#!/bin/sh

PSEUDO\_DIR=”…../”

TMP\_DIR=`pwd`

for ecut in 20 30 40 50 60 ; do

# self-consistent calculation

cat > si.scf.$ecut.in << EOF

&control

calculation = 'scf'

restart\_mode='from\_scratch',

prefix='silicon.$ecut’,

tstress = .true.

tprnfor = .true.

pseudo\_dir = '$PSEUDO\_DIR/',

outdir='$TMP\_DIR/tmp/'

/ &system

ibrav= 2, celldm(1) =10.20, nat= 2, ntyp= 1,

ecutwfc =$ecut,

/

&electrons

diagonalization='$diago'

mixing\_mode = 'plain'

mixing\_beta = 0.7

conv\_thr = 1.0d-8

/

ATOMIC\_SPECIES

Si 28.086 Si.pz-vbc.UPF

ATOMIC\_POSITIONS

Si 0.00 0.00 0.00

Si 0.25 0.25 0.25

K\_POINTS

10

0.1250000 0.1250000 0.1250000 1.00

0.1250000 0.1250000 0.3750000 3.00

0.1250000 0.1250000 0.6250000 3.00

0.1250000 0.1250000 0.8750000 3.00

0.1250000 0.3750000 0.3750000 3.00

0.1250000 0.3750000 0.6250000 6.00

0.1250000 0.3750000 0.8750000 6.00

0.1250000 0.6250000 0.6250000 3.00

0.3750000 0.3750000 0.3750000 1.00

0.3750000 0.3750000 0.6250000 3.00

EOF

………/bin/pw.x < si.scf.$ecut.in > si.scf.$ecut.out

done