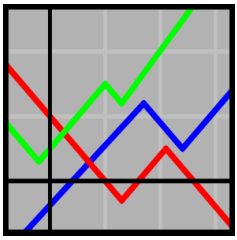
# LAMPIRAN

Lampiran 1. 1 Software


Abinit


Xcrysden



Gnuplot

Lampiran 1. 2 Input file dari germanene didoping atom boron poisisi Bridge

```
#Germanene didoping atom boron posisi Bridge
 ndtset 6
#First dataset : SC run with kpoints in the IBZ
   iscf1  3
  nband1  32
  nstep1 25
 kptopt1 1
 nbdbuf1 0
 prtden1 1   getden1 0   getwfk1 0
#Second dataset : NSC run with large number of bands, and points
in the IBZ
    iscf2 -2
   nband2 32
   nstep2 25
  kptopt2  1
  getwfk2  1   getden2 1
#Third dataset : NSC run with large number of bands, and points
in the the full BZ
    iscf3 -2
   nband3 32
   nstep3 25
  kptopt3  3
  getwfk3  2   getden3 1
#Fourth dataset : ddk response function along axis 1
   iscf4 -3
  nband4 32
  nstep4  1  nline4  0  prtwf4  3
 kptopt4  3
   nqpt4  1  qpt4  0.0d0 0.0d0 0.0d0
  rfdir4  1 0 0
```

```
 rfelfd4  2
 getwfk4  3
#Fifth dataset : ddk response function along axis 2
   iscf5 -3
  nband5 32
  nstep5  1  nline5  0   prtwf5  3
 kptopt5  3
   nqpt5  1  qpt5  0.0d0 0.0d0 0.0d0
  rfdir5  0 1 0
 rfelfd5  2
 getwfk5  3
#Sixth dataset : ddk response function along axis 3
   iscf6 -3
  nband6 32
  nstep6  1  nline6  0    prtwf6  3
 kptopt6  3
   nqpt6  1  qpt6  0.0d0 0.0d0 0.0d0
  rfdir6  0 0 1
 rfelfd6  2
 getwfk6  3
#Data common to all datasets
 nshiftk 1
 shiftk  0.0 0.0 0.0
 ngkpt 18 18 1
 acell   15.5 15.5  29.5
 amu 10.811 72.61
 diemac 12.0
 ecut 30.00


ixc 3
nbdbuf 2
ntypat  2
rprim
0.866 0.5 0
0.0 1.0 0.0
0.0 0.0 1.0
natom 9
typat 1 2 2 2 2 2 2 2 2 tolwfr  1.e-20
xred
1.5/6 3/6 0.34
1/6 1/6 0.15
2/6 2/6 0.15
4/6 1/6 0.15
5/6 2/6 0.15
1/6 4/6 0.15
2/6 5/6 0.15
4/6 4/6 0.15
5/6 5/6 0.15
 tnons 72*0.0
 znucl 5 32
optforces 1
chkprim 0
```

Lampiran 1. 3 Input file dari germanene didoping atom boron posisi Hollow

```
#Germanene didoping boron posisi Hollow
 ndtset 6
#First dataset : SC run with kpoints in the IBZ
   iscf1  3
  nband1  32
  nstep1 25
 kptopt1 1
 nbdbuf1 0
 prtden1 1   getden1 0   getwfk1 0
#Second dataset : NSC run with large number of bands, and points
in the IBZ
    iscf2 -2
   nband2 32
   nstep2 25
  kptopt2  1
  getwfk2  1   getden2 1   ! Usual file handling data
#Third dataset : NSC run with large number of bands, and points
in the the full BZ
    iscf3 -2
   nband3 32
   nstep3 25
  kptopt3  3
  getwfk3  2   getden3 1
#Fourth dataset : ddk response function along axis 1
   iscf4 -3
  nband4 32
  nstep4  1  nline4  0  prtwf4  3
 kptopt4  3
   nqpt4  1  qpt4  0.0d0 0.0d0 0.0d0
  rfdir4  1 0 0
  rfelfd4  2
  getwfk4  3
 #Fifth dataset : ddk response function along axis 2
    iscf5 -3
   nband5 32
   nstep5  1  nline5  0   prtwf5  3
  kptopt5  3
    nqpt5  1  qpt5  0.0d0 0.0d0 0.0d0
   rfdir5  0 1 0
  rfelfd5  2
  getwfk5  3
 #Sixth dataset : ddk response function along axis 3
    iscf6 -3
   nband6 32
   nstep6  1  nline6  0    prtwf6  3
  kptopt6  3
    nqpt6  1  qpt6  0.0d0 0.0d0 0.0d0
   rfdir6  0 0 1
  rfelfd6  2
  getwfk6  3
 #Data common to all datasets
  nshiftk 1
  shiftk  0.0 0.0 0.0
  ngkpt 18 18 1
  acell   15.5 15.5  29.5
  amu 10.811 72.61
  diemac 12.0
  ecut 30.00
  iscf 3
  ixc 3
```

```
 nbdbuf 2
 ntypat  2
rprim
0.866 0.5 0
0.0 1.0 0.0
0.0 0.0 1.0
natom 9
typat 1 2 2 2 2 2 2 2 2 tolwfr  1.e-20
xred
3/6 3/6 0.34
1/6 1/6 0.15
2/6 2/6 0.15
4/6 1/6 0.15
5/6 2/6 0.15
1/6 4/6 0.15
2/6 5/6 0.15
4/6 4/6 0.15
5/6 5/6 0.15
tnons 72*0.0
znucl 5 32
optforces 1
chkprim 0
```

Lampiran 1. 4 Input file dari germanene didoping atom boron posisi Hollow

```
#Germanene didoping boron posisi Top
 ndtset 6
#First dataset : SC run with kpoints in the IBZ
   iscf1  3
  nband1  32
  nstep1 25
 kptopt1 1
 nbdbuf1 0
 prtden1 1   getden1 0   getwfk1 0
#Second dataset : NSC run with large number of bands, and points
in the IBZ
    iscf2 -2
   nband2 32
   nstep2 25
  kptopt2  1
  getwfk2  1   getden2 1
#Third dataset : NSC run with large number of bands, and points
in the the full BZ
    iscf3 -2
   nband3 32
   nstep3 25
  kptopt3  3
  getwfk3  2   getden3 1
#Fourth dataset : ddk response function along axis 1
   iscf4 -3
  nband4 32
  nstep4  1  nline4  0  prtwf4  3
 kptopt4  3
   nqpt4  1  qpt4  0.0d0 0.0d0 0.0d0
  rfdir4  1 0 0
```

```
  rfdir4   1 0 0
 rfelfd4   2
 getwfk4   3
#Fifth dataset : ddk response function along axis 2
   iscf5 -3
  nband5 32
  nstep5   1  nline5   0    prtwf5   3
 kptopt5   3
   nqpt5   1  qpt5   0.0d0 0.0d0 0.0d0
  rfdir5   0 1 0
 rfelfd5   2
 getwfk5   3
#Sixth dataset : ddk response function along axis 3
   iscf6 -3
  nband6 32
  nstep6   1  nline6   0    prtwf6   3
 kptopt6   3
   nqpt6   1  qpt6   0.0d0 0.0d0 0.0d0
  rfdir6   0 0 1
 rfelfd6   2
 getwfk6   3
#Data common to all datasets
 nshiftk 1
 shiftk   0.0 0.0 0.0
 ngkpt 18 18 1
 acell    15.5 15.5  29.5
 amu 10.811 72.61
 diemac 12.0
 ecut 30.00
 iscf 3
  ixc 3
  nbdbuf 2
  ntypat   2
 rprim
 0.866 0.5 0
 0.0 1.0 0.0
 0.0 0.0 1.0
 natom 9
 typat 1 2 2 2 2 2 2 2 2
 tolwfr   1.e-20
 xred
 2/6 2/6 0.34
 1/6 1/6 0.15
 2/6 2/6 0.15
 4/6 1/6 0.15
 5/6 2/6 0.15
 1/6 4/6 0.15
 2/6 5/6 0.15
 4/6 4/6 0.15
 5/6 5/6 0.15

  tnons 72*0.0
  znucl 5 32
 optforces 1
 chkprim 0
```

Lampiran 1. 5 Input file dari germanene didoping atom Nitrogen

```
#Germanene didoping Nitrogen posisi Bridge
 ndtset 6
#First dataset : SC run with kpoints in the IBZ
   iscf1  3
  nband1  32
  nstep1 25
 kptopt1 1
 nbdbuf1 0
 prtden1 1   getden1 0   getwfk1 0
#Second dataset : NSC run with large number of bands, and points
in the IBZ
    iscf2 -2
   nband2 32
   nstep2 25
  kptopt2  1
  getwfk2  1   getden2 1   ! Usual file handling data

#Third dataset : NSC run with large number of bands, and points
in the the full BZ
    iscf3 -2
   nband3 32
   nstep3 25
  kptopt3  3
  getwfk3  2   getden3 1   ! Usual file handling data
#Fourth dataset : ddk response function along axis 1
   iscf4 -3
  nband4 32
  nstep4  1  nline4  0  prtwf4  3
 kptopt4  3
   nqpt4  1  qpt4  0.0d0 0.0d0 0.0d0
  rfdir4  1 0 0
 rfelfd4  2
 getwfk4  3
#Fifth dataset : ddk response function along axis 2
   iscf5 -3
  nband5 32
  nstep5  1  nline5  0   prtwf5  3
 kptopt5  3
   nqpt5  1  qpt5  0.0d0 0.0d0 0.0d0
  rfdir5  0 1 0
 rfelfd5  2
 getwfk5  3
#Sixth dataset : ddk response function along axis 3
   iscf6 -3
  nband6 32
  nstep6  1  nline6  0    prtwf6  3
 kptopt6  3
   nqpt6  1  qpt6  0.0d0 0.0d0 0.0d0
  rfdir6  0 0 1
 rfelfd6  2
 getwfk6  3
#Data common to all datasets
 nshiftk 1
 shiftk  0.0 0.0 0.0
 ngkpt 18 18 1
 acell   15.5 15.5  29.5
 amu 14.00674 72.6
 diemac 12.0
 ecut 30.00
 iscf 3
```

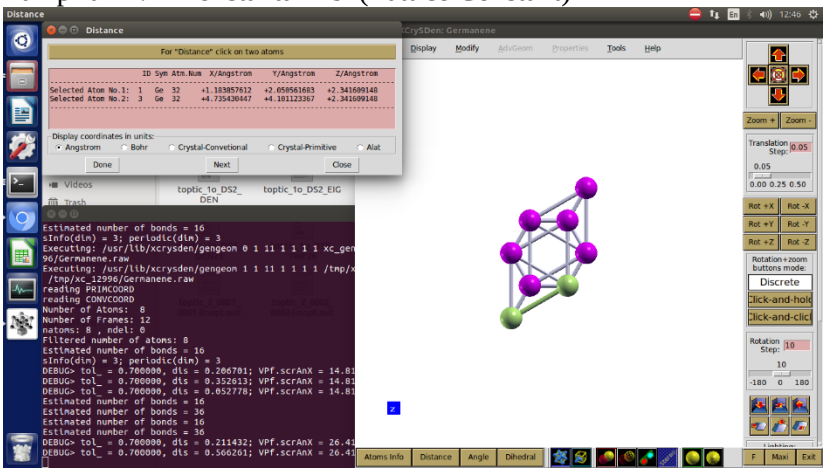
```
 ixc 3
 nbdbuf 2
 ntypat  2
rprim
0.866 0.5 0
0.0 1.0 0.0
0.0 0.0 1.0
natom 9
typat 1 2 2 2 2 2 2 2 2 tolwfr  1.e-20
xred
1.5/6 3/6 0.34
1/6 1/6 0.15
2/6 2/6 0.15
4/6 1/6 0.15
5/6 2/6 0.15
1/6 4/6 0.15
2/6 5/6 0.15
4/6 4/6 0.15
5/6 5/6 0.15

 tnons 72*0.0
 znucl 7 32
optforces 1
chkprim 0
```

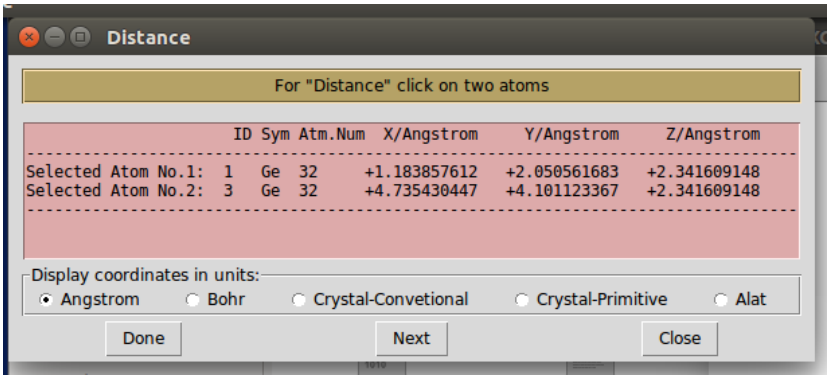
Lampiran 1. 6 Input file dari germanene didoping atom Boron dan Nitrogen

```
#Germanene didoping boron dan nitrogen
 ndtset 6
#First dataset : SC run with kpoints in the IBZ
   iscf1  3
  nband1  32
  nstep1 25
 kptopt1 1
 nbdbuf1 0
 prtden1 1   getden1 0   getwfk1 0
#Second dataset : NSC run with large number of bands, and points
in the IBZ
    iscf2 -2
   nband2 32
   nstep2 25
  kptopt2  1
  getwfk2  1   getden2 1
#Third dataset : NSC run with large number of bands, and points
in the the full BZ
    iscf3 -2
   nband3 32
   nstep3 25
  kptopt3  3
  getwfk3  2   getden3 1   ! Usual file handling data
#Fourth dataset : ddk response function along axis 1
   iscf4 -3
  nband4 32
  nstep4  1  nline4  0  prtwf4  3
 kptopt4  3
   nqpt4  1  qpt4  0.0d0 0.0d0 0.0d0
  rfdir4  1 0 0
```

```
 rfelfd4  2
 getwfk4  3
#Fifth dataset : ddk response function along axis 2
   iscf5 -3
  nband5 32
  nstep5  1  nline5  0   prtwf5  3
 kptopt5  3
   nqpt5  1  qpt5  0.0d0 0.0d0 0.0d0
  rfdir5  0 1 0
 rfelfd5  2
 getwfk5  3
#Sixth dataset : ddk response function along axis 3
   iscf6 -3
  nband6 32
  nstep6  1  nline6  0    prtwf6  3
 kptopt6  3
   nqpt6  1  qpt6  0.0d0 0.0d0 0.0d0
  rfdir6  0 0 1
 rfelfd6  2
 getwfk6  3
#Data common to all datasets
 nshiftk 1
 shiftk  0.0 0.0 0.0
 ngkpt 18 18 1
 acell   15.5 15.5  29.5
 amu 10.811 14.00674 72.61
 diemac 12.0
 ecut 30.00
 iscf 3
 ixc 3
  ixc 3
  nbdbuf 2
  ntypat  3

 rprim
 0.866 0.5 0
 0.0 1.0 0.0
 0.0 0.0 1.0

 natom 10
 typat 1 2 3 3 3 3 3 3 3 3 tolwfr  1.e-20
 xred
 1.5/6 3/6 0.34
 1.5/6 3/6 0
 1/6 1/6 0.15
 2/6 2/6 0.15
 4/6 1/6 0.15
 5/6 2/6 0.15
 1/6 4/6 0.15
 2/6 5/6 0.15
 4/6 4/6 0.15
 5/6 5/6 0.15


  tnons 72*0.0
  znucl 5 7 32
 optforces 1
 chkprim 0
```

Lampiran 1. 7 Konstanta Kisi (Lattice Constant)




Persamaan Garis.

*Lattice Constant* $= \sqrt{\Delta x^2 + \Delta y^2}$

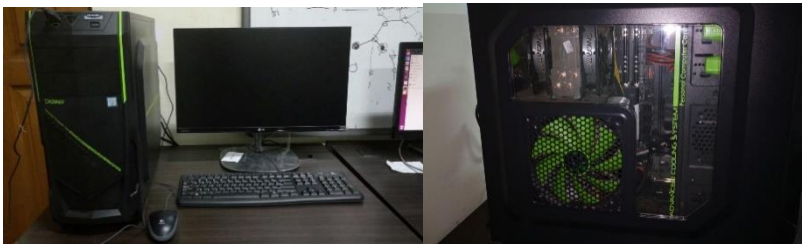
$= \sqrt{(4.74 - 1.18)^2 + (4.10 - 2.05)^2}$

$= \sqrt{12.67 + 4.20}$

$= \sqrt{16.87}$

$= 4.10$

Lampiran 1. 8 Peraltan untuk penelitian



Seperangkat Komputer.

Dengan Spesifikasi:

| | |
|---|---|
| Computer Name | : SIMULASI |
| Processor | : Intel Core i7-5960X |
| Display | : NVIDIA GeForce GTX 960 |
| Ram | : 16GB |
| Monitor | : LG IPS LED |
| Keyboard | : Logitech K120 |
| Mouse | : Logitech |