

LAMPIRAN

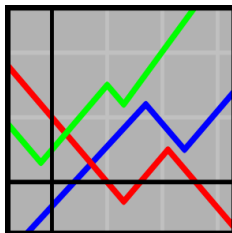
Lampiran 1. 1 Software



Abinit



Xcrysden



Gnuplot

Lampiran 1. 2 Input file dari germanene didoping atom boron posisi 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  prt_wf4 3
  kptopt4 3
  nqpt4 1  qpt4 0.0d0 0.0d0 0.0d0
  rfdir4 1 0 0

  rfelld4 2
  getwfk4 3
#Fifth dataset : ddk response function along axis 2
  iscf5 -3
  nband5 32
  nstep5 1  nline5 0  prt_wf5 3
  kptopt5 3
  nqpt5 1  qpt5 0.0d0 0.0d0 0.0d0
  rfdir5 0 1 0
  rfelld5 2
  getwfk5 3
#Sixth dataset : ddk response function along axis 3
  iscf6 -3
  nband6 32
  nstep6 1  nline6 0  prt_wf6 3
  kptopt6 3
  nqpt6 1  qpt6 0.0d0 0.0d0 0.0d0
  rfdir6 0 0 1
  rfelld6 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

```

```

    rfdird4 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
    rfdird5 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
    rfdird6 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
  prtdden1 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  prt_wf4 3
  kptopt4 3
  ngpt4 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  prt_wf5 3
  kptopt5 3
  ngpt5 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  prt_wf6 3
  kptopt6 3
  ngpt6 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
.
```



```

rfelfd4 2
getwfk4 3
#Fifth dataset : ddk response function along axis 2
  iscf5 -3
  nband5 32
  nstep5 1 nline5 0 prt_wf5 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 prt_wf6 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
nshifk 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)

The screenshot shows the CrystalDien software interface. A 'Distance' dialog box is open, displaying the following table:

ID	Sym	Atm.Num	X/Angstrom	Y/Angstrom	Z/Angstrom
Selected Atom No.1:	1	Ge 32	+1.183857612	+2.050561683	+2.341609148
Selected Atom No.2:	3	Ge 32	+4.735430447	+4.101123367	+2.341609148

Below the table, the 'Display coordinates in units:' section has radio buttons for 'Angstrom' (selected), 'Bohr', 'Crystal-Conventional', 'Crystal-Primitive', and 'Alat'. The 'Next' button is visible.

The background shows a 3D ball-and-stick model of a germanene lattice structure with purple and green spheres representing atoms.

This is a close-up of the 'Distance' dialog box. It contains the following table:

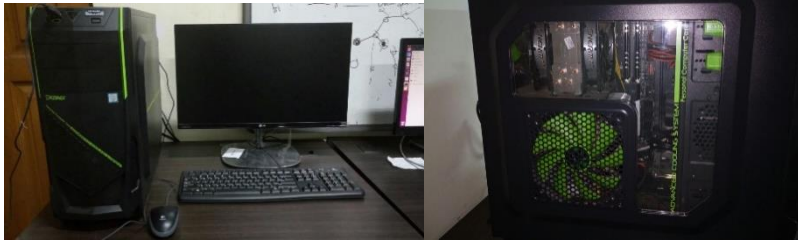
ID	Sym	Atm.Num	X/Angstrom	Y/Angstrom	Z/Angstrom
Selected Atom No.1:	1	Ge 32	+1.183857612	+2.050561683	+2.341609148
Selected Atom No.2:	3	Ge 32	+4.735430447	+4.101123367	+2.341609148

The 'Display coordinates in units:' section has radio buttons for 'Angstrom' (selected), 'Bohr', 'Crystal-Conventional', 'Crystal-Primitive', and 'Alat'. The 'Done', 'Next', and 'Close' buttons are visible at the bottom.

Persamaan Garis.

$$\begin{aligned}
 \text{Lattice Constant} &= \sqrt{\Delta x^2 + \Delta y^2} \\
 &= \sqrt{(4.74 - 1.18)^2 + (4.10 - 2.05)^2} \\
 &= \sqrt{12.67 + 4.20} \\
 &= \sqrt{16.87} \\
 &= 4.10
 \end{aligned}$$

Lampiran 1. 8 Peralatan 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