Convergence w.r.t energy cutoff

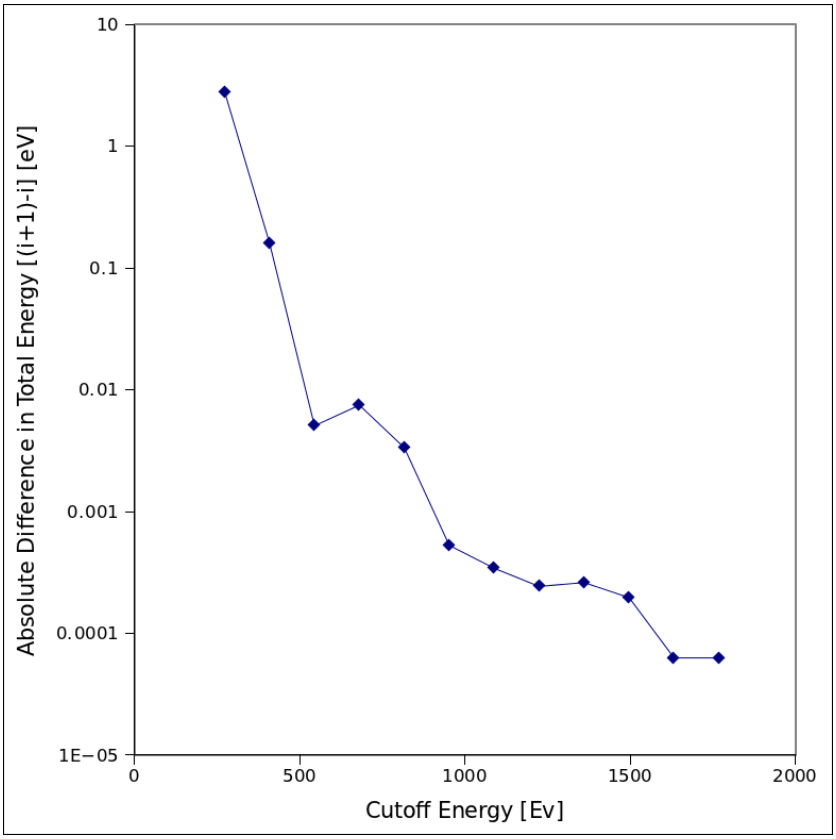

Figure 1: Convergence of Total Energy as a function of energy cutoff

Energy Cutoff [Ry]	Time [CPU s]
20	0.82
30	0.93
40	1.04
50	1.13
60	1.21
70	1.89
80	2.06
90	2.24
100	2.34
110	2.54
120	2.91
130	3.08
140	3.24

Convergence w.r.t k-grid cutoff

K-point grid (nxnxn)	Number of Unique K-points
1	1
2	3
4	8
6	16
8	29
10	47
12	72

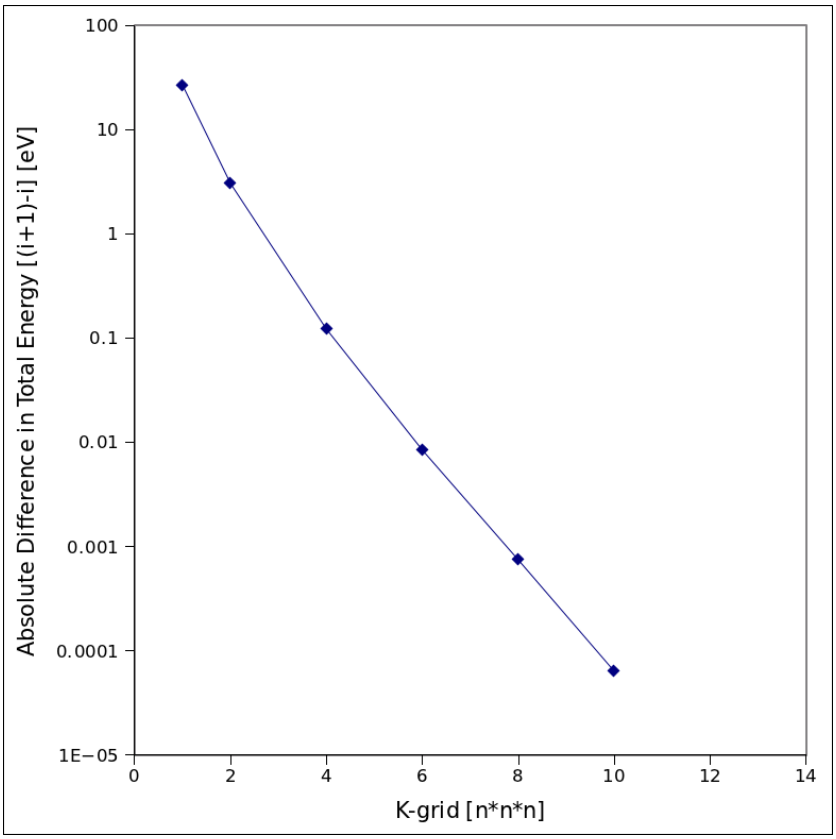

Figure 2: Convergence of Total Energy as a function of k-grid

Convergence of forces w.r.t energy cutoff

Lattice Parameter	6.74 [Bohr]
Pseudopotential	C.pz-kjpaw.UPF
K-grid	4 x 4 x 4 Monkhorst-Pack
Unique K-points	18

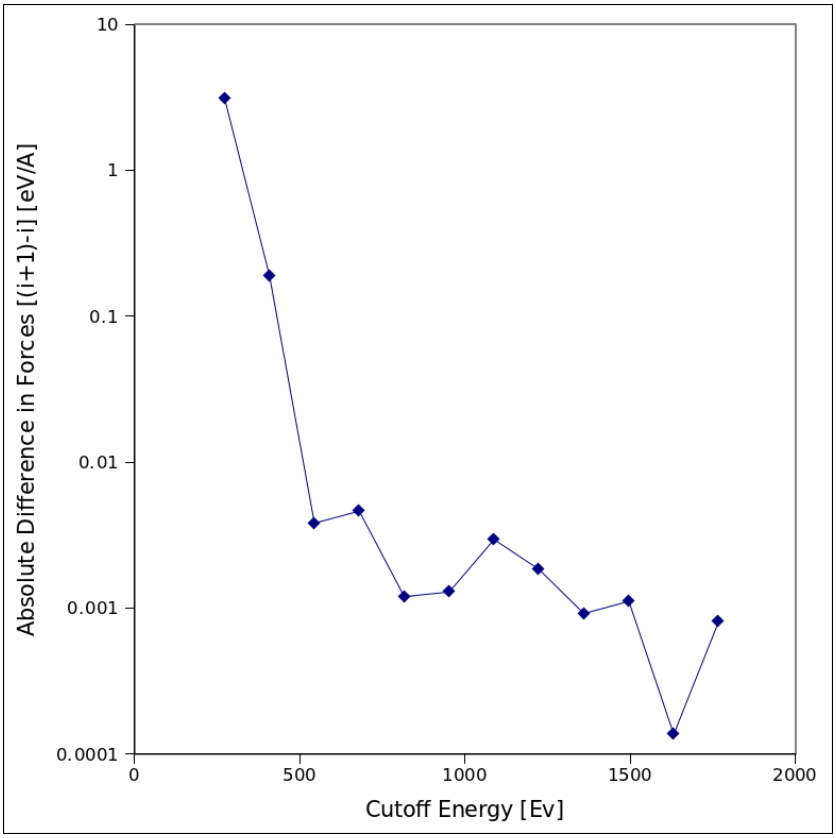

Figure 3: Convergence of Forces as a function of cutoff energy

Equilibrium Lattice Constant

Cutoff	140 [Ry]
K-grid	8 x 8 x 8 Monkhorst-Pack
Unique K-points	95

Pseudopotential	Total Energy [Ry]	Calculated Bulk Modulus [Pa]
C.pz-rrkjus.UPF	-22.8168	3.28E11
C.pz-kjpaw.UPF	-35.5863	No fit

The calculated bulk modulus is on the same order of magnitude as experimental results of 4.42E11 [Pa].

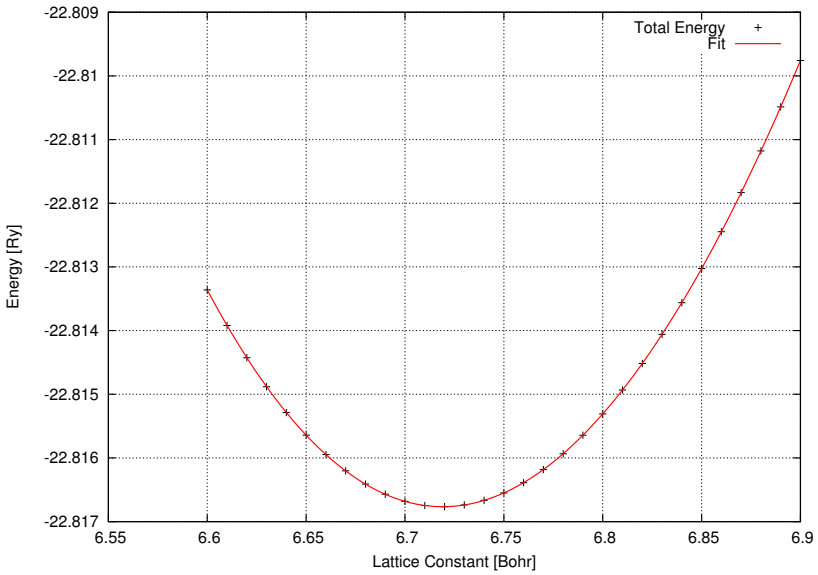

Figure 4: Total energy as a function of lattice constant

Script

```
#!/bin/sh
###############################################################################
LISTECUT='20 30 40 50 60 70 80 90 100 110 120 130 140'

LISTKGRID='1 2 4 6 8 10 12'

LISTALAT='6.60 6.61 6.62 6.63 6.64 6.65 6.66 6.67 6.68
6.69 6.70 6.71 6.72 6.73 6.74 6.75 6.76 6.77 6.78 6.79
6.80 6.81 6.82 6.83 6.84 6.85 6.86 6.87 6.88 6.89 6.90'

PSEUDO_DIR="/home/sam/Documents/espresso-4.3.2/pseudo/"
SCRATCH="/home/sam/Documents/espresso-4.3.2/diac/scratch"
OUTPUT="/home/sam/Documents/espresso-4.3.2/diac"
EXEPATH="/home/sam/Documents/espresso-4.3.2/bin"

if [ ! -d $SCRATCH ]; then
mkdir $SCRATCH
fi

if [ ! -d $PSEUDO_DIR ]; then
mkdir $PSEUDO_DIR
fi

if [ ! -d $OUTPUT ]; then
echo $MYDIR does not exist, please create it first
exit
 fi
```

```
#for ecut in $LISTECUT
#  do
#for kgrid in $LISTKGRID
#  do
for alat in $LISTALAT
  do
#rm -f $OUTPUT/diac.scf.$kgrid.in
#cat > $OUTPUT/diac.scf.$kgrid.in << EOF
#rm -f $OUTPUT/diac.scf.$ecut.in
#cat > $OUTPUT/diac.scf.$ecut.in << EOF
rm -f $OUTPUT/diac.scf.$alat.in
cat > $OUTPUT/diac.scf.$alat.in << EOF



  &control
    prefix='diamond',
    calculation='scf',
    outdir = '$SCRATCH'
    pseudo_dir = '$PSEUDO_DIR'
    tprnfor=.true.
 /
 &system
    ibrav=  2,
    !celldm(1) =6.74,
    celldm(1) =$alat,
    nat=  2, ntyp= 1,
    !ecutwfc = $ecut,
    ecutwfc = 140,
 /
 &electrons
 /
ATOMIC_SPECIES
C  12.0107  C.pz-kjpaw.UPF
ATOMIC_POSITIONS
 C 0.00 0.00 0.05
 C 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
EOF

#$EXEPATH/pw.x < $OUTPUT/diac.scf.$ecut.in >  $OUTPUT/diac.scf.$ecut.out
#$EXEPATH/pw.x < $OUTPUT/diac.scf.$kgrid.in >  $OUTPUT/diac.scf.$kgrid.out
$EXEPATH/pw.x < $OUTPUT/diac.scf.$alat.in >  $OUTPUT/diac.scf.$alat.out
done
```