

LAMPIRAN

Lampiran 1 Silicene didoping dengan Galium posisi *bridge*

#Prepare the computation of linear and non-linear optic properties
#of GaAs crystal : ground-state with few bands,
#then non-SCF with a larger number of bands, then ddk for different directions
#Note that the k point sampling should be finer for significant results. The cut-off energy is also too low.

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 !Usual file handling data
```

#Second dataset : NSC run with large number of bands, and points in the IBZ

```
iscf2 -2
nband2 32 ! This number of bands might be too low for non-linear optics and real part of linear
optics
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 ! This number of bands might be too low for non-linear optics and real part of linear
optics
nstep3 25
kptopt3 3
getwfk3 2 getden3 1 !Usual file handling data
```

#Fourth dataset : ddk response function along axis 1

```
iscf4 -3
nband4 32 ! This number of bands might be too low for non-linear optics and real part of linear
optics
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 ! This number of bands might be too low for non-linear optics and real part of linear optics

nstep5 1 nline5 0 prtwh5 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 ! This number of bands might be too low for non-linear optics and real part of linear optics

nstep6 1 nline6 0 prtwh6 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

#Chksymbreak 1

nshifk 1

shifk 0.0 0.0 0.0 0.0

ngkpt 20 20 1 ! This is much too low : should be at least 24x24x24

acell 7.778905 7.778905 15.0 Angstrom

amu 28.0855 69.72

diemac 12.0

ecut 30.00 ! This is also too low

iscf 3

ixc 11

natom 9 nbdbuf 2

ntypat 2

rprim

0.866 0.5 0

0.0 1.0 0.0

0.0 0.0 1.0

xred

1.5/6 3/6 0.1777

1/6 1/6 0

2/6 2/6 0

4/6 1/6 0

5/6 2/6 0

1/6 4/6 0

2/6 5/6 0

4/6 4/6 0

5/6 5/6 0

#tnons 72*0.0

typat 2 1 1 1 1 1 1 1 1 1 tolwfr 1.e-20

```
znucl 14 31
# add to conserve old < 6.7.2 behavior for calculating forces at each SCF step
  optforces 1
  chkprim 0
  occopt 1

###<BEGIN TEST_INFO>
### [setup]
### executable = abinit
### test_chain = toptic_1.in, toptic_2.in
### [files]
### files_to_test =
### toptic_1.out, tolnlines= 0, tolabs= 0.000e+00, tolrel= 0.000e+00, fld_options = -easy
### psp_files = 31ga.pspnc, 33as.pspnc
### [paral_info]
### max_nprocs = 2
### [extra_info]
### authors =
### keywords = NC, DFPT
### description =
###<END TEST_INFO>
```