# SIMULASI INTERAKSI MOLEKUL GLISIN DI ATAS PERMUKAAN Fe(110) PADA PROSES IMOBILISASI BIORESEPTOR MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)

**SKRIPSI**

**Untuk memenuhi sebagian persyaratan**
**mencapai derajat Sarjana S-1**

**Program Studi Fisika**

**diajukan oleh:**

**Nurul Fajariah**
**13620002**

**Kepada**

**PROGRAM STUDI FISIKA**
**FAKULTAS SAINS DAN TEKNOLOGI**
**UNIVERSITAS ISLAM NEGERI SUNAN KALIJAGA**
**YOGYAKARTA**
**2017**

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**YOGYAKARTA**
**2017**

Universitas Islam Negeri Sunan Kalijaga FM-UINSK-BM-05-07/R0

**PENGESAHAN SKRIPSI/TUGAS AKHIR**

Nomor :B- 687/Un.02/DST/PP.05.3/ 03 /2017

Skripsi/Tugas Akhir dengan judul : Simulasi Interaksi Molekul Glisin di Atas Permukakaan Fe(110) Pada Proses Imobilisasi Bioreseptor Menggunakan Metode *Density Functional Theory* (DFT)

Yang dipersiapkan dan disusun oleh :
Nama : Nurul Fajariah
NIM : 13620002
Telah dimunaqasyahkan pada : 03 Maret 2017
Nilai Munaqasyah : A
Dan dinyatakan telah diterima oleh Fakultas Sains dan Teknologi UIN Sunan Kalijaga

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**SURAT PERSETUJUAN SKRIPSI/TUGAS AKHIR**

Hal : Surat Persetujuan Skripsi/ Tugas Akhir
Lamp : -

Kepada
Yth. Dekan Fakultas Sains dan Teknologi
UIN Sunan Kalijaga Yogyakarta
di Yogyakarta

*Assalamu'alaikum wr. wb.*

Setelah membaca, meneliti, memberikan petunjuk dan mengoreksi serta mengadakan perbaikan seperlunya, maka kami selaku pembimbing berpendapat bahwa skripsi Saudara:

Nama : Nurul Fajariah
NIM : 13620002
Judul Skripsi : Simulasi Interaksi Molekul Gly Di Atas Permukaan Fe(110) Untuk Proses Imobilisasi Bioreseptor Menggunakan Metode DFT

sudah dapat diajukan kembali kepada Program Studi Fisika Fakultas Sains dan Teknologi UIN Sunan Kalijaga Yogyakarta sebagai salah satu syarat untuk memperoleh gelar Sarjana Strata Satu dalam Jurusan Fisika

Dengan ini kami mengharap agar skripsi/tugas akhir Saudara tersebut di atas dapat segera dimunaqsyahkan. Atas perhatiannya kami ucapkan terima kasih.

*Wassalamu'alaikum wr. wb.*

Yogyakarta, 21 Februari 2017

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## SURAT PERNYATAAN KEASLIAN SKRIPSI

Yang bertanda tangan dibawah ini :

| | |
|---|---|
| Nama | : Nurul Fajariah |
| NIM | : 13620002 |
| Program Studi | : Fisika |
| Fakultas | : Sains dan Teknologi |

Dengan ini saya menyatakan bahwa skripsi yang berjudul: Simulasi Interaksi Molekul Gly Di Atas Permukaan Fe(110) untuk Proses Imobilisasi Bioreseptor Menggunakan Metode DFT adalah benar-benar karya saya sendiri. Sepanjang pengetahuan saya tidak terdapat karya atau pendapat yang ditulis atau diterbitkan orang lain kecuali sebagai acuan atau kutipan dengan tata penulisan yang lazim.

Yogyakarta, Februari 2017


ang menyatakan

Nurul Fajariah
NIM : 13620002

## MOTTO

*Nikmati prosesnya!*

*Setiap detik waktu hanya akan menjadi masa lalu.*

*Salam Sukses!*

*-Shaloentzzz-*

## HALAMAN PERSEMBAHAN

**Karya tulis ini saya persembahkan untuk:**

- **Kedua orang tua saya, Bapak Nur'aini Hambali dan Ibu Uju Kusumawati**
- **Saudara-saudara saya, Ibnu Harits, Al Nafis Manarul Huda, Amar Yusuf Bantarja, Aris Firdaus, Ahmad Mubarok dan Putri Hadya Kamila**
- **Keluarga besar saya**
- ***Soulmate* saya, yaitu Farros Haydar Rayhan**
- ***Study Club* Fisika Material UIN Sunan Kalijaga Yogyakarta**
- **Fisika 2013**
- **Keluarga besar UKM JQH Al Mizan UIN Sunan Kalijaga Yogyakarta**
- **Almamater Tercinta Program Studi Fisika UIN Sunan Kalijaga Yogyakarta**

## KATA PENGANTAR

Puji syukur kami panjatkan kehadirat Allah SWT yang telah melimpahkan rahmat dan pertolongan-Nya kepada semua makhluk yang ada di muka bumi ini dengan segala kekuasaan-Nya. *Alhamdulillah,* dengan rahmat dan pertolongan-Nya, penulisan Skripsi yang berjudul "**Simulasi Interaksi Molekul Glisin Di Atas Permukaan Fe(110) Untuk Proses Imobilisasi Bioreseptor Menggunakan Metode *Density Functional Theory* (DFT)"** ini, dapat terselesaikan. Sholawat serta salam semoga tetap tercurahkan kepada baginda Nabi Muhammad saw yang telah menuntun umat manusia untuk terbebas dari kebodohan. Dengan cahayanya, umat manusia dapat mengenal ilmu pengetahuan untuk mencapai kebahagiaan hidup di dunia dan akhirat.

Keberhasilan dalam penulisan Skripsi ini tidak terlepas dari bantuan berupa moril dan materiil berbagai pihak. Untuk itu, penulis mengucapkan terima kasih kepada :

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2. Dr. Thoqibul Fikri N., sekalu Ketua Program Studi Fisika UIN Sunan Kalijaga Yogayakarta.
3. Agung Frida Rahmadi, M.Sc., selaku Dosen Penasehat Akademik (DPA).
4. Asih Melati, M.Sc., selaku Dosen Pembimbing I.
5. Retno Rahmawati, M.Si., selaku Dosen Pembimbing II.
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7. Wahyu Aji E.P., S.Si, M.T., selaku asisten Laboratorium CMD ITB.
8. Dr. Fadjar Fathurrahman, selaku *Research Fellow* di PPNN ITB.
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Penulisan skripsi ini dimaksudkan untuk memenuhi salah satu syarat untuk memperoleh gelar Sarjana Sains Ilmu Fisika di Program Studi Fisika Fakultas Sains dan Teknologi Universitas Islam Negeri Sunan Kalijaga Yogyakarta. Mengingat banyaknya keterbatasan, kami menyadari bahwa dalam penyusunan Skripsi ini masih jauh dari kesempurnaan. Oleh karena itu, kritik dan saran yang bersifat membangun, sangat penulis harapkan dari berbagai pihak. Semoga Skripsi ini memberikan manfaat bagi pembaca. Amin.

Yogyakarta, Februari 2017

Penulis

# SIMULASI INTERAKSI MOLEKUL GLISIN DI ATAS PERMUKAAN Fe(110) UNTUK PROSES IMOBILISASI BIORESEPTOR MENGGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)

**Nurul Fajariah**
**13620002**

## INTISARI

Penelitian yang berada pada ranah komputasi material ini mencakup pemodelan sistem dan aspek lain yang mengacu pada fisika kuantum. Pada penelitian ini, dilakukan simulasi dan pemodelan untuk menginvestigasikan proses adsorpsi molekul Glisin sebagai model bioreseptor di atas permukaan Fe(110) sebagai model material pendukung biosensor. Penelitian dilakukan dengan memodelkan sembilan situs adsorpsi, dengan memvariasikan posisi molekul Glisin di atas permukaan Fe(110) menggunakan metode DFT (*Density Functional Theory*). Hasil menunjukkan bahwa permukaan Fe(110) memiliki kecenderungan berikatan dengan atom O-2 pada molekul Glisin, dengan ikatan yang terbentuk adalah ikatan kovalen. Adsorpsi molekul Glisin di atas permukaan Fe(110) paling stabil terjadi pada posisi molekul **B** di situs *B* (*bridging*), yaitu situs-4 dengan nilai energi adsorpsi sebesar -0,87 eV. Hasil dari penelitian ini dapat merekomendasikan bahwa permukaan Fe mampu mengimobilisasi bioreseptor dalam aplikasi biosensor penanda marker.

**Kata Kunci**: Adsorpsi, Metode DFT, Molekul Glisin, dan Permukaan Fe.

# SIMULATION INTERACTION OF GLYCINE ON Fe(110) SURFACE OF IMMOBILIZATION BIORESEPTOR PROCESS FOR USING DENSITY FUNCTIONAL THEORY (DFT) METHOD

**Nurul Fajariah**
**13620002**

## ABSTRACT

The research of material computation include system modeling and other aspects that refer to quantum physics. In this study, simulating and modeling is needed to investigate the adsorption process Glycine molecules on the surface of Fe(110). The study was conducted by doing nine adsorption sites modeling, by varying the position of Glycine molecules on the surface of Fe(110) using DFT (Density Functional Theory) method. This modeling method showed that the Fe (110) surface has a tendency to bind with O-2 atom, and a covalent bond as a result. The most stable adsorption of Glycine molecule on the surface of Fe (110) is happened in molecule **B** position at site *B* (bridging), namely site-4 which has the value of the adsorption energy is -0.87 eV. The results of this study may recommend that the Fe surface is able to immobilize bioreseptor in biosensor applications.

**Keywords**: Adsorption, DFT method, Glycine, and Fe(110) surface.

## DAFTAR ISI

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## DAFTAR GAMBAR

## DAFTAR LAMPIRAN

# BAB V

# PENUTUP

## 5.1 Kesimpulan

Berdasarkan hasil perhitungan dan simulasi relaksasi sistem dan pembahasan, maka dapat disimpulkan beberapa hal sebagai berikut.

1. Telah dilakukan simulasi dan pemodelan dari interaksi pada level atomik yang terjadi saat proses imobilisasi molekul Glisin oleh permukaan Fe(110) yang dapat dipelajari setelah mengetahui proses adsorpsi. Faktor yang sangat mempengaruhi proses adsorpsi adalah posisi molekul Glisin di atas permukaan Fe(110). Hasil menunjukkan bahwa permukaan Fe(110) memiliki kecenderungan berikatan dengan atom O-2 pada molekul Glisin, dengan ikatan yang terbentuk adalah ikatan kovalen. Sehingga Fe dapat digunakan untuk mengimobilisasi asam amino dalam aplikasi biosensor.
2. Interaksi antara molekul Glisin dengan permukaan Fe(110) direpresentasikan oleh energi adsorpsi. Adsorpsi molekul Glisin di atas permukaan Fe(110) paling stabil terjadi pada posisi molekul **B** di situs *B* (*bridging*), yakni pada situs-4, dengan nilai energi adsorpsi sebesar -0,87 eV.
3. Imobilisasi Glisin oleh permukaan Fe menyebabkan perubahan pada struktur geometri molekul Glisin. Hal ini diakibatkan oleh interaksi elektrostatik dan transfer muatan dari atom-atom pada molekul Glisin dan permukaan Fe yang berikatan. Tranfer elektron dapat

diketahui pada perubahan perubahan puncak dan munculnya keadaan (*state*) baru pada grafik DOS atom dari konstituen-konstituen pada sisten adsorpsi. Selain itu, tranfer elektron juga dapat diketahui perbedaan kerapatan muatan sistem yaitu dengan perbedaan warna yang tergambar yang mengidikasikan terjadinya akumulasi dan deplesi elektron setelah terjadi imobilisasi.

## 5.2 Saran

Terkait dengan kapasitas adsorpasi pada perhitungan dan simulasi relaksasi sistem asam amino pada permukaan Fe, ada beberapa hal yang disarankan oleh penliti.

1. Posisi molekul Glisin saat proses adsorpsi oleh permukaan Fe memiliki banyak probabilitas. Dalam penelitian ini dipilih sembilan situs dengan posisi molekul Glisin yang divariasikan. Perlu dilakukan penelitian dengan variasi posisi lain untuk mendapatkan energi adsorpsi yang paling baik.
2. Molekul Glisin adalah asam amino yang paling sederhana, maka dapat dilipih asam amino lain yang lebih kompleks untuk mengetahui kapasitas adsorpsinya dan interaksinya di level atomik.

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# LAMPIRAN-LAMPIRAN

***Lampiran 1***

## Agenda Kegiatan Penelitian

| No | Nama kegiatan | Minggu | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Okt | | | | Nov | | | | | Des | | | Jan | | | | | Feb | | |
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 1. | **Persiapan:** | | | | | | | | | | | | | | | | | | | | |
| | a. Studi literatur | | | | | | | | | | | | | | | | | | | | |
| | b. Penulisan Proposal | | | | | | | | | | | | | | | | | | | | |
| 2. | **Pelaksanaan:** | | | | | | | | | | | | | | | | | | | | |
| | a. Pembuatan program Quantum Expresso | | | | | | | | | | | | | | | | | | | | |
| | b. Pengambilan data | | | | | | | | | | | | | | | | | | | | |
| | c. Pengolahan data | | | | | | | | | | | | | | | | | | | | |
| | d. Penulisan BAB IV & V | | | | | | | | | | | | | | | | | | | | |

*Lampiran 2*

## Perhitungan Untuk Memperoleh Energi Adsorpsi Sistem

1. **Situs-1**

   -12.277,61415 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,02475342 Ry

   Konversi Satuan: -0,02475342 Ry = -0,336787559 eV

2. **Situs-2**

   -12.277,61966 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,03026642 Ry

   Konversi Satuan: -0.03026642 Ry = -0.411795772 eV

3. **Situs-3**

   -12.277,62154 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,03214195 Ry

   Konversi Satuan: -0,03214195 Ry = -0,437313667 eV

4. **Situs-4**

   -12.277,65328 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,06388726 Ry

   Konversi Satuan: -0,06388726 Ry = -0,86923077 eV

5. **Situs-5**

   -12.277,59058 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,00118885 Ry

   Konversi Satuan: -0,00118885 Ry = -0,016175134 eV

6. **Situs-6**

   -12277.59289 Ry – (-112.734068 Ry + (-12164.85533 Ry)) = -0.00349373 Ry

   Konversi Satuan: -0.00349373 Ry = -0.047534636 eV

7. **Situs-7**

   -12.277,59247 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,00307492 Ry

   Konversi Satuan: -0,00307492 Ry = -0,041836433 eV

8. **Situs-8**

   -12.277,58997 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,0005809 Ry

   Konversi Satuan: -0,0005809 Ry = -0,00790355 eV

9. **Situs-9**

   -12.277,60698 Ry – (-112,734068 Ry + (-12.164,85533 Ry)) = -0,01758967 Ry

   Konversi Satuan: -0,01758967 Ry = -0,239319739 eV

***Lampiran 3***

## INPUT PROGRAM

### Perhitungan *Self-Consistent* (SCF)

```
&CONTROL
  calculation = 'scf'
  title         = 'optimasi parameter'
  prefix        = 'FeGlisin'
  restart_mode = 'from_scratch'
  outdir = './Fe'
  pseudo_dir = '/home/ganda/WAHYU/pseudo'
  wf_collect = .TRUE.
/

&SYSTEM
  ibrav = 0
  nat   = 58
  ntyp  = 5
  ecutwfc = 40
  occupations = 'smearing'
  smearing = 'mv'
  degauss = 0.01
  starting_magnetization(5)=0.5
  nspin = 2
/

&ELECTRONS
  mixing_beta = 0.1
  electron_maxstep = 500
  conv_thr = 1.d-6
  diagonalization = 'david'
/
 f
&IONS
  ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
  H    1.00797      H.pbe-van_ak.UPF
  C    12.01115     C.pbe-van_ak.UPF
  N    14.0067      N.pbe-van_ak.UPF
  O    15.9994      O.pbe-van_ak.UPF
 Fe    55.845    Fe.pbe-sp-van_ak.UPF

ATOMIC_POSITIONS {angstrom}
Fe      1.516176820   0.055095870   0.080504280    0   0   0
Fe      4.382676010   0.056520840   0.078889020    0   0   0
Fe      7.249175200   0.057945800   0.077273760    0   0   0
Fe      1.514159740   4.108937180   0.077182830    0   0   0
Fe      4.380658930   4.110362150   0.075567570    0   0   0
Fe      7.247158120   4.111787120   0.073952310    0   0   0
Fe      0.081918680   2.081304040   0.079651190    0   0   0
Fe      1.516309610   2.083677820   2.105764140    0   0   0
Fe      2.948417870   2.082729010   0.078035930    0   0   0
Fe      4.382808800   2.085102780   2.104148880    0   0   0
```

```
Fe       5.814917060   2.084153980   0.076420670    0    0    0
Fe       7.249308000   2.086527750   2.102533620    0    0    0
Fe       0.084068560   0.056044680   2.108232500    0    0    0
Fe       2.950567750   0.057469640   2.106617240    0    0    0
Fe       5.817066940   0.058894610   2.105001980    0    0    0
Fe       0.079901600   6.135145360   0.076329740    0    0    0
Fe       1.514292530   6.137519130   2.102442700    0    0    0
Fe       2.946400790   6.136570320   0.074714480    0    0    0
Fe       4.380791730   6.138944100   2.100827440    0    0    0
Fe       5.812899990   6.137995290   0.073099220    0    0    0
Fe       7.247290920   6.140369070   2.099212180    0    0    0
Fe       0.082051480   4.109885990   2.104911050    0    0    0
Fe       2.948550670   4.111310960   2.103295790    0    0    0
Fe       5.815049860   4.112735920   2.101680530    0    0    0
Fe       1.517629298   0.058970770   4.143532430
Fe       4.384026281   0.059526296   4.142131062
Fe       7.249184606   0.059595919   4.142238757
Fe       1.517165304   4.113128821   4.141555533
Fe       4.383563786   4.113680288   4.140152080
Fe       7.248725295   4.113742818   4.140262163
Fe       0.084261362   2.086284561   4.142606606
Fe       1.518592363   2.087491404   6.132350964
Fe       2.950894484   2.086369004   4.142008188
Fe       4.384022306   2.087783349   6.131592430
Fe       5.816546628   2.086911607   4.140837828
Fe       7.249098199   2.087965236   6.131162499
Fe       0.084201574   0.060022748   6.132996670
Fe       2.951340551   0.060220720   6.132139708
Fe       5.817231480   0.060515251   6.131791397
Fe       0.083811854   6.140079015   4.140476207
Fe       1.518461489   6.141014327   6.130563029
Fe       2.950445134   6.140163373   4.139869088
Fe       4.383876509   6.141295990   6.129806761
Fe       5.816099372   6.140707541   4.138706967
Fe       7.248970286   6.141502292   6.129391897
Fe       0.084042913   4.114523353   6.131335622
Fe       2.951188190   4.114716185   6.130473366
Fe       5.817093451   4.115009597   6.130122333
O        3.40177791    2.15265537   10.08892945
O        4.44484333    2.13554401    8.06492867
N        7.02959818    2.14690259    9.32810856
C        5.79563553    2.13636701   10.10122216
C        4.50587958    2.14104177    9.28222366
H        5.76905963    3.00720107   10.77827636
H        5.77195927    1.24837512   10.75576911
H        7.03539887    2.96410597    8.71134338
H        7.04142906    1.33963158    8.69828171
H        2.61497256    2.15170880    9.49880759

K_POINTS automatic
3 3 1 0 0 0

CELL_PARAMETERS {bohr}
    16.247864050    0.000000000    0.000000000
     0.000000000   15.321898315    0.000000000
     0.000000000    0.000000000   36.108884190
```

**Perhitungan Relaksasi Sistem**

```
&CONTROL
  calculation = 'relax'
  title         = 'Structure optimization of Fe-Glisincine'
  prefix        = 'FeGlisin'
  restart_mode = 'from_scratch'
  outdir = './Fe'
  pseudo_dir = '/home/ganda/WAHYU/pseudo'
  wf_collect = .TRUE.
/

&SYSTEM
  ibrav = 0
  nat   = 58
  ntyp  = 5
  ecutwfc = 40
  occupations = 'smearing'
  smearing = 'mv'
  degauss = 0.01
  starting_magnetization(5)=0.5
  nspin = 2
/

&ELECTRONS
  mixing_beta = 0.1
  electron_maxstep = 500
  conv_thr = 1.d-6
  diagonalization = 'david'
/
 f
&IONS
  ion_dynamics = 'bfgs'
/

ATOMIC_SPECIES
  H    1.00797      H.pbe-van_ak.UPF
  C    12.01115     C.pbe-van_ak.UPF
  N    14.0067      N.pbe-van_ak.UPF
  O    15.9994      O.pbe-van_ak.UPF
 Fe    55.845    Fe.pbe-sp-van_ak.UPF

ATOMIC_POSITIONS {angstrom}
Fe      1.516176820   0.055095870   0.080504280    0   0   0
Fe      4.382676010   0.056520840   0.078889020    0   0   0
Fe      7.249175200   0.057945800   0.077273760    0   0   0
Fe      1.514159740   4.108937180   0.077182830    0   0   0
Fe      4.380658930   4.110362150   0.075567570    0   0   0
Fe      7.247158120   4.111787120   0.073952310    0   0   0
Fe      0.081918680   2.081304040   0.079651190    0   0   0
Fe      1.516309610   2.083677820   2.105764140    0   0   0
Fe      2.948417870   2.082729010   0.078035930    0   0   0
Fe      4.382808800   2.085102780   2.104148880    0   0   0
Fe      5.814917060   2.084153980   0.076420670    0   0   0
Fe      7.249308000   2.086527750   2.102533620    0   0   0
Fe      0.084068560   0.056044680   2.108232500    0   0   0
```

```
Fe      2.950567750   0.057469640   2.106617240    0    0    0
Fe      5.817066940   0.058894610   2.105001980    0    0    0
Fe      0.079901600   6.135145360   0.076329740    0    0    0
Fe      1.514292530   6.137519130   2.102442700    0    0    0
Fe      2.946400790   6.136570320   0.074714480    0    0    0
Fe      4.380791730   6.138944100   2.100827440    0    0    0
Fe      5.812899990   6.137995290   0.073099220    0    0    0
Fe      7.247290920   6.140369070   2.099212180    0    0    0
Fe      0.082051480   4.109885990   2.104911050    0    0    0
Fe      2.948550670   4.111310960   2.103295790    0    0    0
Fe      5.815049860   4.112735920   2.101680530    0    0    0
Fe      1.517629298   0.058970770   4.143532430
Fe      4.384026281   0.059526296   4.142131062
Fe      7.249184606   0.059595919   4.142238757
Fe      1.517165304   4.113128821   4.141555533
Fe      4.383563786   4.113680288   4.140152080
Fe      7.248725295   4.113742818   4.140262163
Fe      0.084261362   2.086284561   4.142606606
Fe      1.518592363   2.087491404   6.132350964
Fe      2.950894484   2.086369004   4.142008188
Fe      4.384022306   2.087783349   6.131592430
Fe      5.816546628   2.086911607   4.140837828
Fe      7.249098199   2.087965236   6.131162499
Fe      0.084201574   0.060022748   6.132996670
Fe      2.951340551   0.060220720   6.132139708
Fe      5.817231480   0.060515251   6.131791397
Fe      0.083811854   6.140079015   4.140476207
Fe      1.518461489   6.141014327   6.130563029
Fe      2.950445134   6.140163373   4.139869088
Fe      4.383876509   6.141295990   6.129806761
Fe      5.816099372   6.140707541   4.138706967
Fe      7.248970286   6.141502292   6.129391897
Fe      0.084042913   4.114523353   6.131335622
Fe      2.951188190   4.114716185   6.130473366
Fe      5.817093451   4.115009597   6.130122333
O       3.40177791    2.15265537   10.08892945
O       4.44484333    2.13554401    8.06492867
N       7.02959818    2.14690259    9.32810856
C       5.79563553    2.13636701   10.10122216
C       4.50587958    2.14104177    9.28222366
H       5.76905963    3.00720107   10.77827636
H       5.77195927    1.24837512   10.75576911
H       7.03539887    2.96410597    8.71134338
H       7.04142906    1.33963158    8.69828171
H       2.61497256    2.15170880    9.49880759

K_POINTS automatic
3 3 1 0 0 0

CELL_PARAMETERS {bohr}
    16.247864050    0.000000000    0.000000000
     0.000000000   15.321898315    0.000000000
     0.000000000    0.000000000   36.108884190
```

***Lampiran 4***

## OUTPUT PROGRAM

```
     Program PWSCF v.5.0.2 (svn rev. 9392) starts on  6Jan2017 at
7:41:50

     This program is part of the open-source Quantum ESPRESSO
suite
     for quantum simulation of materials; please cite
         "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502
(2009);
          URL http://www.quantum-espresso.org",
     in publications or presentations arising from this work. More
details at
     http://www.quantum-espresso.org/quote.php

     Parallel version (MPI), running on    20 processors
     R & G space division:  proc/nbgrp/npool/nimage =      20

     Current dimensions of program PWSCF are:
     Max number of different atomic species (ntypx) = 10
     Max number of k-points (npk) =  40000
     Max angular momentum in pseudopotentials (lmaxx) =  3
     Waiting for input...
     Reading input from standard input

     Subspace diagonalization in iterative solution of the
eigenvalue problem:
     scalapack distributed-memory algorithm (size of sub-group:
3*  3 procs)


     Parallelization info
     --------------------
      .     .     .
      .     .     .
      .     .     .
Self-consistent Calculation

      iteration #  1     ecut=    40.00 Ry     beta=0.10
      Davidson diagonalization with overlap
      ethr =  1.00E-02,  avg # of iterations =  3.9

      negative rho (up, down):  0.773E-03 0.617E-03

      total cpu time spent up to now is      597.9 secs

      total energy              =  -12254.34711800 Ry
      Harris-Foulkes estimate   =  -12282.89262173 Ry
      estimated scf accuracy    <     226.18016927 Ry
```

```
total magnetization       =   160.00 Bohr mag/cell
absolute magnetization    =   164.90 Bohr mag/cell

iteration #  2     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  4.0

negative rho (up, down):  0.667E-03 0.499E-03

total cpu time spent up to now is     1166.9 secs

total energy              =  -12232.29126929 Ry
Harris-Foulkes estimate   =  -12302.22465613 Ry
estimated scf accuracy    <    2055.49765337 Ry

total magnetization       =   116.30 Bohr mag/cell
absolute magnetization    =   120.35 Bohr mag/cell

iteration #  3     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  4.3

negative rho (up, down):  0.383E-03 0.247E-03

total cpu time spent up to now is     1569.5 secs

total energy              =  -12264.65626145 Ry
Harris-Foulkes estimate   =  -12271.02067028 Ry
estimated scf accuracy    <      82.92959020 Ry

total magnetization       =   160.00 Bohr mag/cell
absolute magnetization    =   167.75 Bohr mag/cell

iteration #  4     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  2.3

negative rho (up, down):  0.213E-03 0.121E-03

total cpu time spent up to now is     1854.1 secs

total energy              =  -12266.71651117 Ry
Harris-Foulkes estimate   =  -12268.72424549 Ry
estimated scf accuracy    <      51.82030940 Ry

total magnetization       =   159.92 Bohr mag/cell
absolute magnetization    =   167.86 Bohr mag/cell

iteration #  5     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  6.49E-03,  avg # of iterations =  2.7
```

```
negative rho (up, down):  0.178E-03 0.972E-04

total cpu time spent up to now is     2154.6 secs

total energy              =  -12270.44339913 Ry
Harris-Foulkes estimate   =  -12269.37259964 Ry
estimated scf accuracy    <      16.68317178 Ry

total magnetization       =   158.43 Bohr mag/cell
absolute magnetization    =   164.11 Bohr mag/cell

iteration #  6     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.09E-03,  avg # of iterations =  2.1

negative rho (up, down):  0.204E-03 0.112E-03

total cpu time spent up to now is     2429.5 secs

total energy              =  -12272.69403203 Ry
Harris-Foulkes estimate   =  -12270.96665162 Ry
estimated scf accuracy    <      11.83952529 Ry

total magnetization       =   156.74 Bohr mag/cell
absolute magnetization    =   162.91 Bohr mag/cell

iteration #  7     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.48E-03,  avg # of iterations =  3.0

negative rho (up, down):  0.329E-03 0.202E-03

total cpu time spent up to now is     2726.2 secs

total energy              =  -12274.42413926 Ry
Harris-Foulkes estimate   =  -12272.98617608 Ry
estimated scf accuracy    <       7.98839649 Ry

total magnetization       =   151.26 Bohr mag/cell
absolute magnetization    =   158.42 Bohr mag/cell

iteration #  8     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-03,  avg # of iterations =  2.6

negative rho (up, down):  0.770E-03 0.572E-03

total cpu time spent up to now is     3017.9 secs

total energy              =  -12276.21680324 Ry
```

```
Harris-Foulkes estimate   =  -12274.62928813 Ry
estimated scf accuracy    <       6.05549123 Ry

total magnetization       =   145.29 Bohr mag/cell
absolute magnetization    =   153.98 Bohr mag/cell

iteration #  9     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  7.59E-04,  avg # of iterations =  1.9

negative rho (up, down):  0.149E-02 0.119E-02

total cpu time spent up to now is     3290.4 secs

total energy              =  -12277.13063502 Ry
Harris-Foulkes estimate   =  -12276.50694608 Ry
estimated scf accuracy    <       5.31516880 Ry

total magnetization       =   139.48 Bohr mag/cell
absolute magnetization    =   148.84 Bohr mag/cell

iteration # 10     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  6.66E-04,  avg # of iterations =  1.9

negative rho (up, down):  0.189E-02 0.150E-02

total cpu time spent up to now is     3560.2 secs

total energy              =  -12277.44295243 Ry
Harris-Foulkes estimate   =  -12277.35975642 Ry
estimated scf accuracy    <       1.07076542 Ry

total magnetization       =   134.28 Bohr mag/cell
absolute magnetization    =   143.22 Bohr mag/cell

iteration # 11     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.34E-04,  avg # of iterations =  4.2

negative rho (up, down):  0.214E-02 0.170E-02

total cpu time spent up to now is     3890.7 secs

total energy              =  -12277.55093215 Ry
Harris-Foulkes estimate   =  -12277.55936125 Ry
estimated scf accuracy    <       0.73236797 Ry

total magnetization       =   130.56 Bohr mag/cell
absolute magnetization    =   138.82 Bohr mag/cell
```

```
iteration # 12     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  9.18E-05,  avg # of iterations =  2.2

negative rho (up, down):  0.213E-02 0.169E-02

total cpu time spent up to now is     4171.5 secs

total energy              =  -12277.57856451 Ry
Harris-Foulkes estimate   =  -12277.58688785 Ry
estimated scf accuracy    <       0.19600242 Ry

total magnetization       =   128.31 Bohr mag/cell
absolute magnetization    =   136.40 Bohr mag/cell

iteration # 13     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.46E-05,  avg # of iterations =  4.3

negative rho (up, down):  0.212E-02 0.169E-02

total cpu time spent up to now is     4498.6 secs

total energy              =  -12277.58378682 Ry
Harris-Foulkes estimate   =  -12277.58962658 Ry
estimated scf accuracy    <       0.28656650 Ry

total magnetization       =   128.28 Bohr mag/cell
absolute magnetization    =   136.19 Bohr mag/cell

iteration # 14     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.46E-05,  avg # of iterations =  1.0

negative rho (up, down):  0.204E-02 0.163E-02

total cpu time spent up to now is     4750.0 secs

total energy              =  -12277.58673429 Ry
Harris-Foulkes estimate   =  -12277.58997837 Ry
estimated scf accuracy    <       0.08239460 Ry

total magnetization       =   127.58 Bohr mag/cell
absolute magnetization    =   135.46 Bohr mag/cell

iteration # 15     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.03E-05,  avg # of iterations =  2.6

negative rho (up, down):  0.183E-02 0.148E-02
```

```
total cpu time spent up to now is     5037.6 secs

total energy              =  -12277.58717157 Ry
Harris-Foulkes estimate   =  -12277.58917904 Ry
estimated scf accuracy    <       0.04132004 Ry

total magnetization       =   127.10 Bohr mag/cell
absolute magnetization    =   134.83 Bohr mag/cell

iteration # 16     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  5.18E-06,  avg # of iterations =  6.3

negative rho (up, down):  0.175E-02 0.143E-02

total cpu time spent up to now is     5424.6 secs

total energy              =  -12277.58914443 Ry
Harris-Foulkes estimate   =  -12277.58931244 Ry
estimated scf accuracy    <       0.02155234 Ry

total magnetization       =   126.95 Bohr mag/cell
absolute magnetization    =   134.40 Bohr mag/cell

iteration # 17     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.70E-06,  avg # of iterations =  1.9

negative rho (up, down):  0.156E-02 0.130E-02

total cpu time spent up to now is     5696.4 secs

total energy              =  -12277.59132825 Ry
Harris-Foulkes estimate   =  -12277.58982433 Ry
estimated scf accuracy    <       0.01365832 Ry

total magnetization       =   126.83 Bohr mag/cell
absolute magnetization    =   134.16 Bohr mag/cell

iteration # 18     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.71E-06,  avg # of iterations =  5.4

negative rho (up, down):  0.150E-02 0.125E-02

total cpu time spent up to now is     6068.0 secs

total energy              =  -12277.59281486 Ry
Harris-Foulkes estimate   =  -12277.59232161 Ry
estimated scf accuracy    <       0.00761157 Ry
```

```
total magnetization       =   127.20 Bohr mag/cell
absolute magnetization    =   134.23 Bohr mag/cell

iteration # 19     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  9.54E-07,  avg # of iterations =  1.5

negative rho (up, down):  0.149E-02 0.125E-02

total cpu time spent up to now is     6327.4 secs

total energy              =  -12277.59328950 Ry
Harris-Foulkes estimate   =  -12277.59327187 Ry
estimated scf accuracy    <       0.00291087 Ry

total magnetization       =   127.27 Bohr mag/cell
absolute magnetization    =   134.16 Bohr mag/cell

iteration # 20     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.65E-07,  avg # of iterations =  1.5

negative rho (up, down):  0.148E-02 0.124E-02

total cpu time spent up to now is     6587.4 secs

total energy              =  -12277.59365790 Ry
Harris-Foulkes estimate   =  -12277.59349320 Ry
estimated scf accuracy    <       0.00283216 Ry

total magnetization       =   127.25 Bohr mag/cell
absolute magnetization    =   134.11 Bohr mag/cell

iteration # 21     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.55E-07,  avg # of iterations =  1.0

negative rho (up, down):  0.147E-02 0.124E-02

total cpu time spent up to now is     6838.2 secs

total energy              =  -12277.59397538 Ry
Harris-Foulkes estimate   =  -12277.59377080 Ry
estimated scf accuracy    <       0.00099739 Ry

total magnetization       =   127.21 Bohr mag/cell
absolute magnetization    =   134.02 Bohr mag/cell

iteration # 22     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.25E-07,  avg # of iterations =  1.4
```

```
negative rho (up, down):  0.146E-02 0.124E-02

total cpu time spent up to now is     7099.6 secs

total energy              =  -12277.59431453 Ry
Harris-Foulkes estimate   =  -12277.59402258 Ry
estimated scf accuracy    <       0.00079007 Ry

total magnetization       =   127.27 Bohr mag/cell
absolute magnetization    =   134.03 Bohr mag/cell

iteration # 23     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  9.90E-08,  avg # of iterations =  2.9

negative rho (up, down):  0.145E-02 0.123E-02

total cpu time spent up to now is     7438.0 secs

total energy              =  -12277.59453865 Ry
Harris-Foulkes estimate   =  -12277.59442545 Ry
estimated scf accuracy    <       0.00028991 Ry

total magnetization       =   127.19 Bohr mag/cell
absolute magnetization    =   133.84 Bohr mag/cell

iteration # 24     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.63E-08,  avg # of iterations =  1.0

negative rho (up, down):  0.145E-02 0.123E-02

total cpu time spent up to now is     7687.4 secs

total energy              =  -12277.59458799 Ry
Harris-Foulkes estimate   =  -12277.59455979 Ry
estimated scf accuracy    <       0.00076280 Ry

total magnetization       =   127.22 Bohr mag/cell
absolute magnetization    =   133.84 Bohr mag/cell

iteration # 25     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.63E-08,  avg # of iterations =  1.0

negative rho (up, down):  0.144E-02 0.123E-02

total cpu time spent up to now is     7938.7 secs

total energy              =  -12277.59474677 Ry
```

```
Harris-Foulkes estimate   =  -12277.59460911 Ry
estimated scf accuracy    <       0.00036974 Ry

total magnetization       =   127.22 Bohr mag/cell
absolute magnetization    =   133.82 Bohr mag/cell

iteration # 26     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.63E-08,  avg # of iterations =  1.8

negative rho (up, down):  0.144E-02 0.123E-02

total cpu time spent up to now is     8208.9 secs

total energy              =  -12277.59480996 Ry
Harris-Foulkes estimate   =  -12277.59476151 Ry
estimated scf accuracy    <       0.00009252 Ry

total magnetization       =   127.24 Bohr mag/cell
absolute magnetization    =   133.80 Bohr mag/cell

iteration # 27     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.16E-08,  avg # of iterations =  2.0

negative rho (up, down):  0.143E-02 0.123E-02

total cpu time spent up to now is     8489.0 secs

total energy              =  -12277.59491379 Ry
Harris-Foulkes estimate   =  -12277.59481593 Ry
estimated scf accuracy    <       0.00007865 Ry

total magnetization       =   127.25 Bohr mag/cell
absolute magnetization    =   133.79 Bohr mag/cell

iteration # 28     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  9.86E-09,  avg # of iterations =  2.3

negative rho (up, down):  0.143E-02 0.123E-02

total cpu time spent up to now is     8798.7 secs

total energy              =  -12277.59496118 Ry
Harris-Foulkes estimate   =  -12277.59492350 Ry
estimated scf accuracy    <       0.00003354 Ry

total magnetization       =   127.29 Bohr mag/cell
absolute magnetization    =   133.79 Bohr mag/cell
```

```
iteration # 29     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  4.20E-09,  avg # of iterations =  2.1

negative rho (up, down):  0.142E-02 0.123E-02

total cpu time spent up to now is     9078.0 secs

total energy              =  -12277.59499051 Ry
Harris-Foulkes estimate   =  -12277.59496420 Ry
estimated scf accuracy    <       0.00002607 Ry

total magnetization       =   127.32 Bohr mag/cell
absolute magnetization    =   133.78 Bohr mag/cell

iteration # 30     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  3.27E-09,  avg # of iterations =  2.1

negative rho (up, down):  0.142E-02 0.123E-02

total cpu time spent up to now is     9377.4 secs

total energy              =  -12277.59500534 Ry
Harris-Foulkes estimate   =  -12277.59499363 Ry
estimated scf accuracy    <       0.00002067 Ry

total magnetization       =   127.34 Bohr mag/cell
absolute magnetization    =   133.78 Bohr mag/cell

iteration # 31     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.59E-09,  avg # of iterations =  1.3

negative rho (up, down):  0.142E-02 0.123E-02

total cpu time spent up to now is     9636.7 secs

total energy              =  -12277.59501344 Ry
Harris-Foulkes estimate   =  -12277.59500648 Ry
estimated scf accuracy    <       0.00001184 Ry

total magnetization       =   127.35 Bohr mag/cell
absolute magnetization    =   133.78 Bohr mag/cell

iteration # 32     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.48E-09,  avg # of iterations =  2.4

negative rho (up, down):  0.142E-02 0.123E-02
```

```
total cpu time spent up to now is     9928.2 secs

total energy              =  -12277.59501817 Ry
Harris-Foulkes estimate   =  -12277.59501438 Ry
estimated scf accuracy    <       0.00001168 Ry

total magnetization       =   127.36 Bohr mag/cell
absolute magnetization    =   133.77 Bohr mag/cell

iteration # 33     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.46E-09,  avg # of iterations =  1.6

negative rho (up, down):  0.142E-02 0.123E-02

total cpu time spent up to now is    10192.2 secs

total energy              =  -12277.59502048 Ry
Harris-Foulkes estimate   =  -12277.59501877 Ry
estimated scf accuracy    <       0.00000801 Ry

total magnetization       =   127.36 Bohr mag/cell
absolute magnetization    =   133.77 Bohr mag/cell

iteration # 34     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-09,  avg # of iterations =  1.7

negative rho (up, down):  0.142E-02 0.123E-02

total cpu time spent up to now is    10466.1 secs

total energy              =  -12277.59502442 Ry
Harris-Foulkes estimate   =  -12277.59502132 Ry
estimated scf accuracy    <       0.00003468 Ry

total magnetization       =   127.36 Bohr mag/cell
absolute magnetization    =   133.77 Bohr mag/cell

iteration # 35     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-09,  avg # of iterations =  2.3

negative rho (up, down):  0.142E-02 0.124E-02

total cpu time spent up to now is    10752.3 secs

total energy              =  -12277.59502671 Ry
Harris-Foulkes estimate   =  -12277.59502579 Ry
estimated scf accuracy    <       0.00001522 Ry
```

```
total magnetization       =   127.37 Bohr mag/cell
absolute magnetization    =   133.77 Bohr mag/cell

iteration # 36     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.00E-09,  avg # of iterations =  1.1

negative rho (up, down):  0.142E-02 0.124E-02

total cpu time spent up to now is    11008.0 secs

total energy              =  -12277.59502754 Ry
Harris-Foulkes estimate   =  -12277.59502709 Ry
estimated scf accuracy    <       0.00000236 Ry

total magnetization       =   127.37 Bohr mag/cell
absolute magnetization    =   133.77 Bohr mag/cell

iteration # 37     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.96E-10,  avg # of iterations =  1.7

negative rho (up, down):  0.142E-02 0.124E-02

total cpu time spent up to now is    11274.9 secs

total energy              =  -12277.59502827 Ry
Harris-Foulkes estimate   =  -12277.59502762 Ry
estimated scf accuracy    <       0.00000203 Ry

total magnetization       =   127.37 Bohr mag/cell
absolute magnetization    =   133.76 Bohr mag/cell

iteration # 38     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  2.54E-10,  avg # of iterations =  1.5

negative rho (up, down):  0.142E-02 0.124E-02

total cpu time spent up to now is    11533.9 secs

total energy              =  -12277.59502874 Ry
Harris-Foulkes estimate   =  -12277.59502833 Ry
estimated scf accuracy    <       0.00000144 Ry

total magnetization       =   127.37 Bohr mag/cell
absolute magnetization    =   133.76 Bohr mag/cell

iteration # 39     ecut=    40.00 Ry     beta=0.10
Davidson diagonalization with overlap
ethr =  1.80E-10,  avg # of iterations =  1.9
```

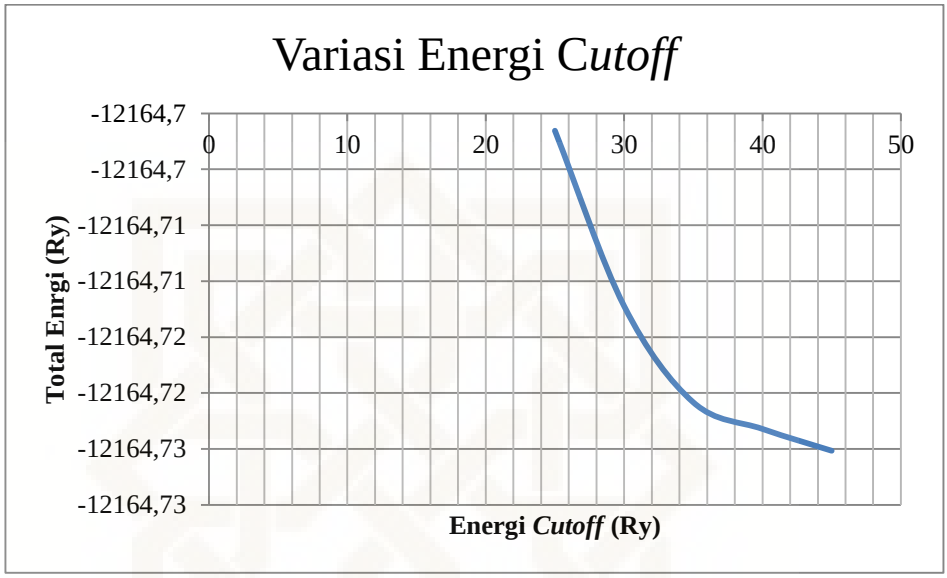
```
     negative rho (up, down):  0.142E-02 0.124E-02

     total cpu time spent up to now is    11810.0 secs

     total energy              =  -12277.59502943 Ry
     Harris-Foulkes estimate   =  -12277.59502879 Ry
     estimated scf accuracy    <       0.00000124 Ry

     total magnetization       =   127.37 Bohr mag/cell
     absolute magnetization    =   133.76 Bohr mag/cell

     iteration # 40     ecut=    40.00 Ry     beta=0.10
     Davidson diagonalization with overlap
     ethr =  1.55E-10,  avg # of iterations =  2.3

     negative rho (up, down):  0.142E-02 0.124E-02

     total cpu time spent up to now is    12093.5 secs

     End of self-consistent calculation

------ SPIN UP ------------
      .     .     .
      .     .     .
      .     .     .

    Writing output data file FeGlisin.save

    init_run  :    113.46s CPU    131.40s WALL (1 calls)
    electrons : 275785.56s CPU 340418.99s WALL (50 calls)
    update_pot:     54.58s CPU     58.56s WALL (49 calls)
    forces    :   3079.49s CPU   3334.99s WALL (50 calls)

    Called by init_run:
    wfcinit   :    109.92s CPU    127.69s WALL (1 calls)
    potinit   :      0.59s CPU      0.63s WALL (1 calls)

    Called by electrons:
    c_bands   : 245102.74s CPU 304340.42s WALL (1126 calls)
    sum_band  :  27903.23s CPU  32923.47s WALL (1126 calls)
    v_of_rho  :    122.81s CPU    142.79s WALL (1170 calls)
    newd      :   2582.89s CPU   2658.87s WALL (1170 calls)
    mix_rho   :     31.49s CPU     37.10s WALL (1126 calls)

    Called by c_bands:
    init_us_2: 288.98s CPU    297.32s WALL (23030 calls)
    cegterg  : 241919.86s CPU 298629.27s WALL (11260 calls)

    Called by *egterg:
    h_psi     : 93219.44s CPU 106799.20s WALL (34831 calls)
    s_psi     : 28582.17s CPU  28685.82s WALL (34831 calls)
    g_psi     : 367.13s CPU    367.60s WALL   (23561 calls)
    cdiaghg   : 38458.18s CPU  68443.25s WALL (34271 calls)
```

```
     Called by h_psi:
     add_vuspsi: 28911.52s CPU  29057.54s WALL (34831 calls)

     General routines
     calbec:  46579.68s CPU  50934.52s WALL (46591 calls)
     fft   :    227.16s CPU    497.99s WALL (29236 calls)
     fftw  :  38386.59s CPU  51952.17s WALL (27990712 calls)
     davcio:      1.33s CPU   2847.40s WALL (34300 calls)

     Parallel routines
     fft_scatter :  11975.19s CPU  23743.75s WALL (28019948 calls)

     PWSCF       :     3d    5h32m CPU     3d   23h35m WALL


   This run was terminated on:   7:17:40  10Jan2017

=------------------------------------------------------------------=
   JOB DONE.
=------------------------------------------------------------------=
```

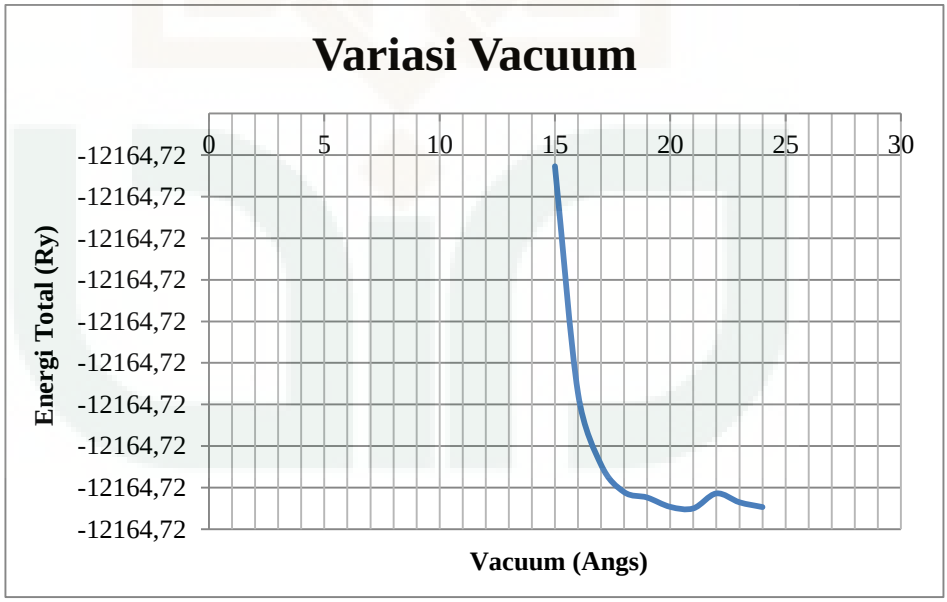
***Lampiran 5***

**Optimasi Parameter**

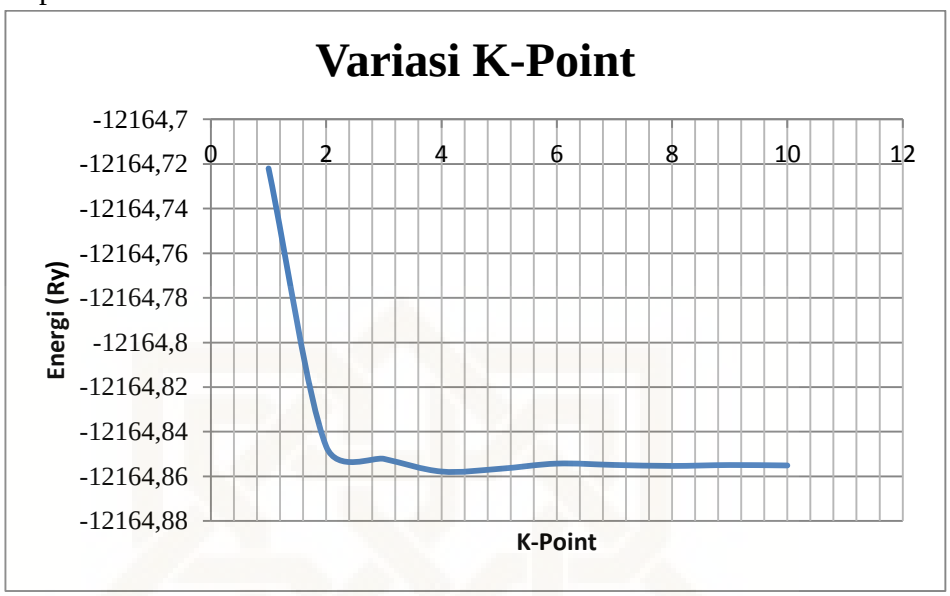
1. Energi *Cutoff*




2. Tinggi Ruang Vacuum

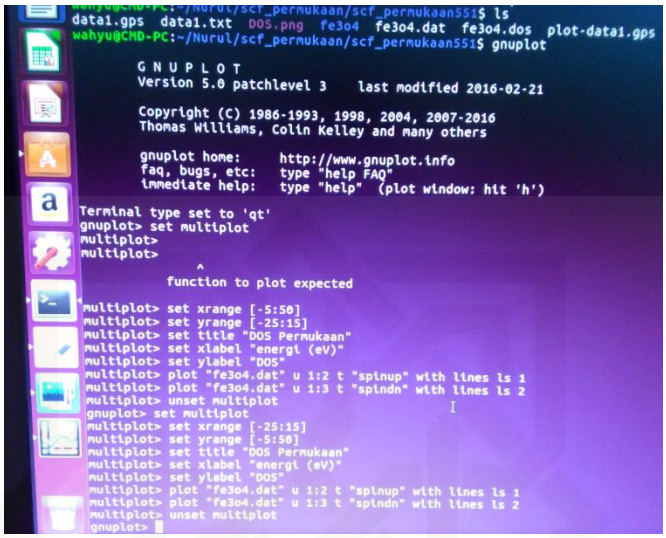


3. K-point

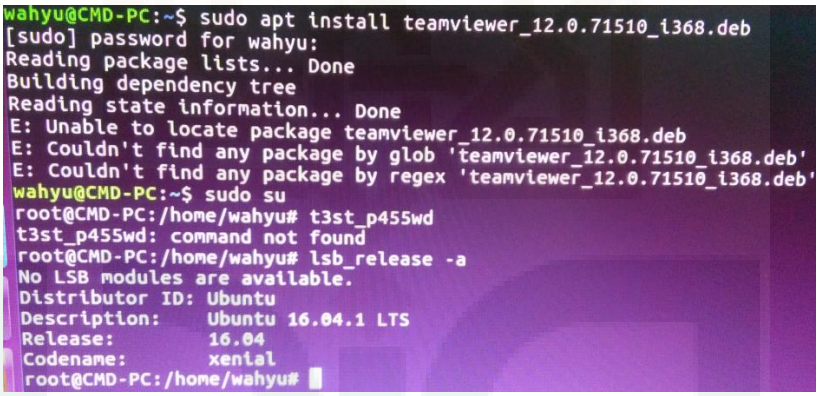

Variasi K-Point
-12164,7
-12164,72
-12164,74
-12164,76
-12164,78
-12164,8
-12164,82
-12164,84
-12164,86
-12164,88
Energi (Ry)
0
2
4
6
8
10
12
K-Point

*Lampiran 6*

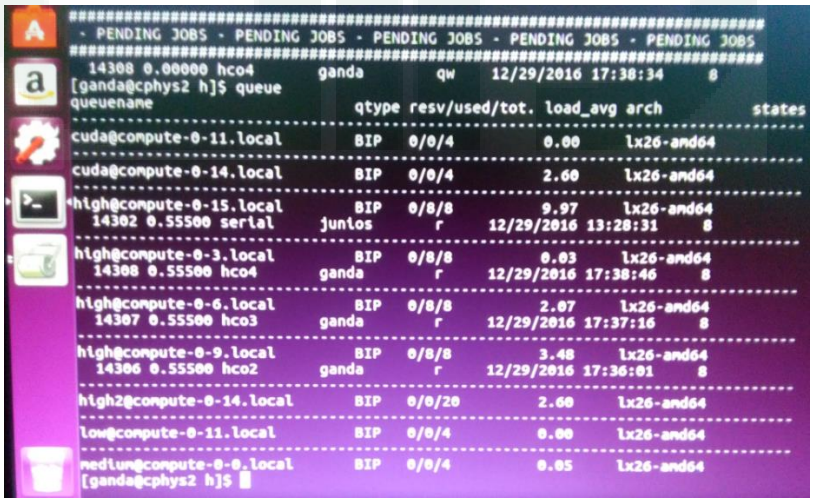
## DOKUMENTASI KEGIATAN RUNNING




**Tampilan Saat Memplot Grafik DOS**




**Seri Ubuntu yang Digunakan**




**Tampilan Saat Submit Input**

***Lampiran 7***

# Curriculum Vitae


## Data Pribadi

| | |
|---|---|
| Nama | : Nurul Fajariah |
| Tempat, tanggal lahir | : Serang, 24 Mei 1995 |
| Jenis Kelamin | : Perempuan |
| Agama | : Islam |
| Golongan darah | : O |
| Alamat | : Sapen GK I, RT/RW 22/07 No. 401 Gondokusuman, Yogyakarta, D.I Yogyakarta |
| Telepon | : 085780945402 |
| Email | : cahayafajar80@gmail.com |

## Latar Belakang Pendidikan

**Formal**

| | |
|---|---|
| 2001-2007 | : SD N Cilengo, Serang, Banten |
| 2007-2010 | : MTs N Model Padarincang, Serang, Banten |
| 2010-2013 | : SMA N 1 Padarincang, Serang, Banten |
| 2013-sekarang | : UIN Sunan Kalijaga Yogyakarta, DIY |

**Non Formal**

| | |
|---|---|
| 2004-2006 | : Madrasah Diniyyah Awaliyah al-Hikmah |
| 2012 | : Lembaga Bimbingan Belajar Nurul Fikri |

## Pengalaman Organisasi

| | |
|---|---|
| 2010-2012 | : Ketua OSIS SMAN 1 Padarincang |
| 2012 | : Sekeretaris Forum Anak Kabupaten Serang |
| 2014-2015 | : Sekretaris Divisi Tilawah UKM al-Mizan UIN Sunan Kalijaga |
| 2015-sekarang | : Sekretaris *study club* Fisika Material UIN Sunan Kalijaga |
| 2015-sekarang | : Bendahara Umum UKM al-Mizan UIN Sunan Kalijaga |