

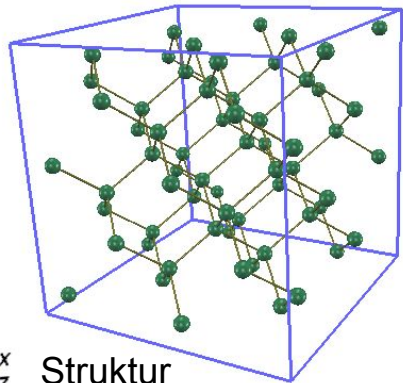
Fisika Magnet: Komputasi Material Iron (Fe)

Zohan Syah Fatomi

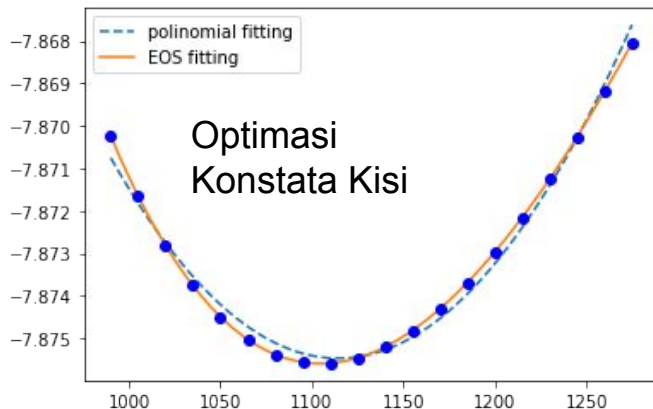


Jurusan Fisika
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Jenderal Soedirman

Rekayasa Komputasi Material

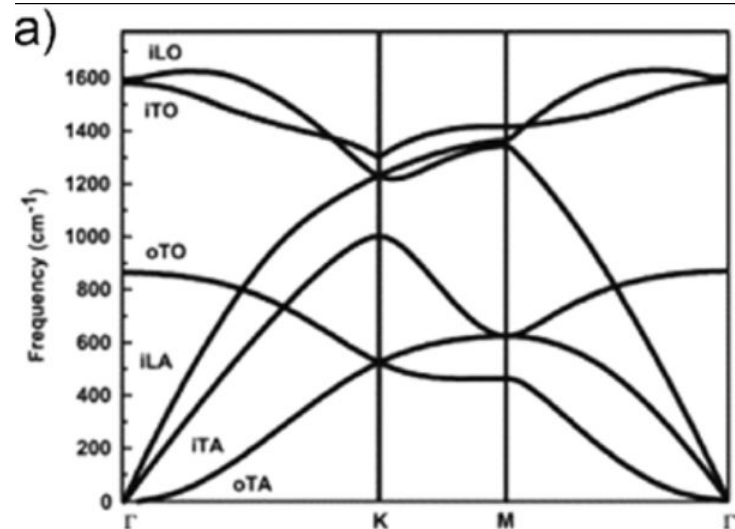


Struktur kristal

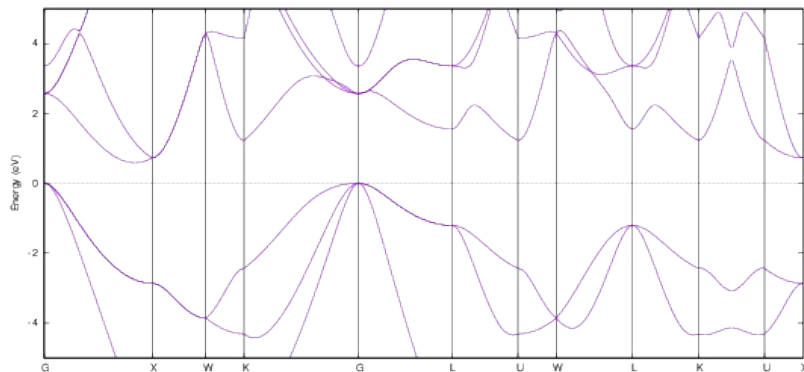


**Density Functional
Theory (DFT) +
Komputasi Numerik
+ Komputer**

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



Sifat vibrasi
(phonon dispersion)



Struktur elektronik

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

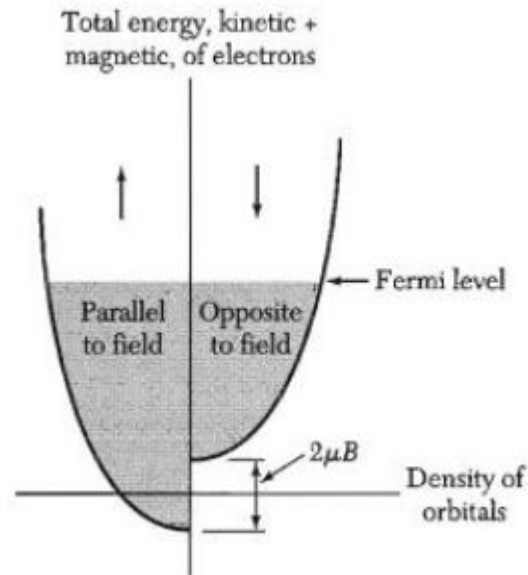
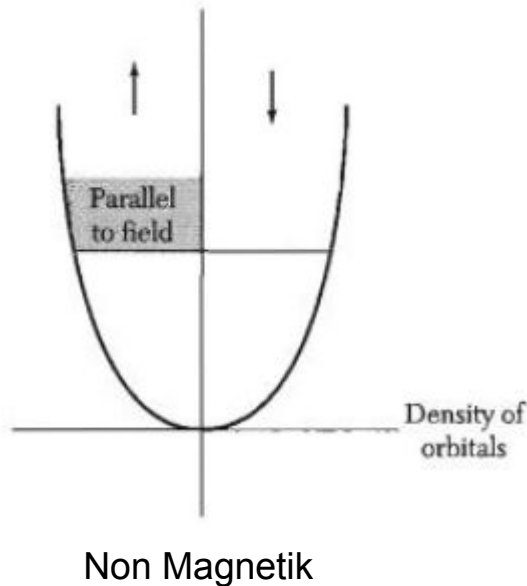
Berdasarkan kemagnetannya material dibedakan menjadi 3:

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

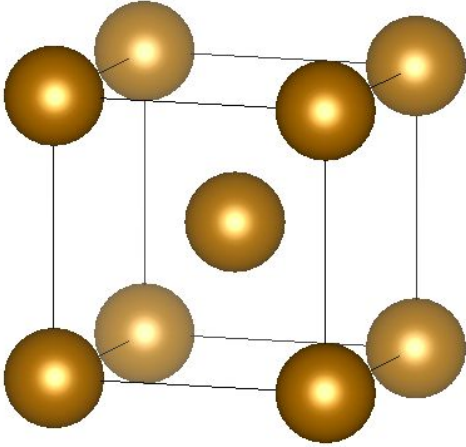
Sifat Magnet pada Material

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



Iron (Fe)

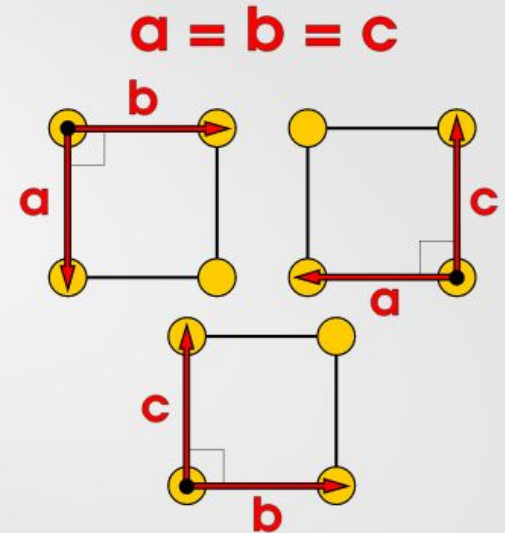
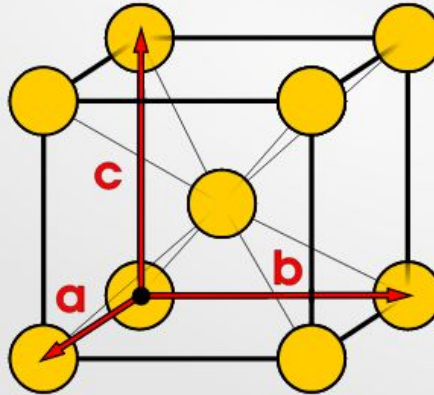


Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

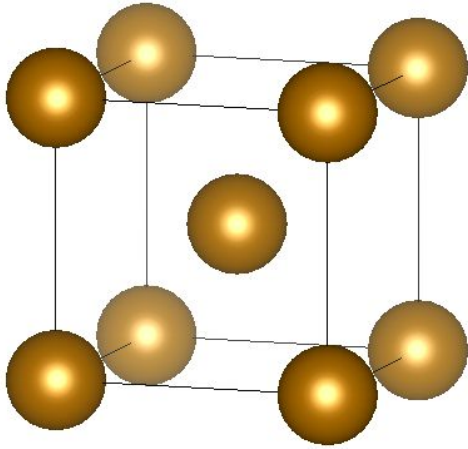
Berapa atom Fe pada sebuah unit sel Iron?

Berapa atom tetangga terdekat pada sebuah atom Fe?

Body-Centered Cubic (BCC) Crystal Structure



Iron (Fe)



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

Berapa atom tetangga pada sebuah atom Fe?

Body-Centered Cubic (BCC)

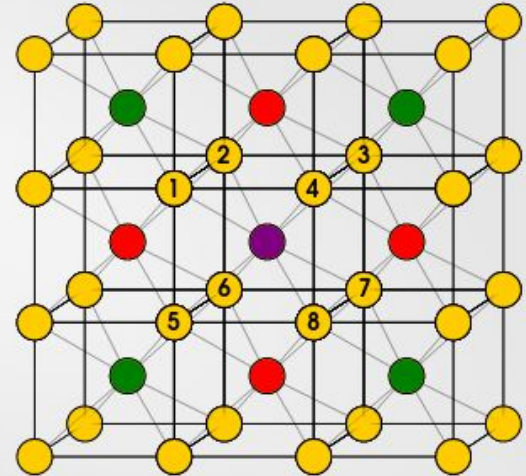
Coordination number: 8

1, 2, 3, 4, 5, 6, 7, 8

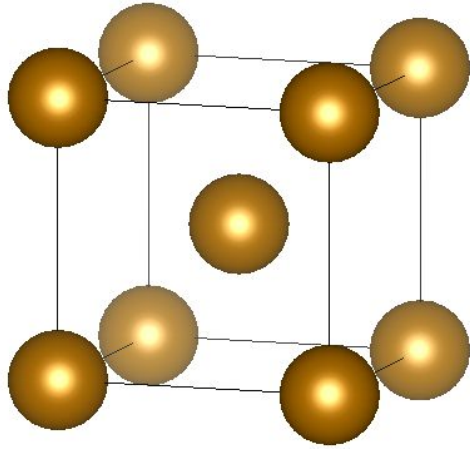
Nearest neighbors (NN)

Next-nearest neighbors (NNN)

Next-next nearest neighbors (NNNN)

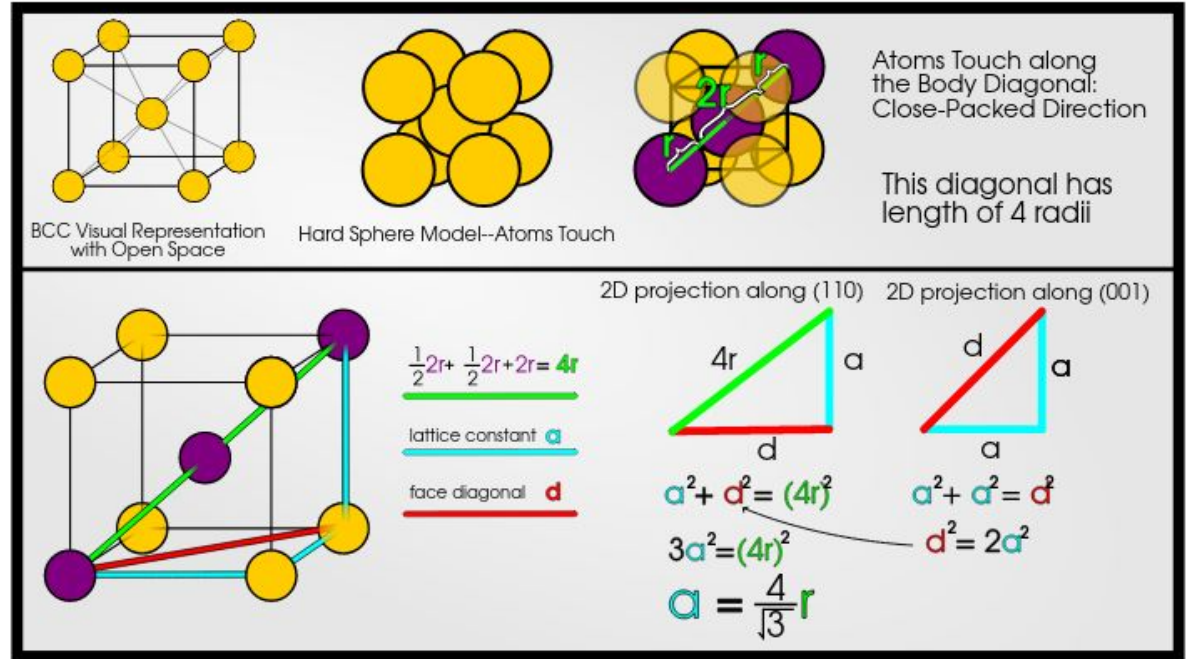


Iron (Fe)



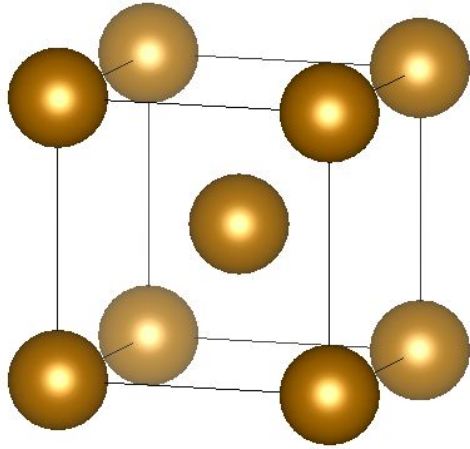
Struktur kristal unit sel Iron (Fe) adalah Body Center Cubic (BCC).

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



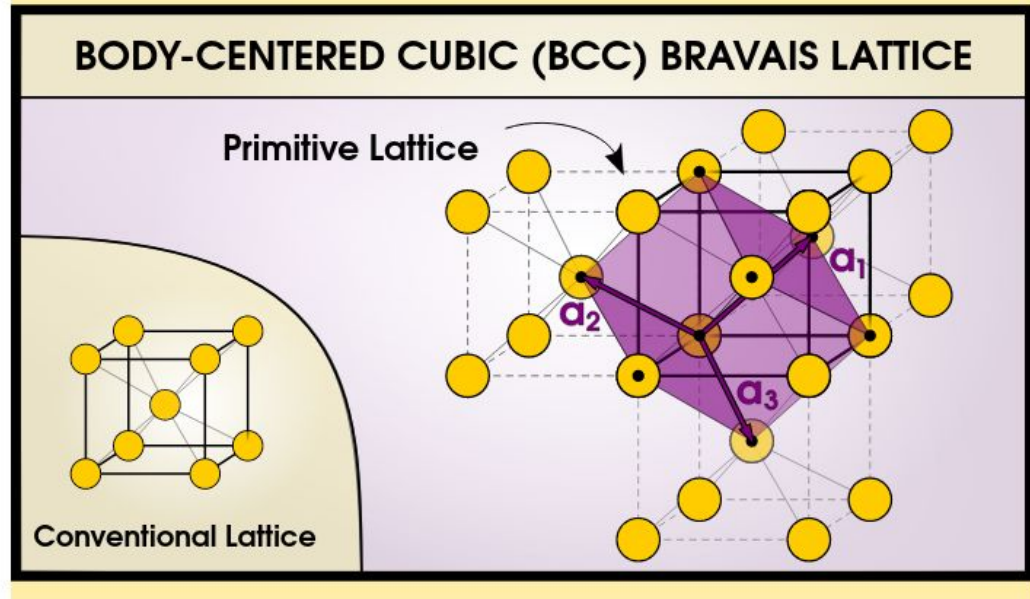
r = jari-jari atom Fe

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)?

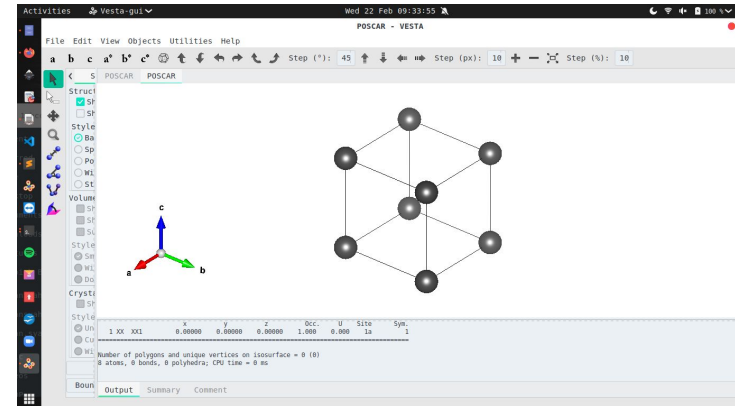
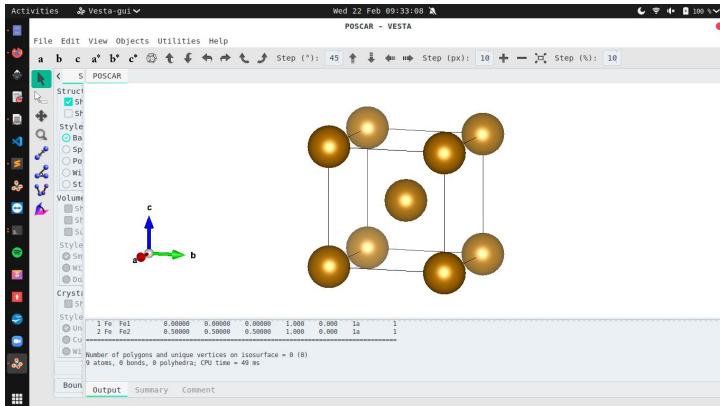
Konstruksi Iron (Fe)

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

The screenshot shows the Materials Project website interface. At the top, there is a search bar with the text "Search for materials information by chemistry, composition, or property". Below the search bar, there is a navigation bar with the text "Explore Materials" and "Advanced Search Syntax". The main content area displays a periodic table of elements. The element Carbon (C) is highlighted with a red circle. To the right of the periodic table, there is a sidebar with various filters and options, including "Number of elements", "Excluded elements", "External Provenance", "Material Tags", "Band Gap (eV)", "Energy Above Hull", and "Formation Energy".

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 terdekat)



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_CAMPUS/1_Fisi
1 &fnames
2 F_INP      = './input_bcc_Fe.data'
3 F_POT(1)   = '../pp/Fe_ggapbe_paw_us_02.pp'
4 F_ENERG    = './nfenergy.data'
5 F_CHGT     = './nfcharge.data'
6 F_ZAJ      = './zaj.data'
7 /
8
```

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**)

nfnp.data

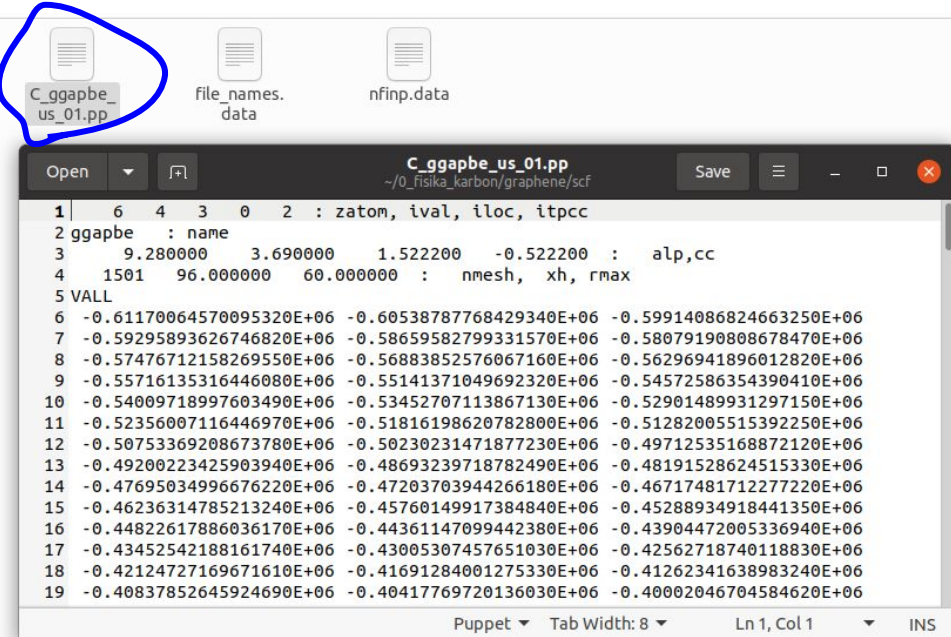
```
1 Control{
2     cpumax = 3600 sec
3     condition = Initial
4 }
5 accuracy{
6     cutoff_wf = 25.00 rydberg
7     cutoff_cd = 225.00 rydberg
8     num_bands = 16
9     ksampling{
10         mesh{
11             nx = 2
12             ny = 2
13             nz = 1
14         }
15     }
16 }
17 structure{
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 **Iron (Fe)**, **graphene**, **diamond**, **stanene**, **silicine** dlsb, tergantung konfigurasi pada block tsb.

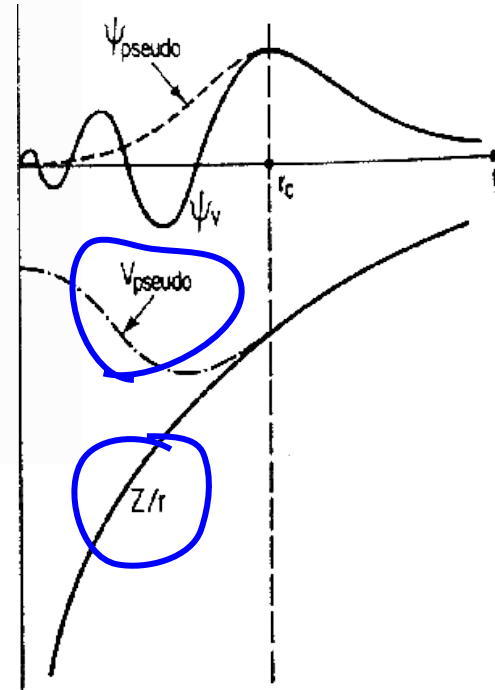
File pseudopotential



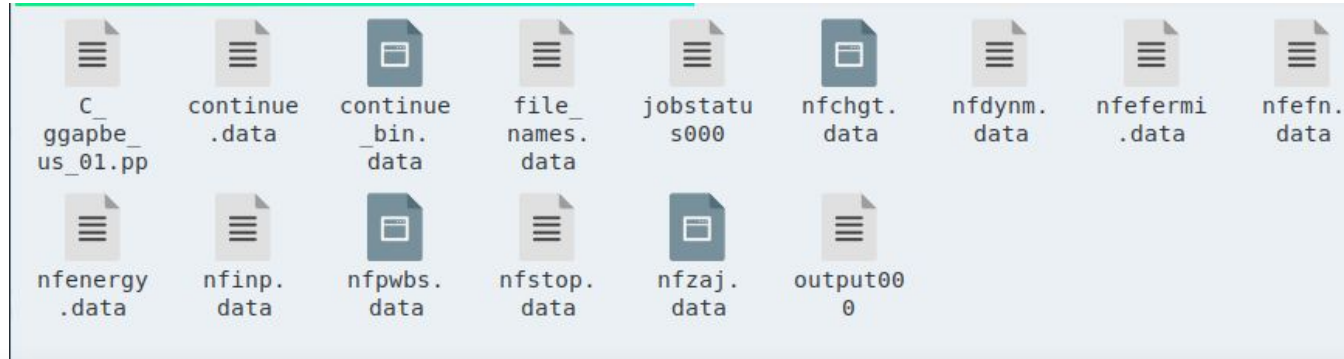
File pseudopotential ada di **phase/samples**

Pseudopotential digunakan untuk mengaproksimasi bentuk potensial yang ekstrim.

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



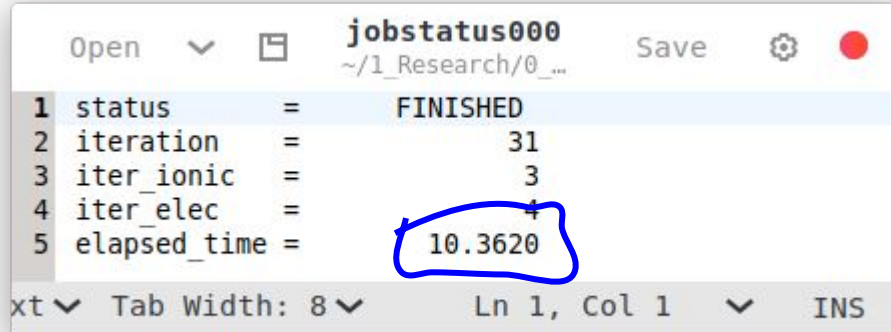
SCF Iron (Fe)



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

mpirun -np 2 phase

Kalkulasi SCF Iron (Fe)

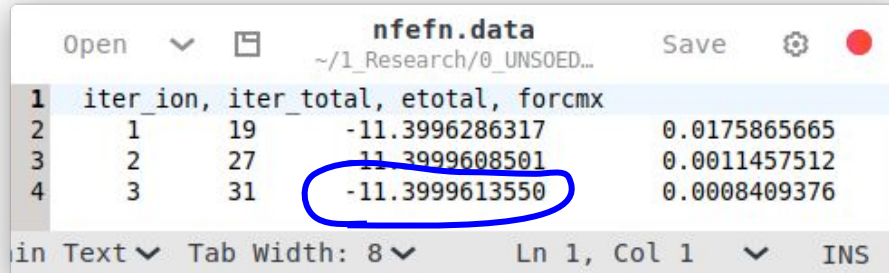


A screenshot of a text editor window titled 'jobstatus000' showing the output of an SCF calculation. The file path is '~/.1_Research/0_...'. The content is as follows:

Line	Key	Value
1	status	FINISHED
2	iteration	31
3	iter_ionic	3
4	iter_elec	4
5	elapsed_time	10.3620

The value '10.3620' is circled in blue. The editor status bar at the bottom shows 'Ln 1, Col 1'.

Kalkulasi telah selesai
dengan waktu 10 detik



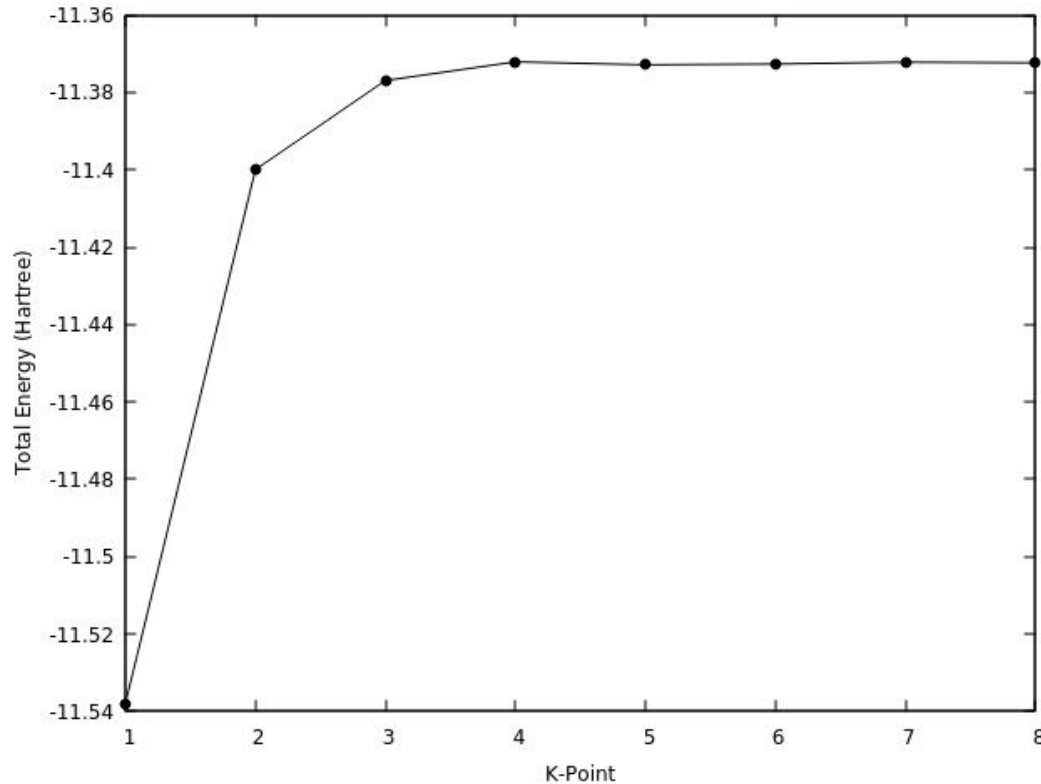
A screenshot of a text editor window titled 'nfeffn.data' showing the output of an SCF calculation. The file path is '~/.1_Research/0_UNSOED...'. The content is as follows:

Line	iter_ion	iter_total	etotal	forcmx
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

The value '-11.3999613550' is circled in blue. The editor status bar at the bottom shows 'Ln 1, Col 1'.

Energi Total -11.399 Hartree

Konvergensi Kpoint



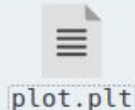
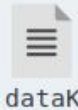
Buatlah diagram konvergensi
akurasi kpoint-mesh.

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

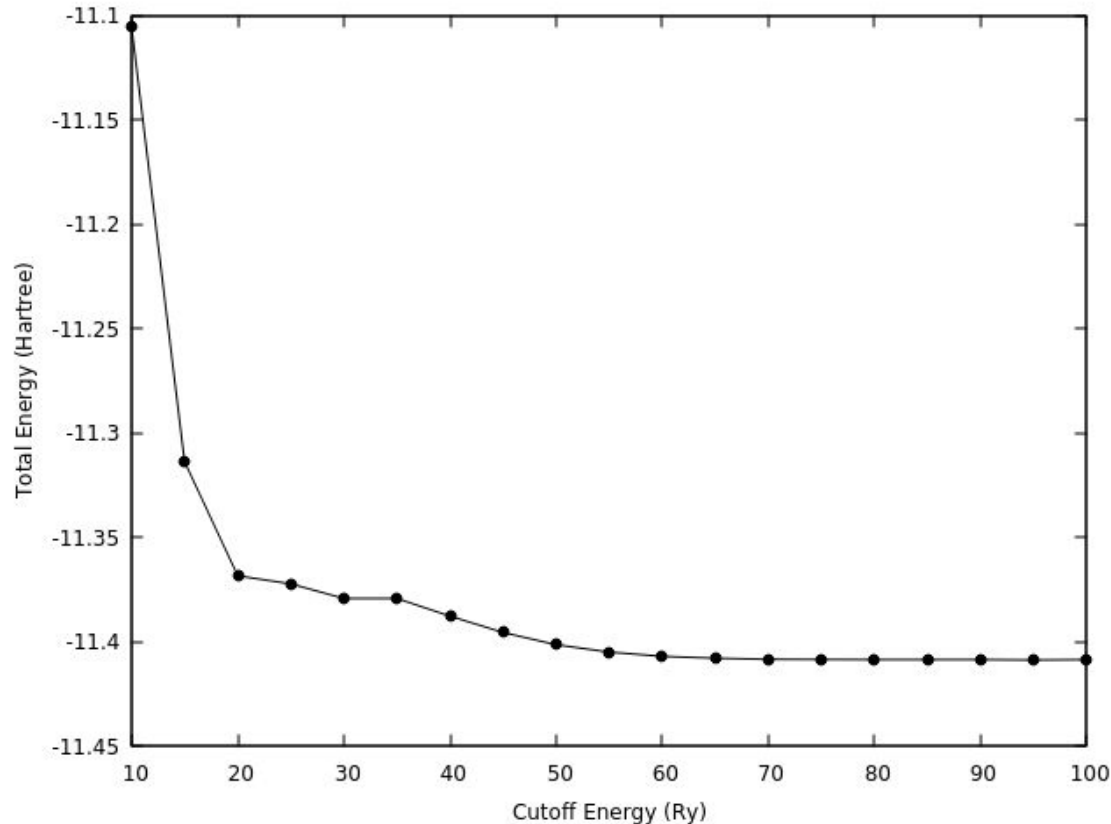
Visualisasi data (GNUPlot)

```
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!**

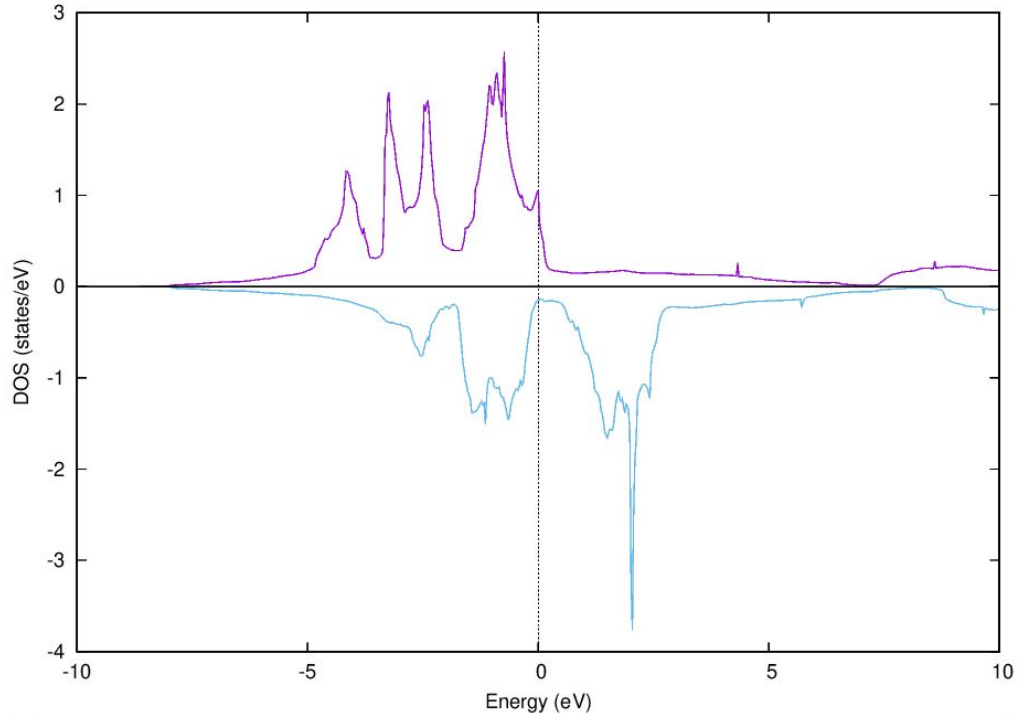
Atomic Magnetic Moment

```
Terminal
!OLD total charge (UP, DOWN, SUM) = 5.10000000 (+) 2.90000000 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.07040837 (+) 2.92959163 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.06645934 (+) 2.93354066 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.06640315 (+) 2.93359685 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.07100773 (+) 2.92899227 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.08827691 (+) 2.91172309 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.09810418 (+) 2.90189582 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.10998692 (+) 2.89001308 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11139059 (+) 2.88860941 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11322200 (+) 2.88677800 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11344641 (+) 2.88655359 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11326129 (+) 2.88673871 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11324102 (+) 2.88675898 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11323939 (+) 2.88676061 (=) 8.00000000
!NEW total charge (UP, DOWN, SUM) = 5.11324209 (+) 2.88675791 (=) 8.00000000
F_CHGT = ./nfcharge.data , newly opened
→ scf 3~
```

Atomic Magnetic
Moment:
 $Q = n_{\text{up}} - n_{\text{down}}$

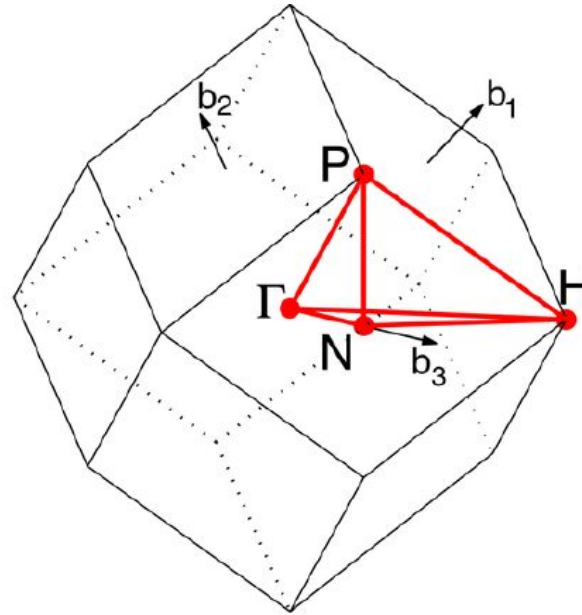
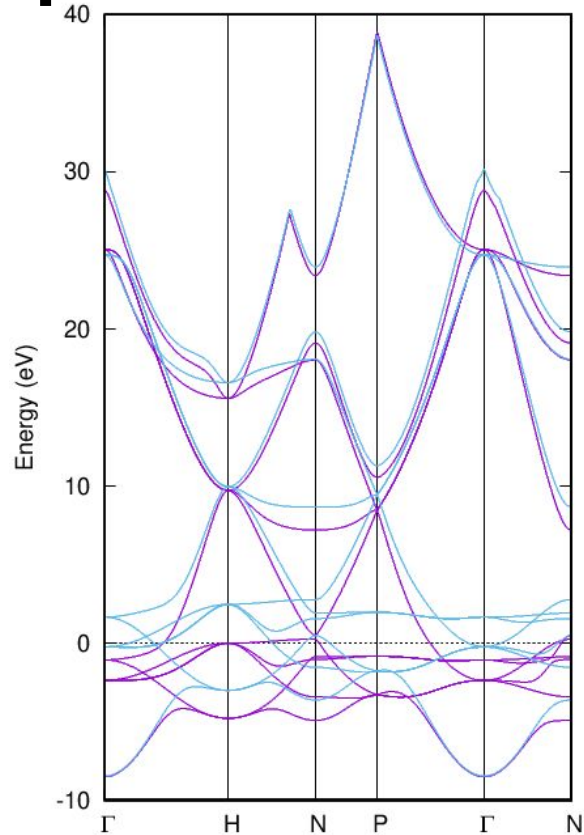
grep charge output000

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
```