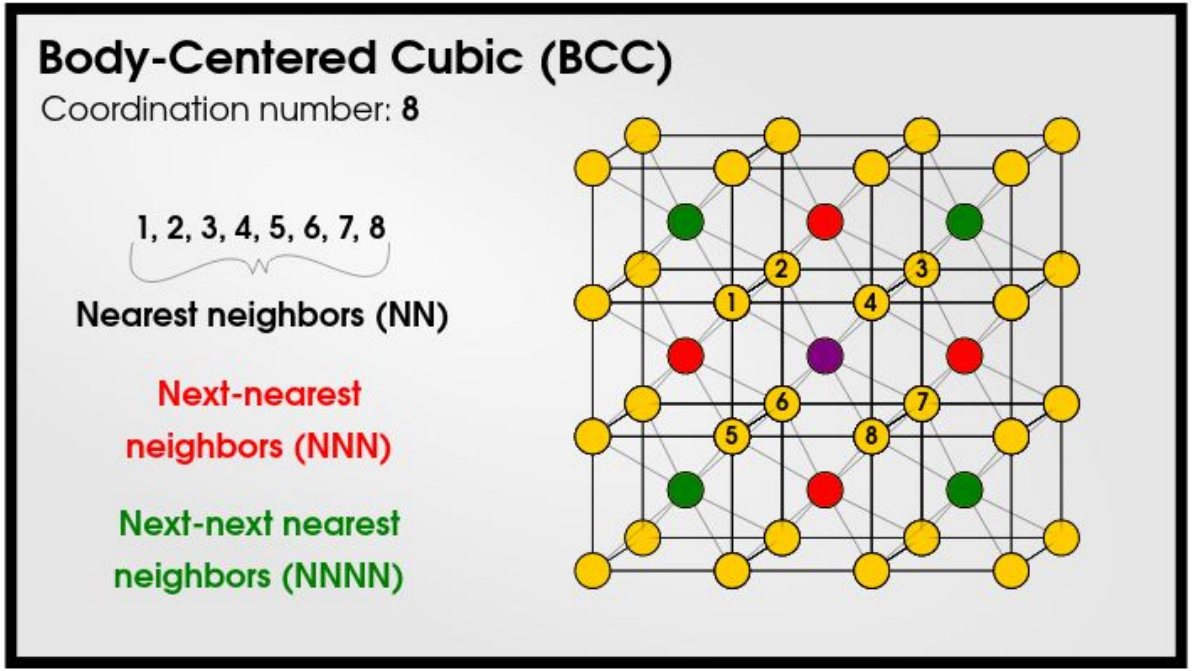


Iron (Fe)

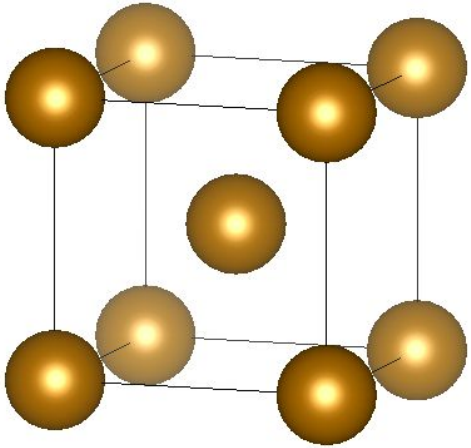


Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

Berapa atom tetangga pada sebuah atom Fe?

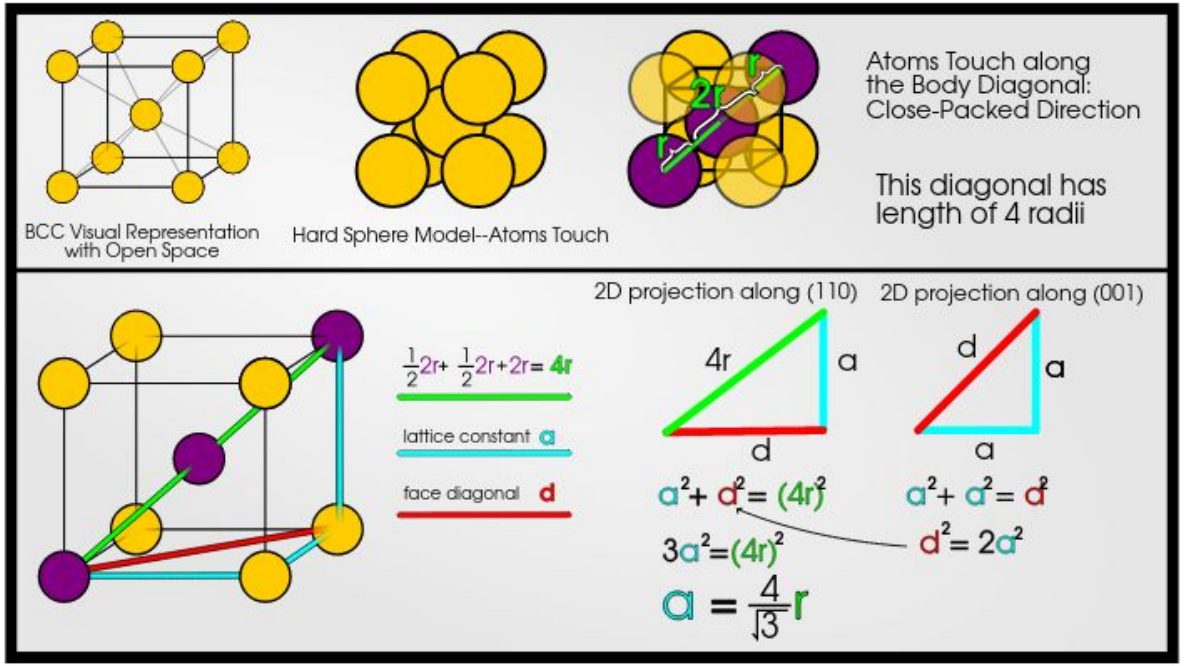


Iron (Fe)



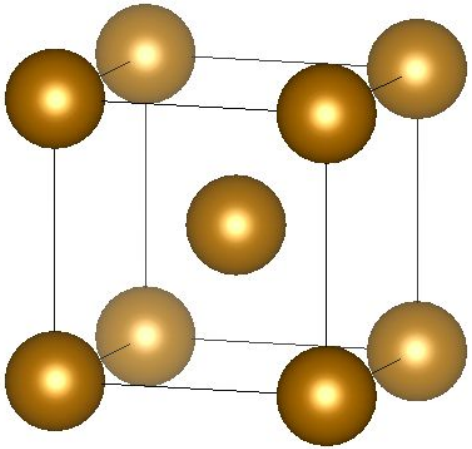
Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

Berapa Angstrom konstanta kisi (lattice constant) pada unit sel Fe?



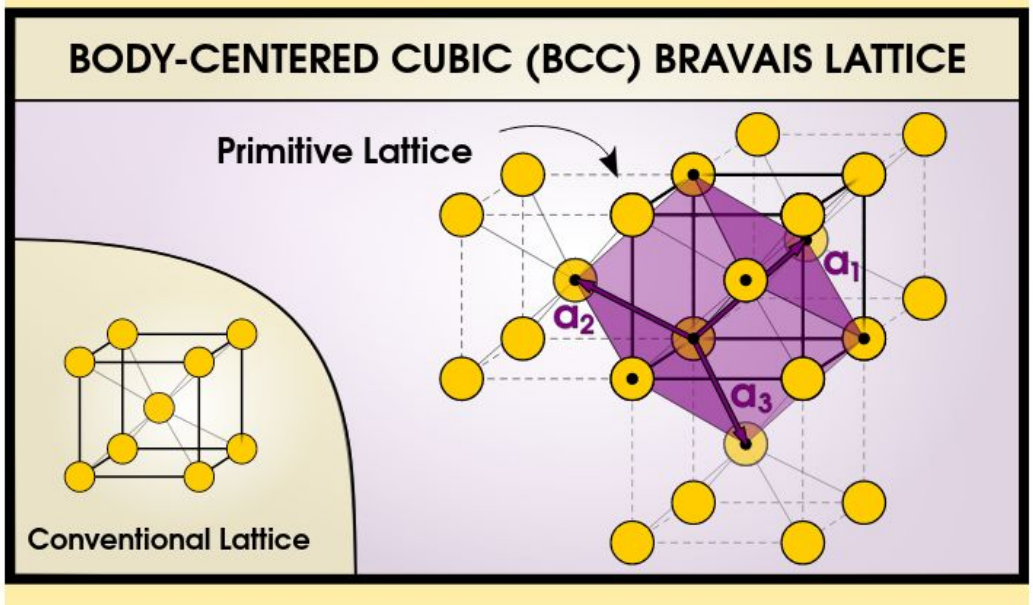
r = jari-jari atom Fe

Iron (Fe)



Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

Unit sel Primitif Iron (Fe)



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

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

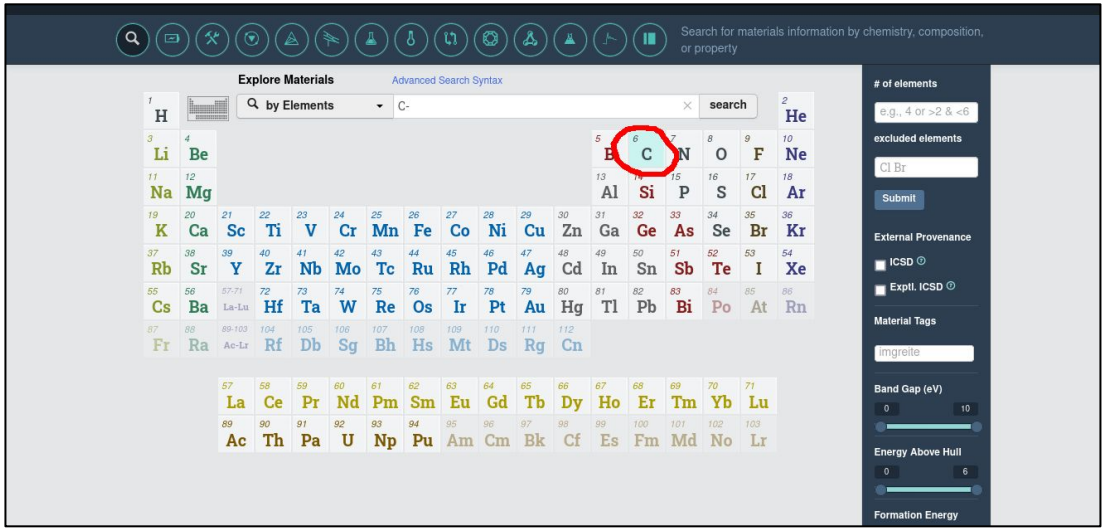
$$a_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{x} - \frac{a}{2}\hat{z}$$

Vektor unit sel primitif Iron (Fe)

Berapa atom Fe pada sebuah unit sel primitif Iron (Fe)?

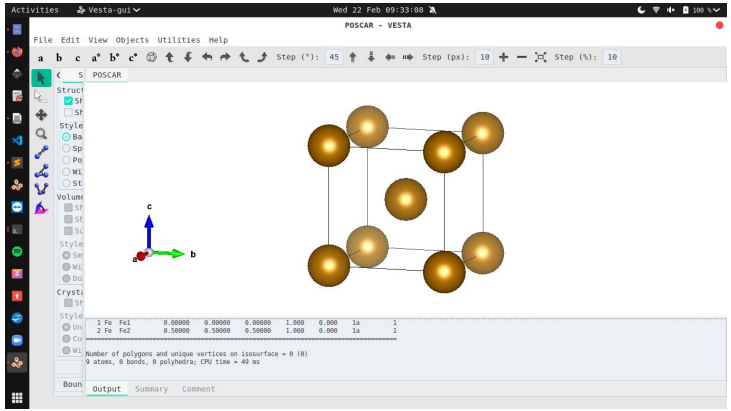
Konstruksi Iron (Fe)

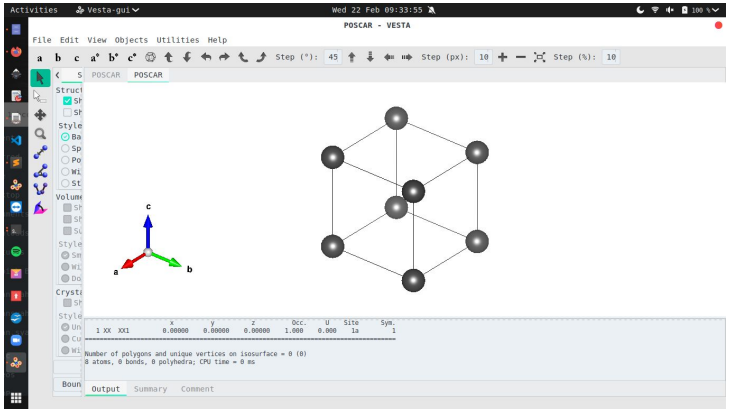
1. Buka https://materialsproject.org/
2. Buat akun dengan email anda.
3. Carilah **Space Group** Fe!
4. Pilih unsur **Iron (Fe)** di halaman utama material project.
5. Pilih material dengan **Space Group** yang sesuai untuk Fe



Konstruksi Iron (Fe)

1. Buat folder **1_Fisika_Magnet** di Home (~)
2. Di dalam folder 1_Fisika_Magnet buat folder **1_bcc_Fe**
3. Download file CIF & POSCAR letakan di folder **1_bcc_Fe**
4. Buka **VESTA** dan masukan file **POSCAR** ke **VESTA**.
5. Analisa Struktur Fe:
   - Ukur panjang ***bondlength*** Fe (Jarak tetangga atom Fe tedekat)





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/fisika_magnet

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

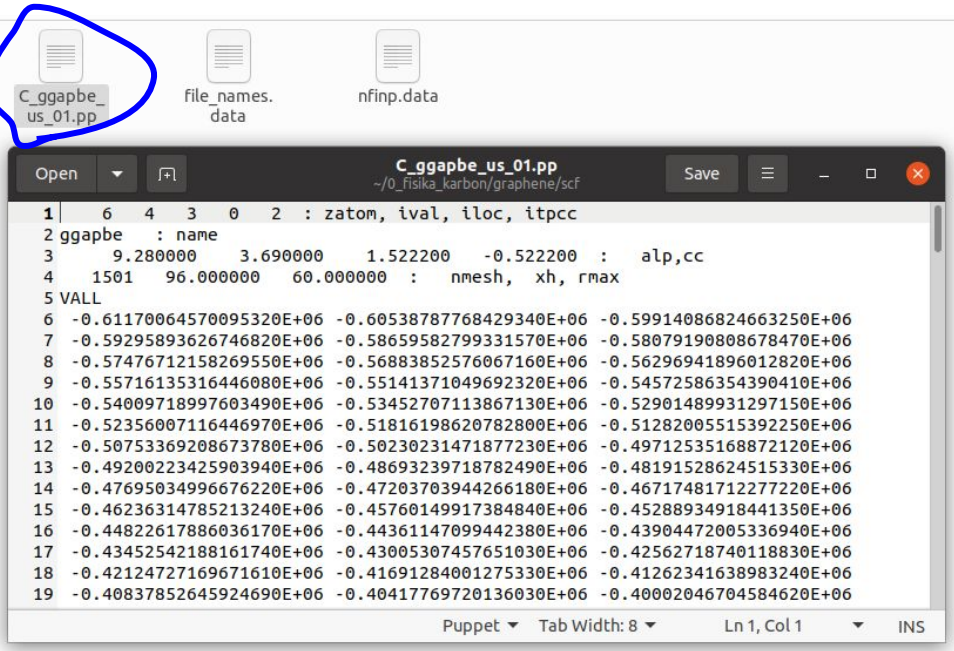
```
Control{
    cpumax = 3600 sec
    condition = Initial
}
accuracy{
    cutoff_wf = 25.00 rydberg
    cutoff_cd = 225.00 rydberg
    num_bands = 16
    ksampling{
        mesh{
            nx = 2
            ny = 2
            nz = 1
        }
    }
}
structure{
    unit_cell_type = primitive
   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

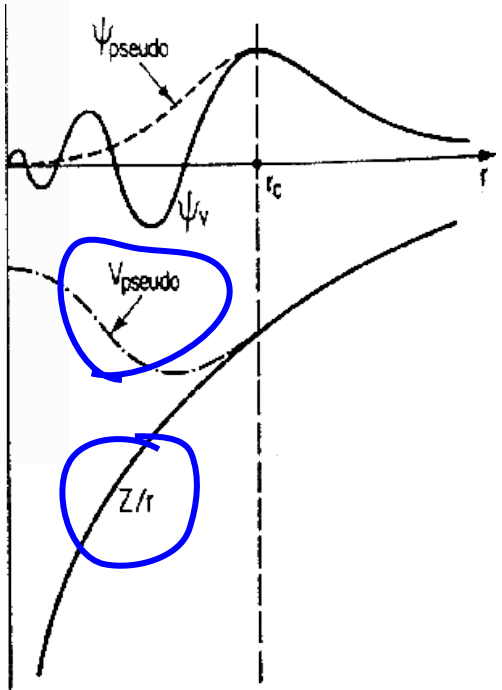
File pseudopotential



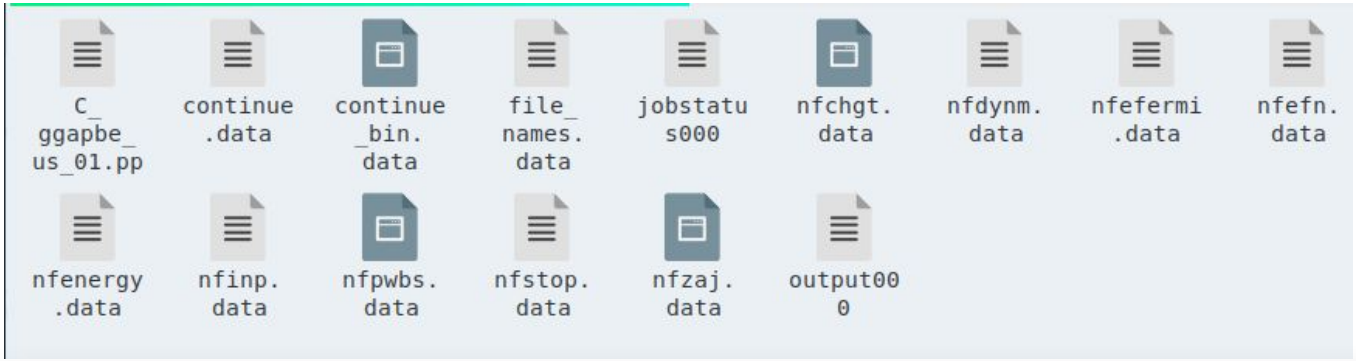
File pseudopotential ada di **phase/samples**

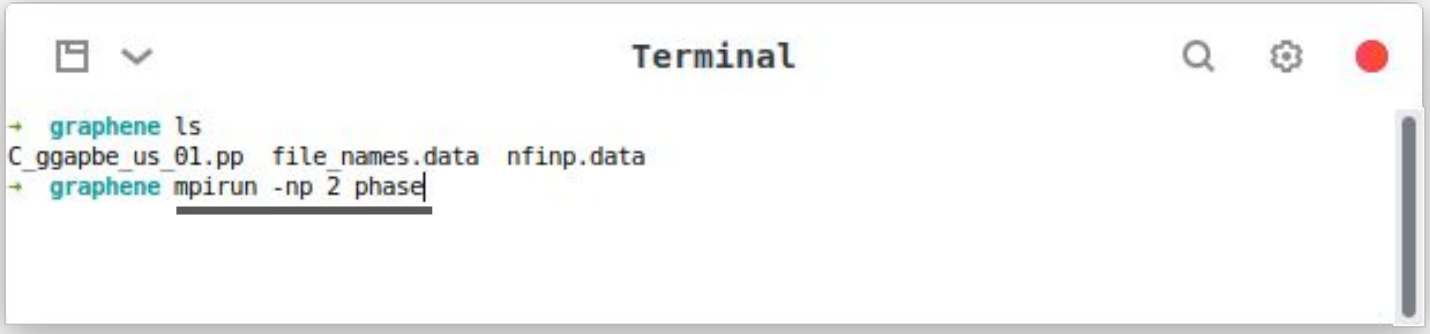
Pseudopotential digunakan untuk mengaproksimasi bentuk potential yang ekstrim.

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



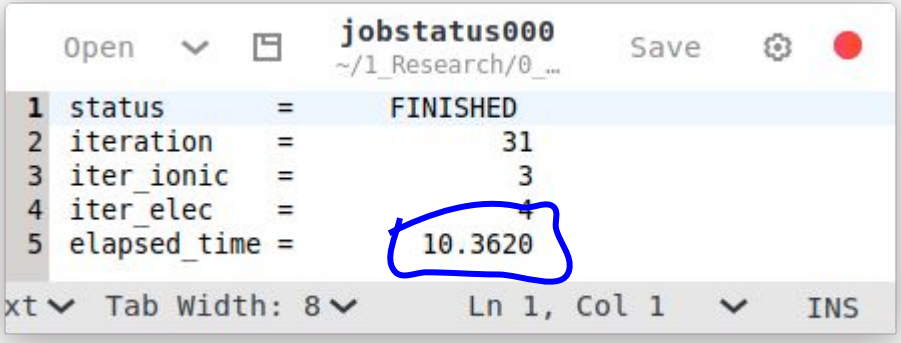
SCF Iron (Fe)





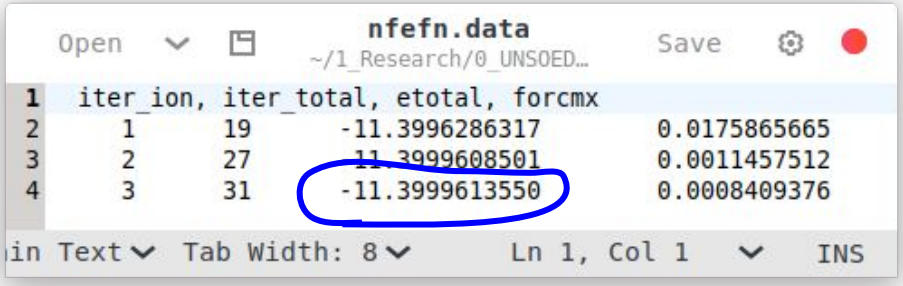
mpirun -np 2 phase

Kalkulasi SCF Iron (Fe)



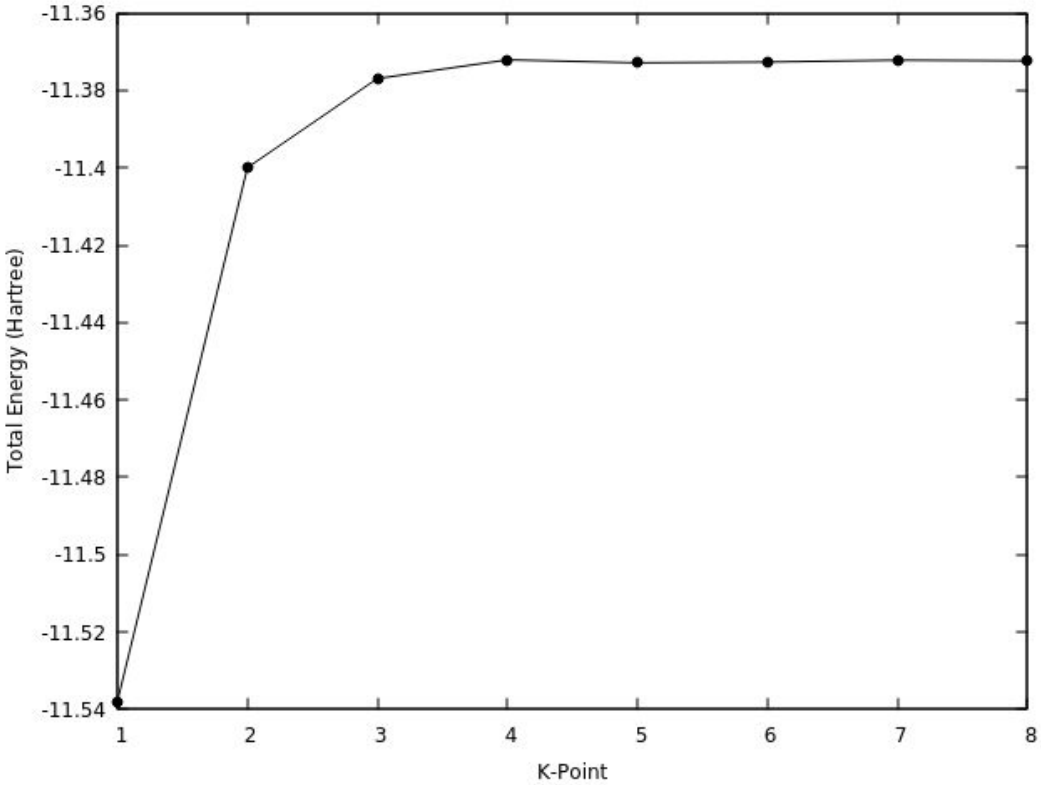
Kalkulasi telah selesai

dengan waktu 10 detik



Energi Total -11.399 Hartree

Konvergensi Kpoint



Buatlah diagram konvergensi akurasi kpoint-mesh.

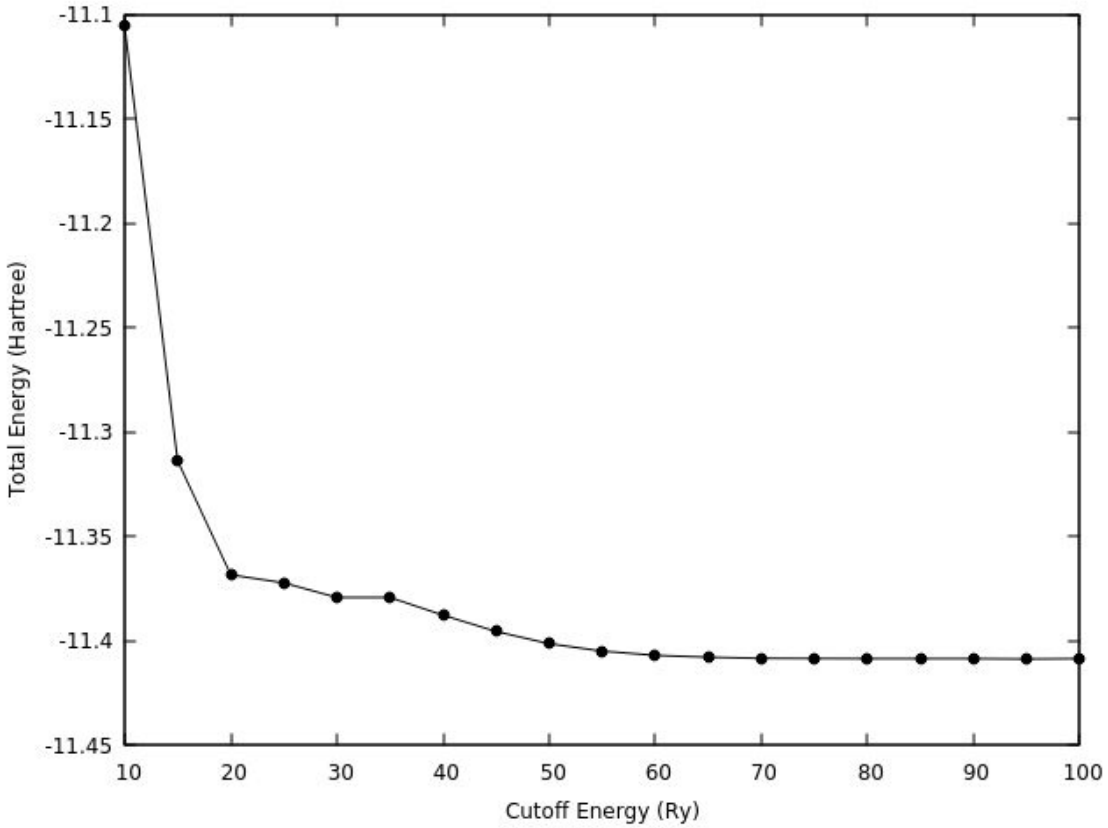
Dari 1x1x1, 2x2x1 … s.d. 10x10x1!

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
```

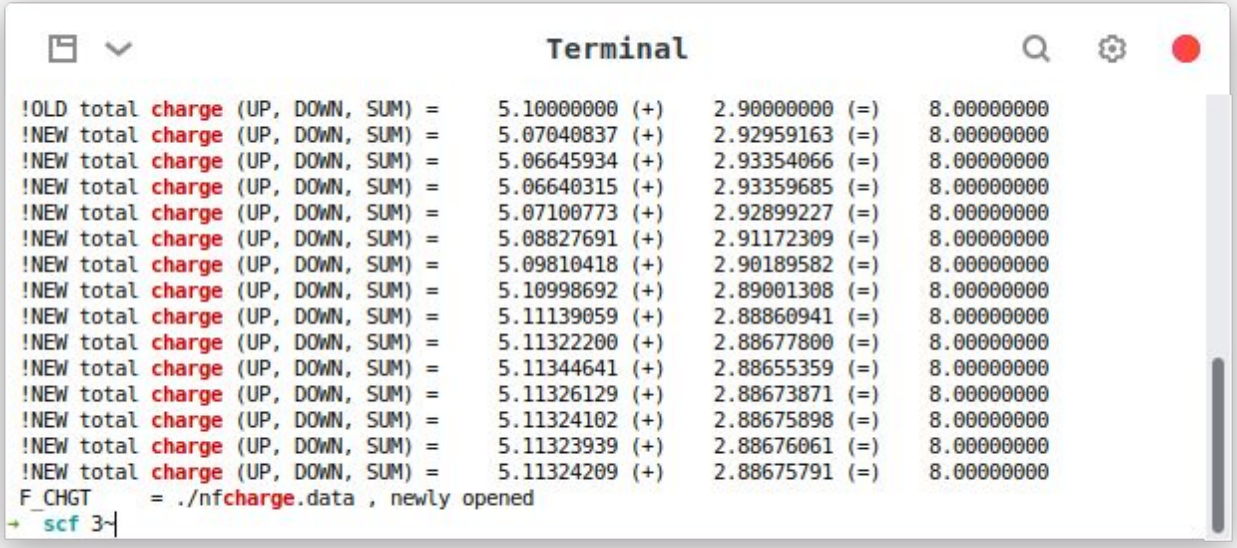
Plotting grafik dapat dilakukan dengan GnuPlot.

Konvergensi Energi Cutoff



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

Atomic Magnetic Moment

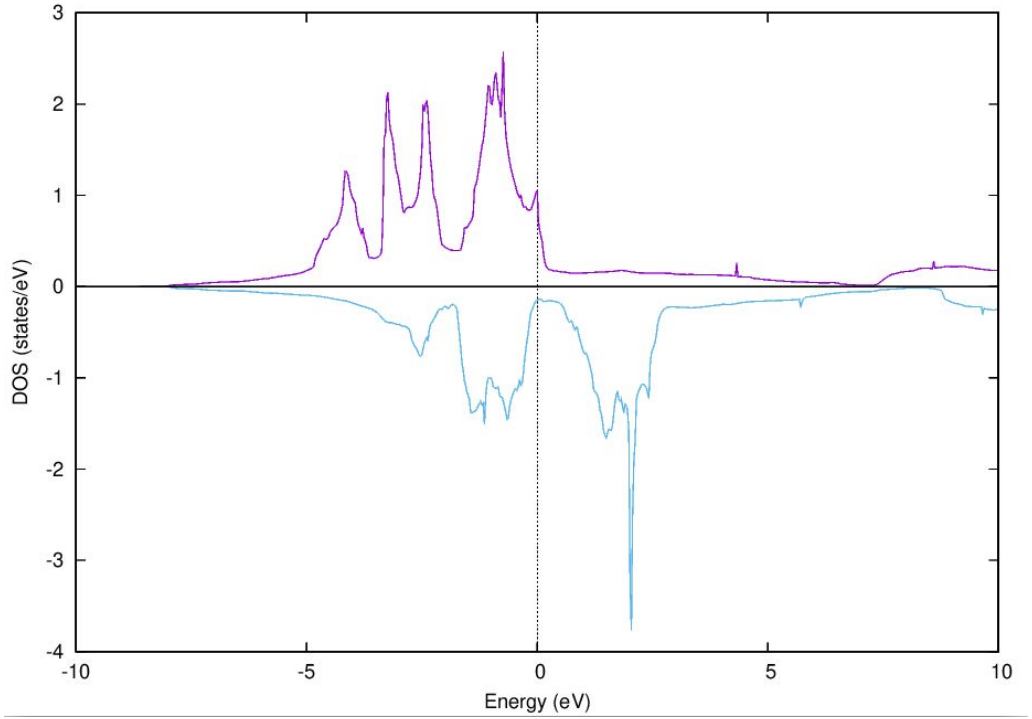


Atomic Magnetic Moment:

Q = n_up - n_down

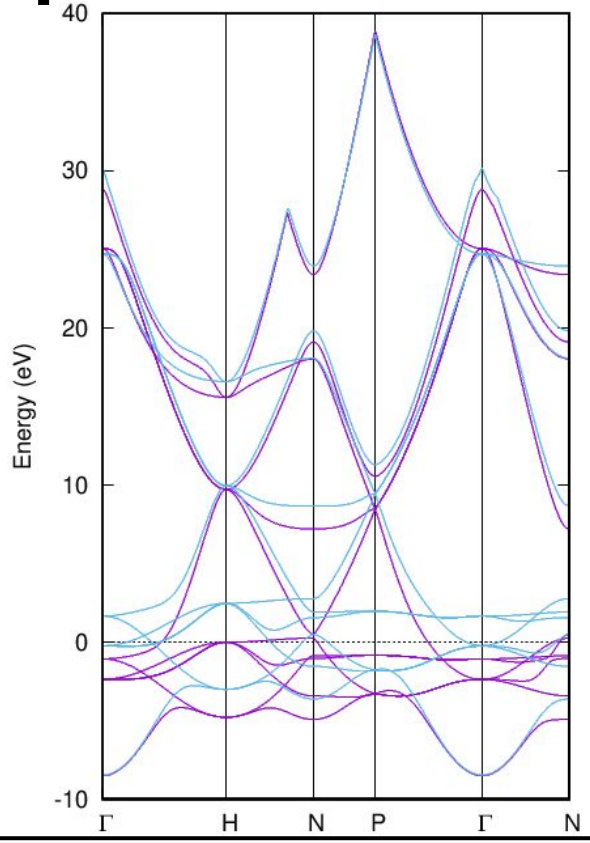
grep charge output000

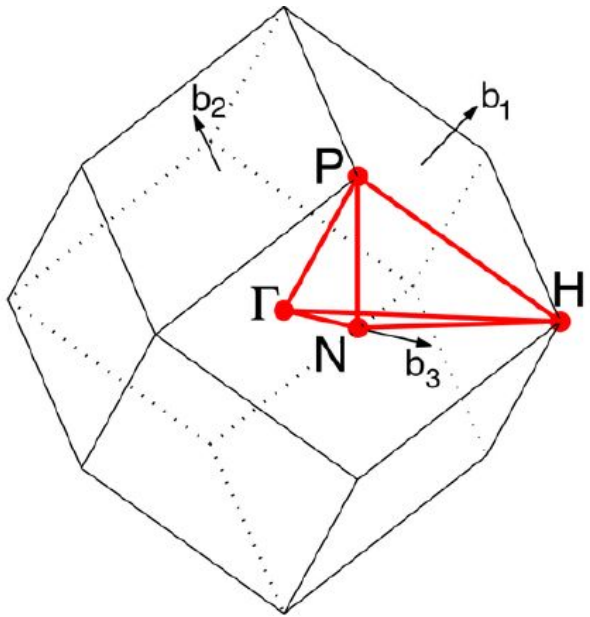
Spin Polarized DOS



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

Spin Polarized Band Structure





BCC path: Γ-H-N-Γ-P-H|P-N

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

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