Propriedades Quânticas de Nanomateriais utilizando a Teoria do Funcional Densidade (DFT)

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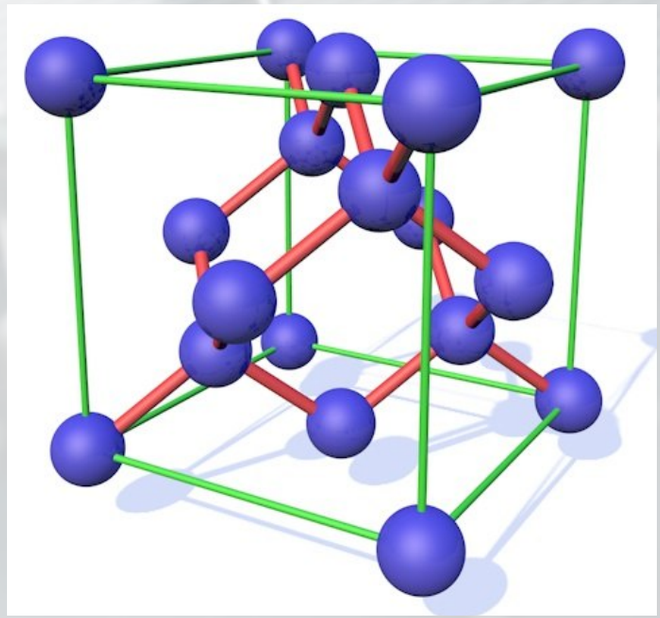
Practical Part

Silicon

- Bulk SCF (initial convergency tests)
- Total and projected density of states
- Bulk band structure
- FCC lattice parameter (convergency tests)
- FCC bulk modulus
- FCC lattice parameter - VC-relax

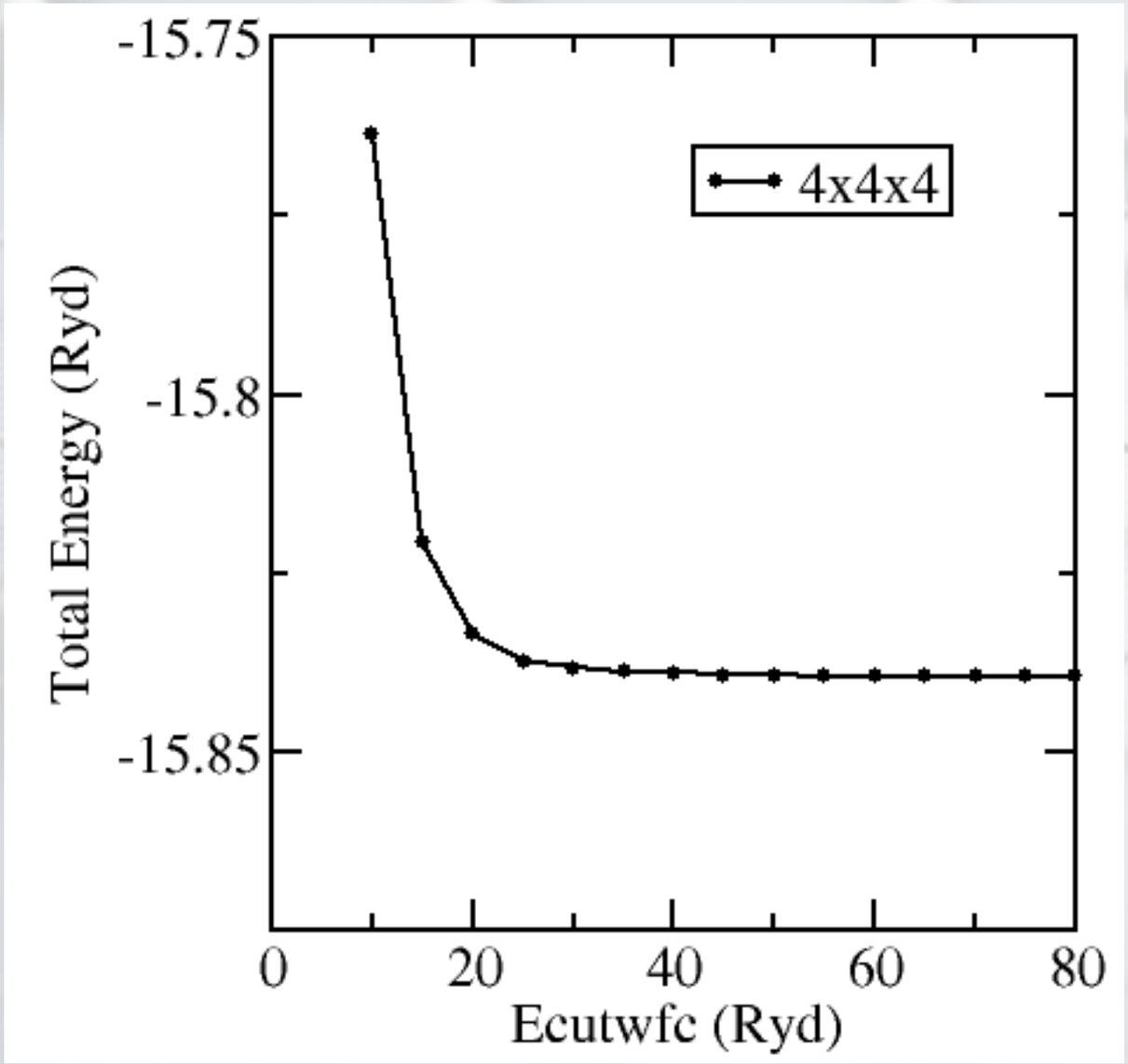


Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

Convergency Tests

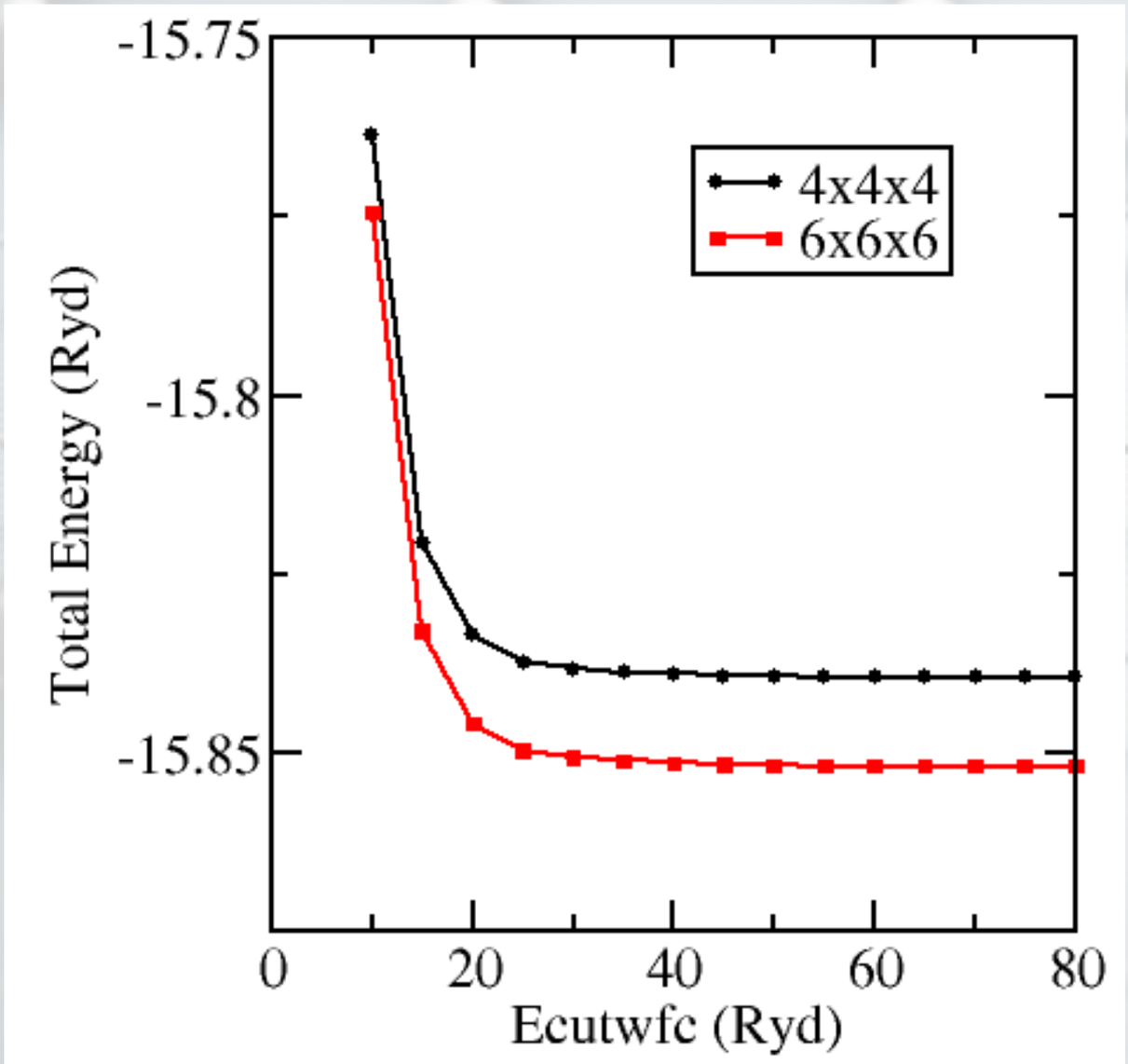
Wave function expansion cutoff energy - ecutwfc




```
for ecutwfc in `seq 10 5 80`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/
&system
    ibrav=  2,
    celldm(1) =10.20,
    nat=  2,
    ntyp= 1,
    ecutwfc =$ecutwfc,
/
```

Convergency Tests

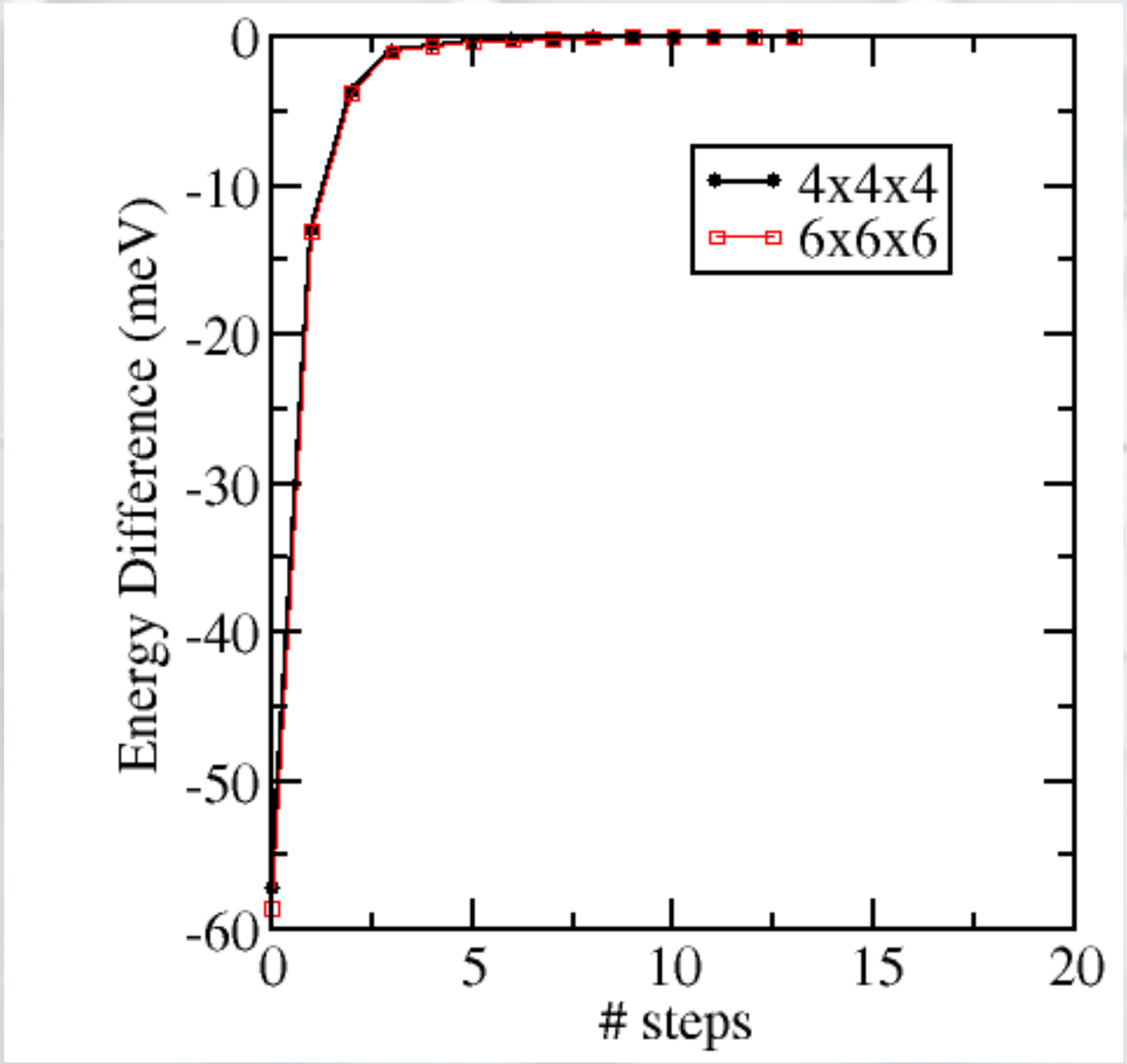
Wave function expansion cutoff energy - ecutwfc




```
for ecutwfc in `seq 10 5 80`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/
&system
    ibrav=  2,
    celldm(1) =10.20,
    nat=  2,
    ntyp= 1,
    ecutwfc =$ecutwfc,
/
```

Convergency Tests

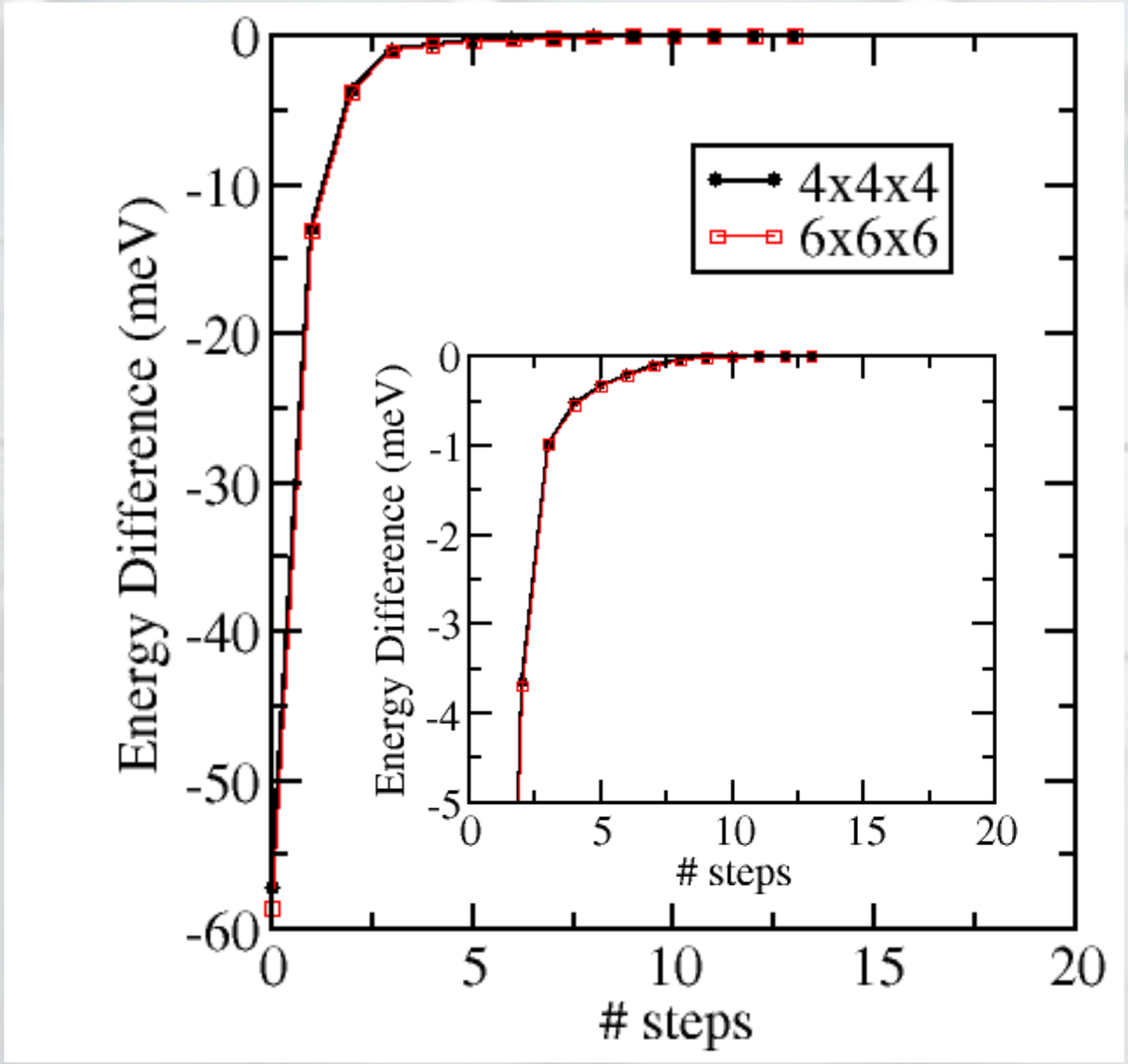
Wave function expansion cutoff energy - ecutwfc




```
for ecutwfc in `seq 10 5 80`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/
&system
    ibrav=  2,
    celldm(1) =10.20,
    nat=  2,
    ntyp= 1,
    ecutwfc =$ecutwfc,
/
```

Convergency Tests

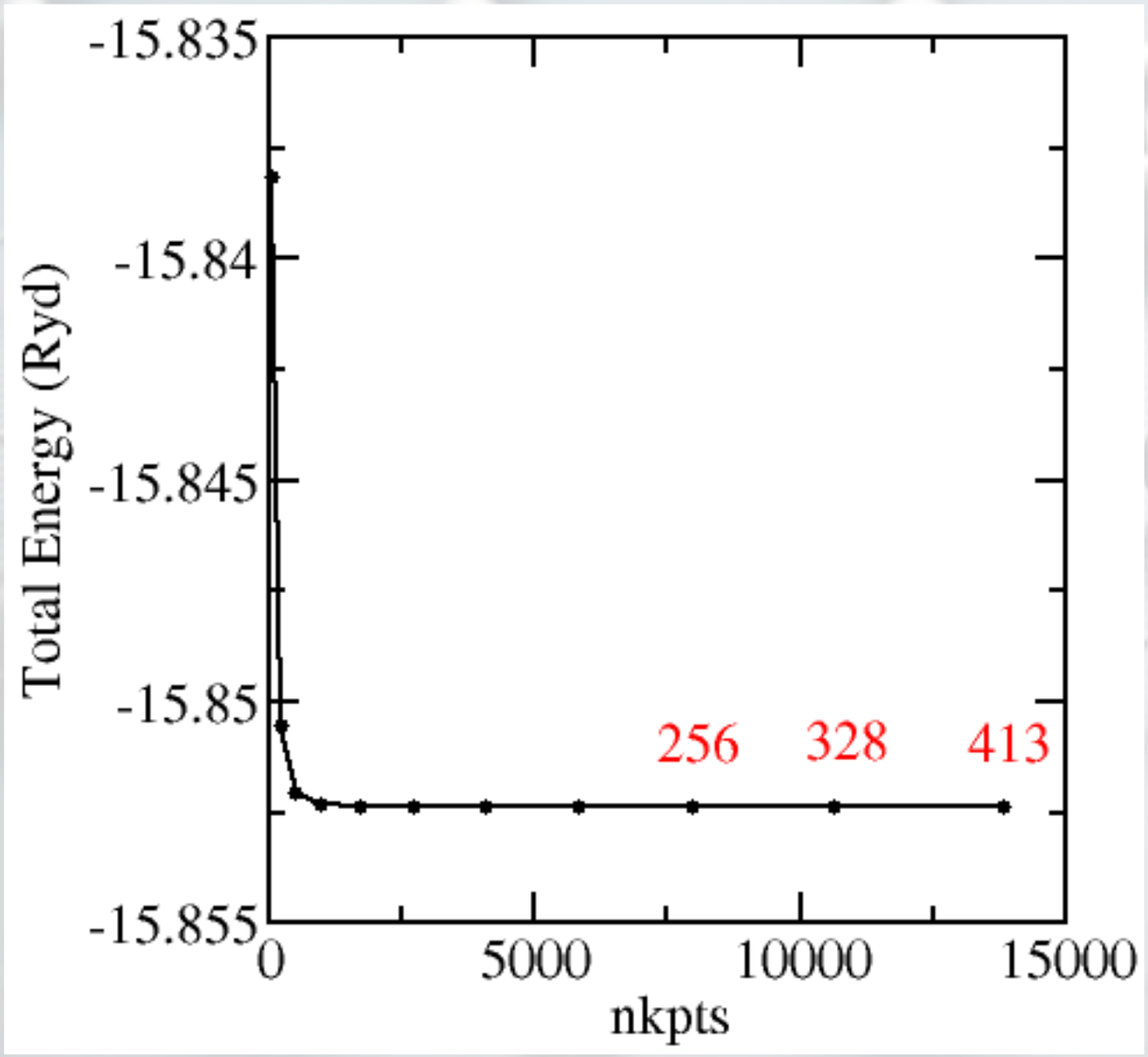
Wave function expansion cutoff energy - ecutwfc




```
for ecutwfc in `seq 10 5 80`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/
&system
    ibrav=  2,
    celldm(1) =10.20,
    nat=  2,
    ntyp= 1,
    ecutwfc =$ecutwfc,
/
```

Convergency Tests

Reciprocal space sampling - K_POINTS




```
for nkpts in `seq 4 2 24`; do

cat > si.scf.$nkpts.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/
                              .
                              .
                              .
K_POINTS automatic
 $nkpts $nkpts $nkpts 0 0 0
EOF
```

Convergency Tests

Reciprocal space sampling - K_POINTS

```
     atomic species   valence    mass     pseudopotential
        Si             4.00    28.08600     Si( 1.00)

     48 Sym. Ops., with inversion, found (24 have fractional translation)


                                s                          frac. trans.

      isym =  1     identity

cryst.   s( 1) = (     1          0          0      )
                 (     0          1          0      )
                 (     0          0          1      )

cart.    s( 1) = (  1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


      isym =  2     180 deg rotation - cart. axis [0,0,1]

cryst.   s( 2) = (     0          1         -1      )
                 (     1          0         -1      )
                 (     0          0         -1      )

cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000 -1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


      isym =  3     180 deg rotation - cart. axis [0,1,0]

cryst.   s( 3) = (    -1          0          0      )
                 (    -1          0          1      )
                 (    -1          1          0      )

cart.    s( 3) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000 -1.0000000 )
```

Convergency Tests

Reciprocal space sampling - K_POINTS

```
     atomic species   valence    mass     pseudopotential
        Si             4.00    28.08600     Si( 1.00)

     48 Sym. Ops., with inversion, found (24 have fractional translation)


                                s                          frac. trans.

      isym =  1     identity

cryst.   s( 1) = (     1          0          0      )
                 (     0          1          0      )
                 (     0          0          1      )

cart.    s( 1) = (  1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


      isym =  2     180 deg rotation - cart. axis [0,0,1]

cryst.   s( 2) = (     0          1         -1      )
                 (     1          0         -1      )
                 (     0          0         -1      )

cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000 -1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


      isym =  3     180 deg rotation - cart. axis [0,1,0]

cryst.   s( 3) = (    -1          0          0      )
                 (    -1          0          1      )
                 (    -1          1          0      )

cart.    s( 3) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000 -1.0000000 )
```

```
for nkpts in `seq 4 2 24`; do

cat > si.scf.$nkpts.in <<EOF
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '$pseudo_dir',
   outdir='./'
/

.
.
.

K_POINTS automatic
 $nkpts $nkpts $nkpts 0 0 0
EOF
```

Convergency Tests

Reciprocal space sampling - K_POINTS

```
Cartesian axes

  site n.     atom                  positions (alat units)
      1           Si  tau(   1) = (   0.0000000   0.0000000   0.0000000  )
      2           Si  tau(   2) = (   0.2500000   0.2500000   0.2500000  )

Crystallographic axes

  site n.     atom                  positions (cryst. coord.)
      1           Si  tau(   1) = (  0.0000000  0.0000000  0.0000000  )
      2           Si  tau(   2) = ( -0.2500000  0.7500000 -0.2500000  )

  number of k points=     8
                    cart. coord. in units 2pi/alat
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
     k(    2) = (  -0.2500000   0.2500000  -0.2500000), wk =   0.2500000
     k(    3) = (   0.5000000  -0.5000000   0.5000000), wk =   0.1250000
     k(    4) = (   0.0000000   0.5000000   0.0000000), wk =   0.1875000
     k(    5) = (   0.7500000  -0.2500000   0.7500000), wk =   0.7500000
     k(    6) = (   0.5000000   0.0000000   0.5000000), wk =   0.3750000
     k(    7) = (   0.0000000  -1.0000000   0.0000000), wk =   0.0937500
     k(    8) = (  -0.5000000  -1.0000000   0.0000000), wk =   0.1875000

                    cryst. coord.
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
     k(    2) = (   0.0000000   0.0000000   0.2500000), wk =   0.2500000
     k(    3) = (   0.0000000   0.0000000  -0.5000000), wk =   0.1250000
     k(    4) = (   0.0000000   0.2500000   0.2500000), wk =   0.1875000
     k(    5) = (   0.0000000   0.2500000  -0.5000000), wk =   0.7500000
     k(    6) = (   0.0000000   0.2500000  -0.2500000), wk =   0.3750000
     k(    7) = (   0.0000000  -0.5000000  -0.5000000), wk =   0.0937500
     k(    8) = (   0.2500000  -0.5000000  -0.2500000), wk =   0.1875000
```

Convergency Tests

Reciprocal space sampling - K_POINTS

```
Cartesian axes

  site n.     atom                  positions (alat units)
      1           Si  tau(   1) = (   0.0000000   0.0000000   0.0000000  )
      2           Si  tau(   2) = (   0.2500000   0.2500000   0.2500000  )

Crystallographic axes

  site n.     atom                  positions (cryst. coord.)
      1           Si  tau(   1) = (  0.0000000  0.0000000  0.0000000  )
      2           Si  tau(   2) = ( -0.2500000  0.7500000 -0.2500000  )

 number of k points=     8
                  cart. coord. in units 2pi/alat
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
     k(    2) = (  -0.2500000   0.2500000  -0.2500000), wk =   0.2500000
     k(    3) = (   0.5000000  -0.5000000   0.5000000), wk =   0.1250000
     k(    4) = (   0.0000000   0.5000000   0.0000000), wk =   0.1875000
     k(    5) = (   0.7500000  -0.2500000   0.7500000), wk =   0.7500000
     k(    6) = (   0.5000000   0.0000000   0.5000000), wk =   0.3750000
     k(    7) = (   0.0000000  -1.0000000   0.0000000), wk =   0.0937500
     k(    8) = (  -0.5000000  -1.0000000   0.0000000), wk =   0.1875000

                  cryst. coord.
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
     k(    2) = (   0.0000000   0.0000000   0.2500000), wk =   0.2500000
     k(    3) = (   0.0000000   0.0000000  -0.5000000), wk =   0.1250000
     k(    4) = (   0.0000000   0.2500000   0.2500000), wk =   0.1875000
     k(    5) = (   0.0000000   0.2500000  -0.5000000), wk =   0.7500000
     k(    6) = (   0.0000000   0.2500000  -0.2500000), wk =   0.3750000
     k(    7) = (   0.0000000  -0.5000000  -0.5000000), wk =   0.0937500
     k(    8) = (   0.2500000  -0.5000000  -0.2500000), wk =   0.1875000
```

Convergency Tests

Reciprocal space sampling - K_POINTS

noinv	LOGICAL
Default:	.FALSE.

if (.TRUE.) disable the usage of k => -k symmetry
(time reversal) in k-point generation

Convergency Tests

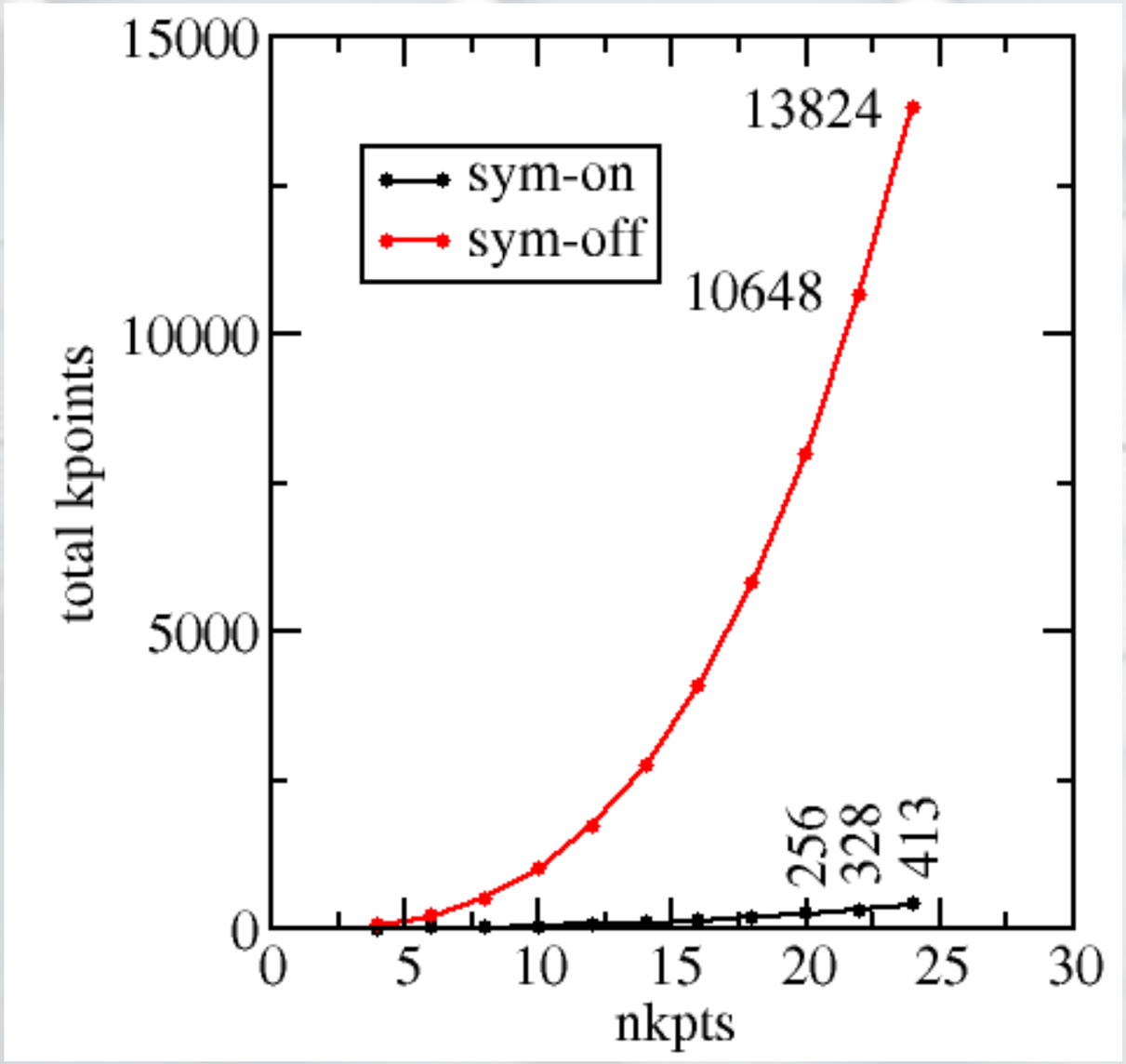
Reciprocal space sampling - K_POINTS

nosym	LOGICAL
Default:	.FALSE.

```
if (.TRUE.) symmetry is not used. Consequences:

- if a list of k points is provided in input, it is used
  "as is": symmetry-inequivalent k-points are not generated,
  and the charge density is not symmetrized;

- if a uniform (Monkhorst-Pack) k-point grid is provided in
  input, it is expanded to cover the entire Brillouin Zone,
  irrespective of the crystal symmetry.
  Time reversal symmetry is assumed so k and -k are considered
  as equivalent unless noinv=.true. is specified.

Do not use this option unless you know exactly what you want
and what you get. May be useful in the following cases:
- in low-symmetry large cells, if you cannot afford a k-point
  grid with the correct symmetry
- in MD simulations
- in calculations for isolated atoms
```

Convergency Tests

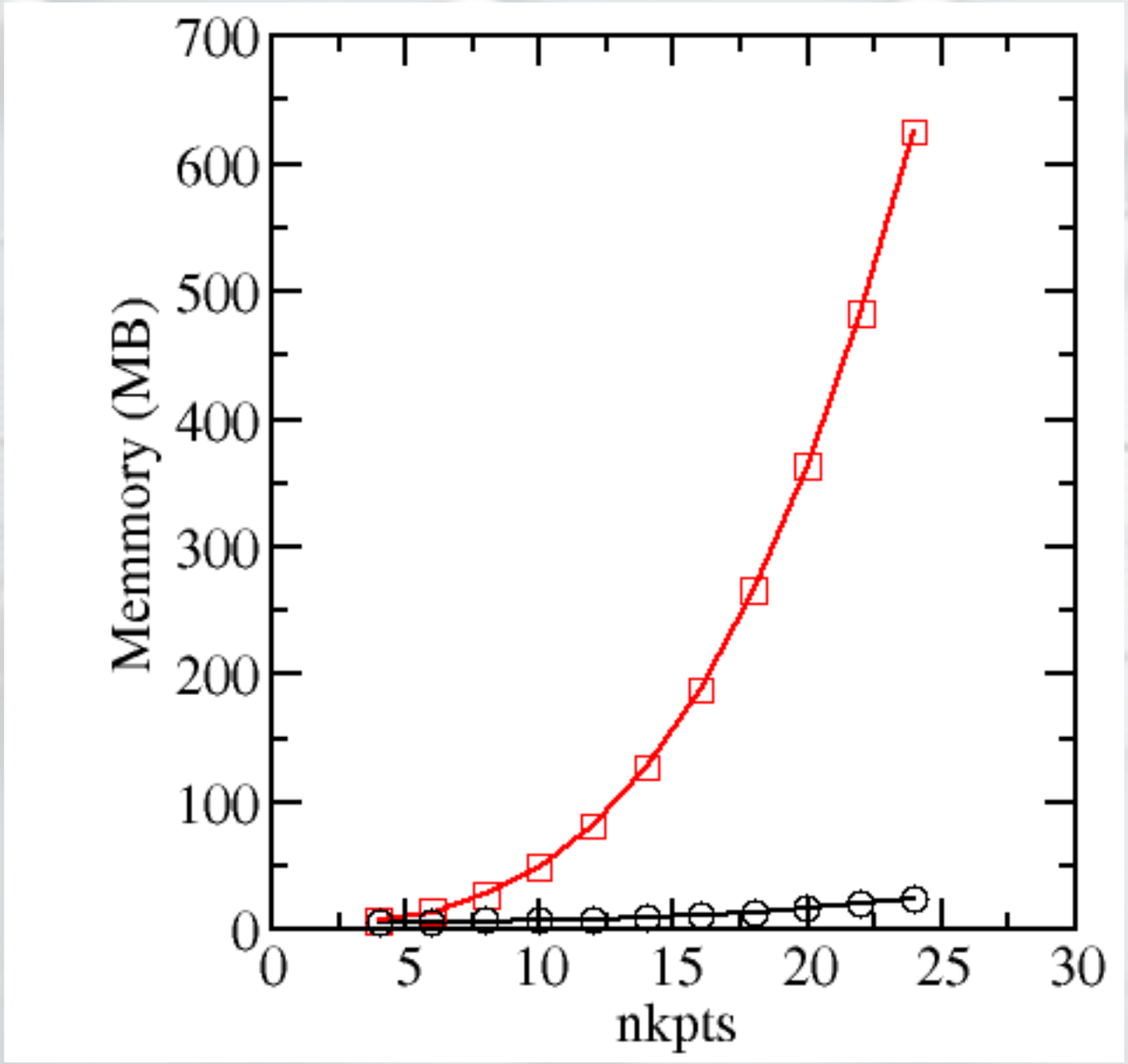
Reciprocal space sampling - K_POINTS




```
for nkpts in `seq 4 2 24`; do

cat > si.scf.$nkpts.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/

.
.
.

K_POINTS automatic
 $nkpts $nkpts $nkpts 0 0 0
EOF
```

Convergency Tests

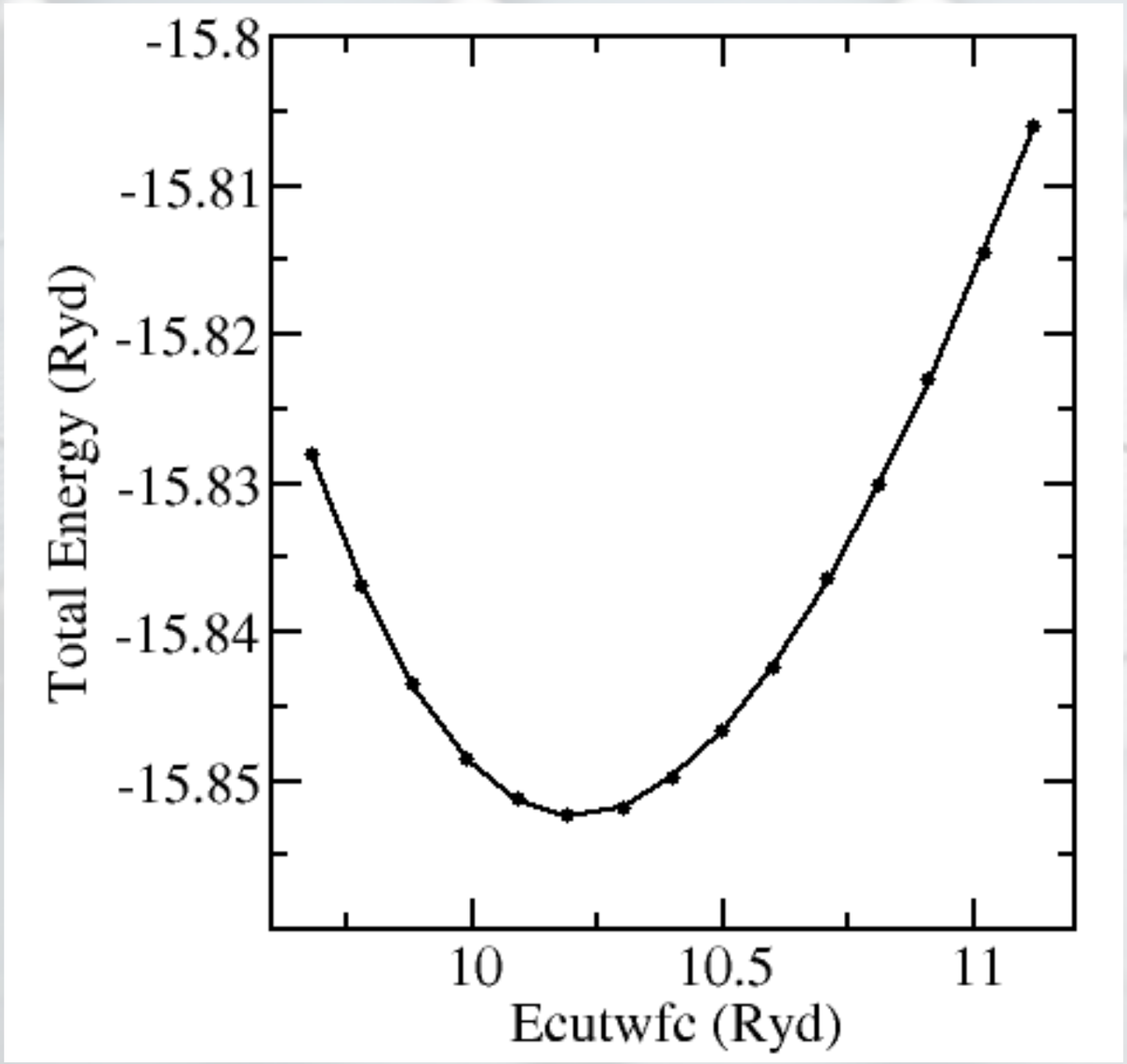
Reciprocal space sampling - K_POINTS



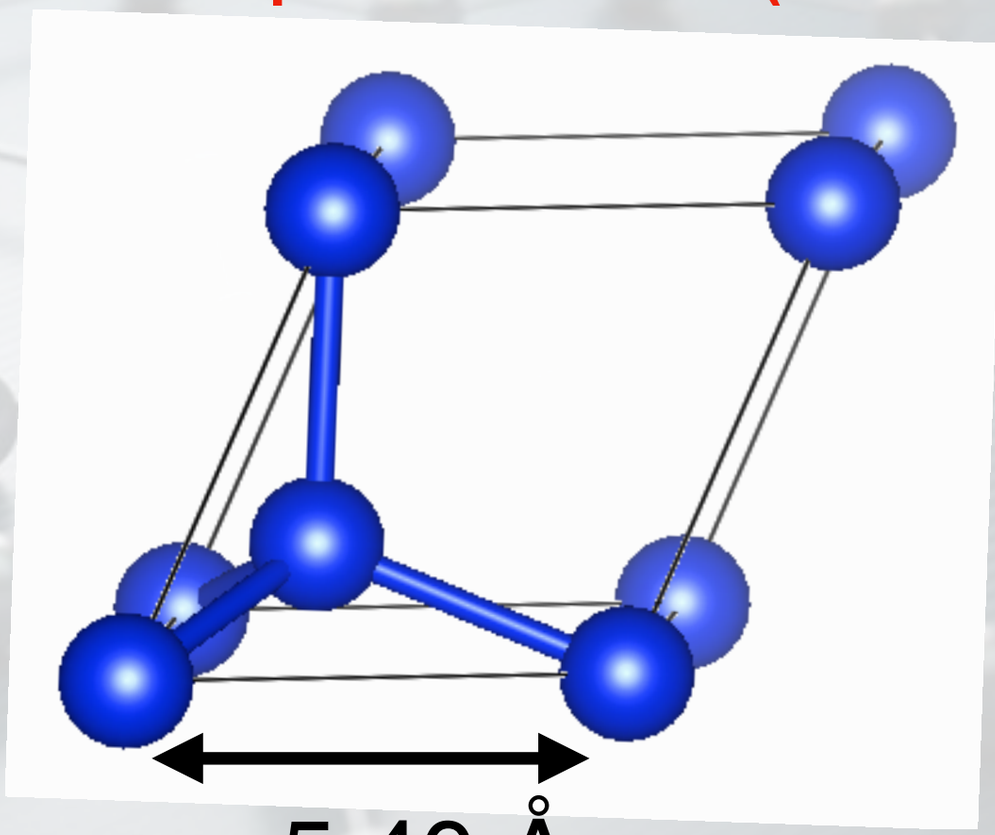

```
for nkpts in `seq 4 2 24`; do

cat > si.scf.$nkpts.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '$pseudo_dir',
    outdir='./'
/

.
.
.

K_POINTS automatic
 $nkpts $nkpts $nkpts 0 0 0
EOF
```

Lattice Parameter

Lattice Parameter -PZ-VBC(LDA)



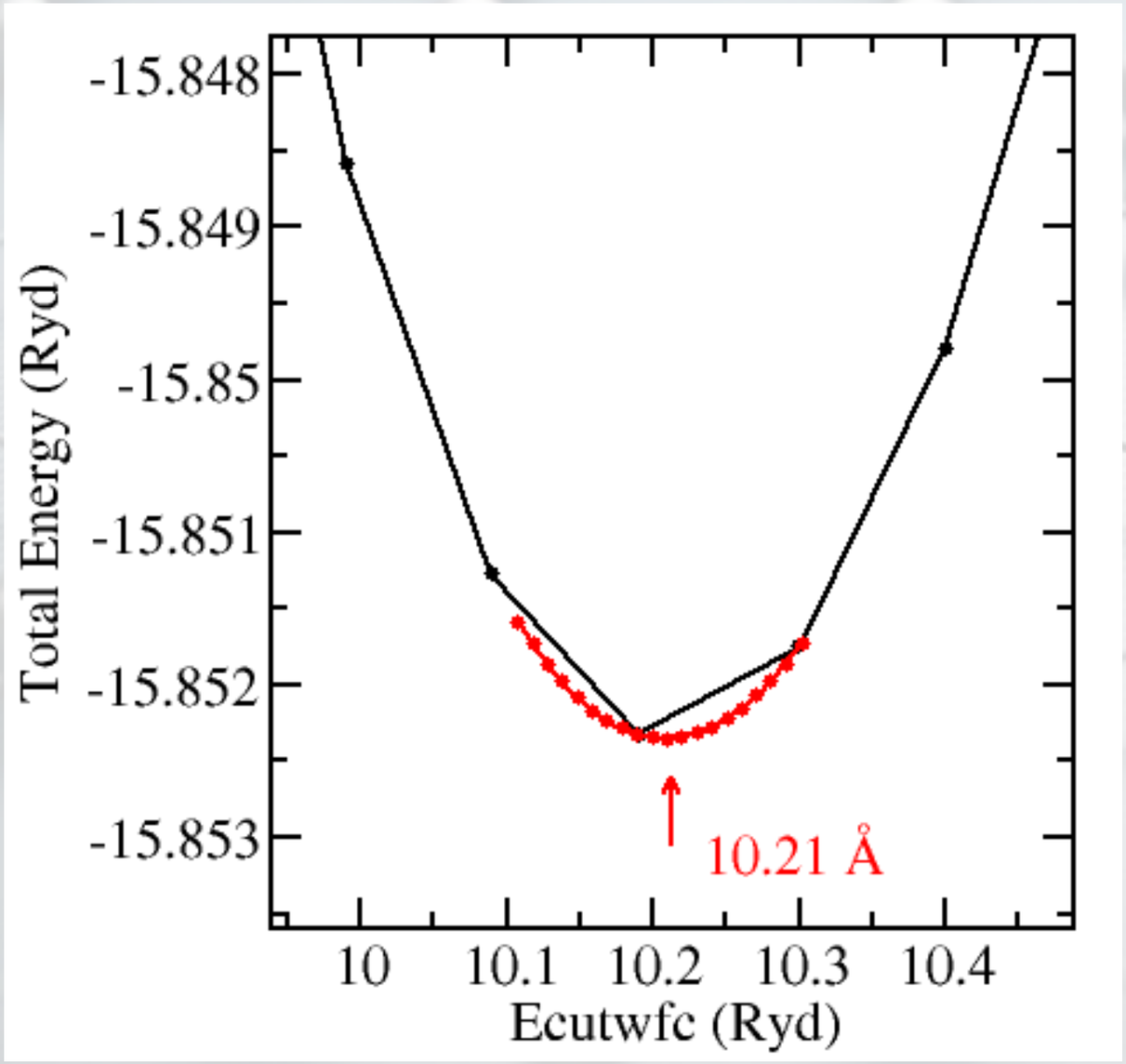
lattice parameter (Bohr)



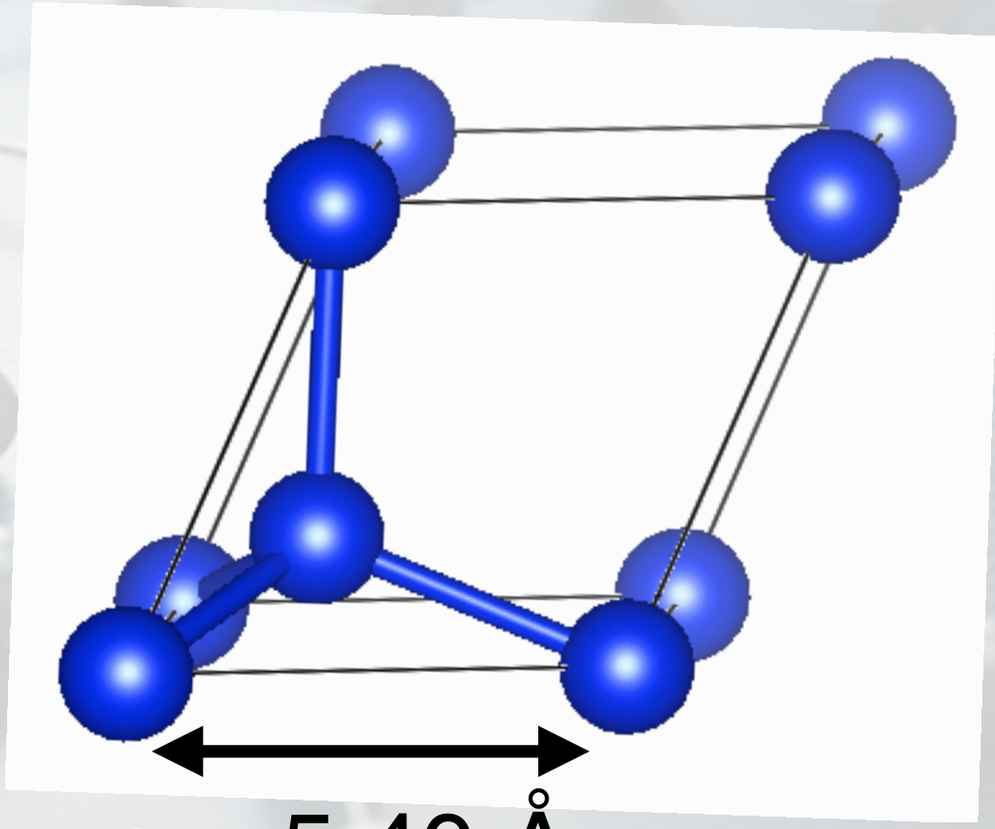
a = 5.40 Å

Lattice Parameter

Lattice Parameter -PZ-VBC(LDA)



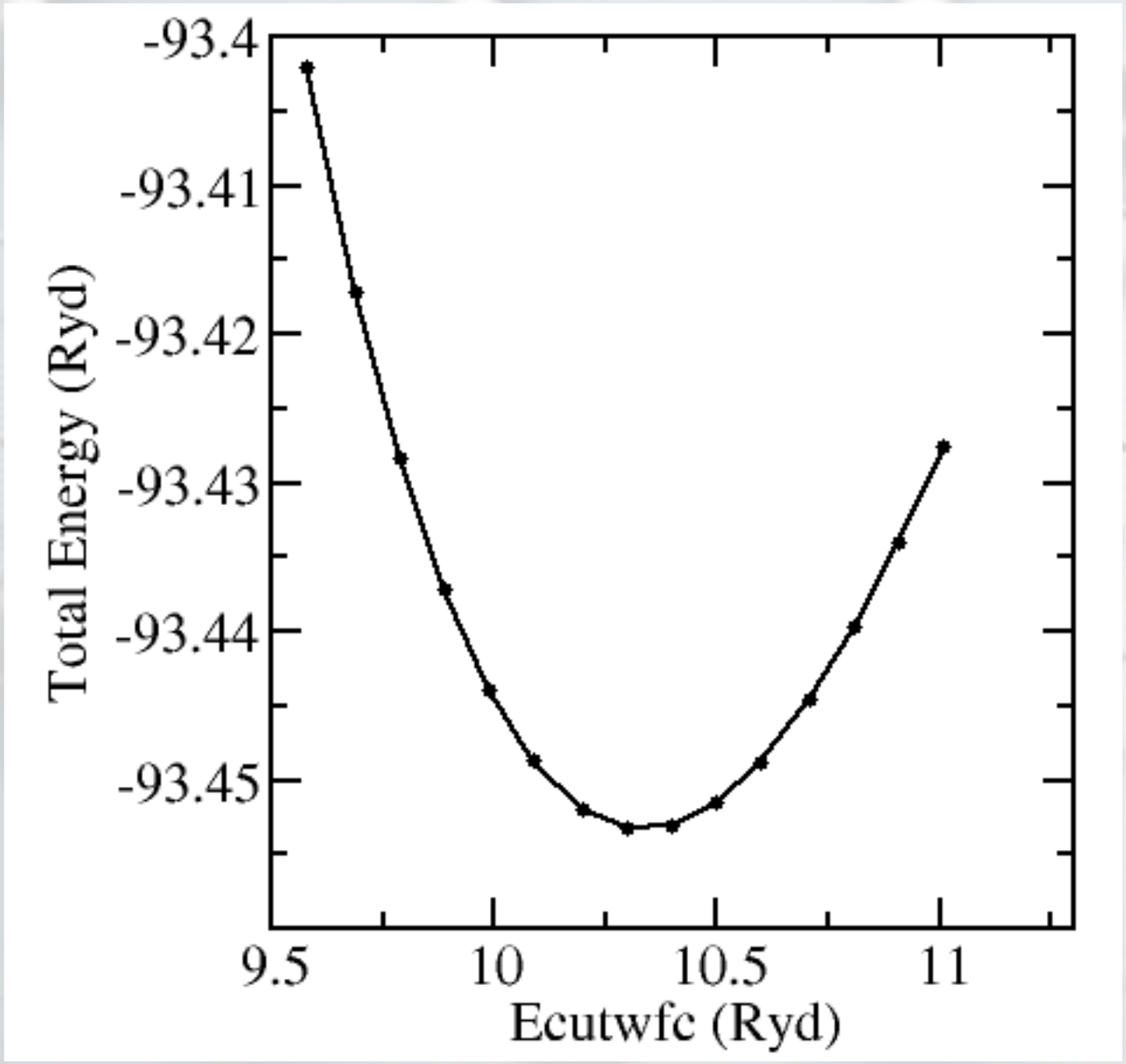
lattice parameter (Bohr)



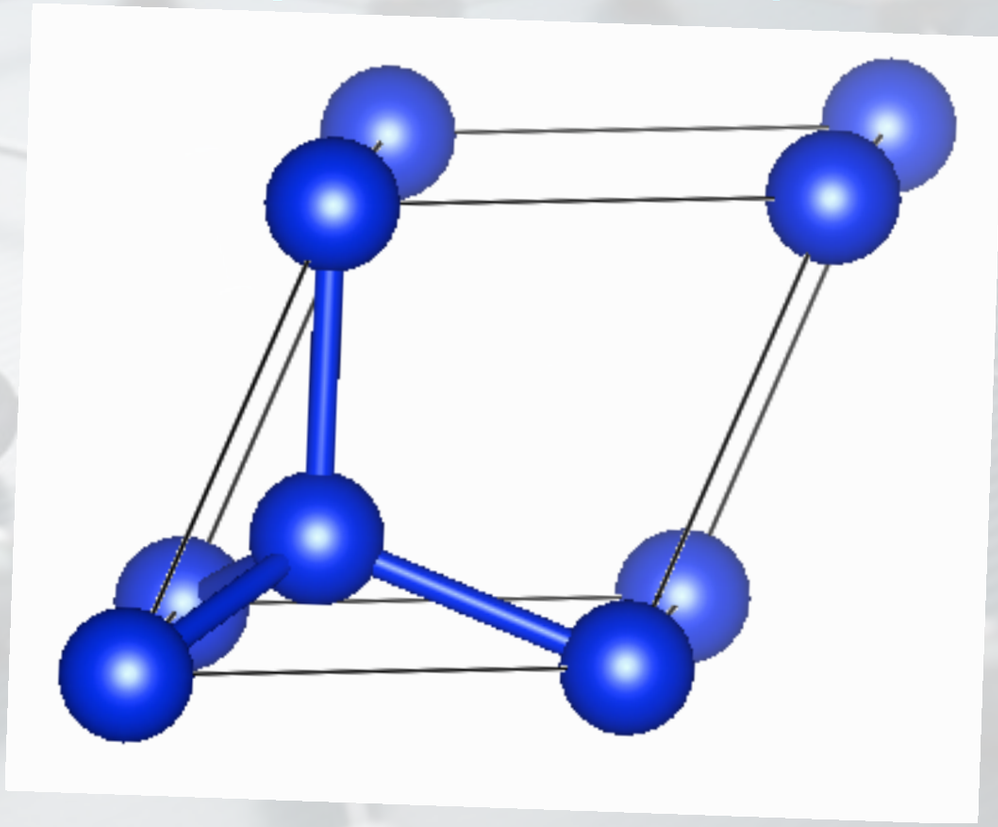
a = 5.40 Å

Lattice Parameter

Lattice Parameter - PAW-PBE (GGA)

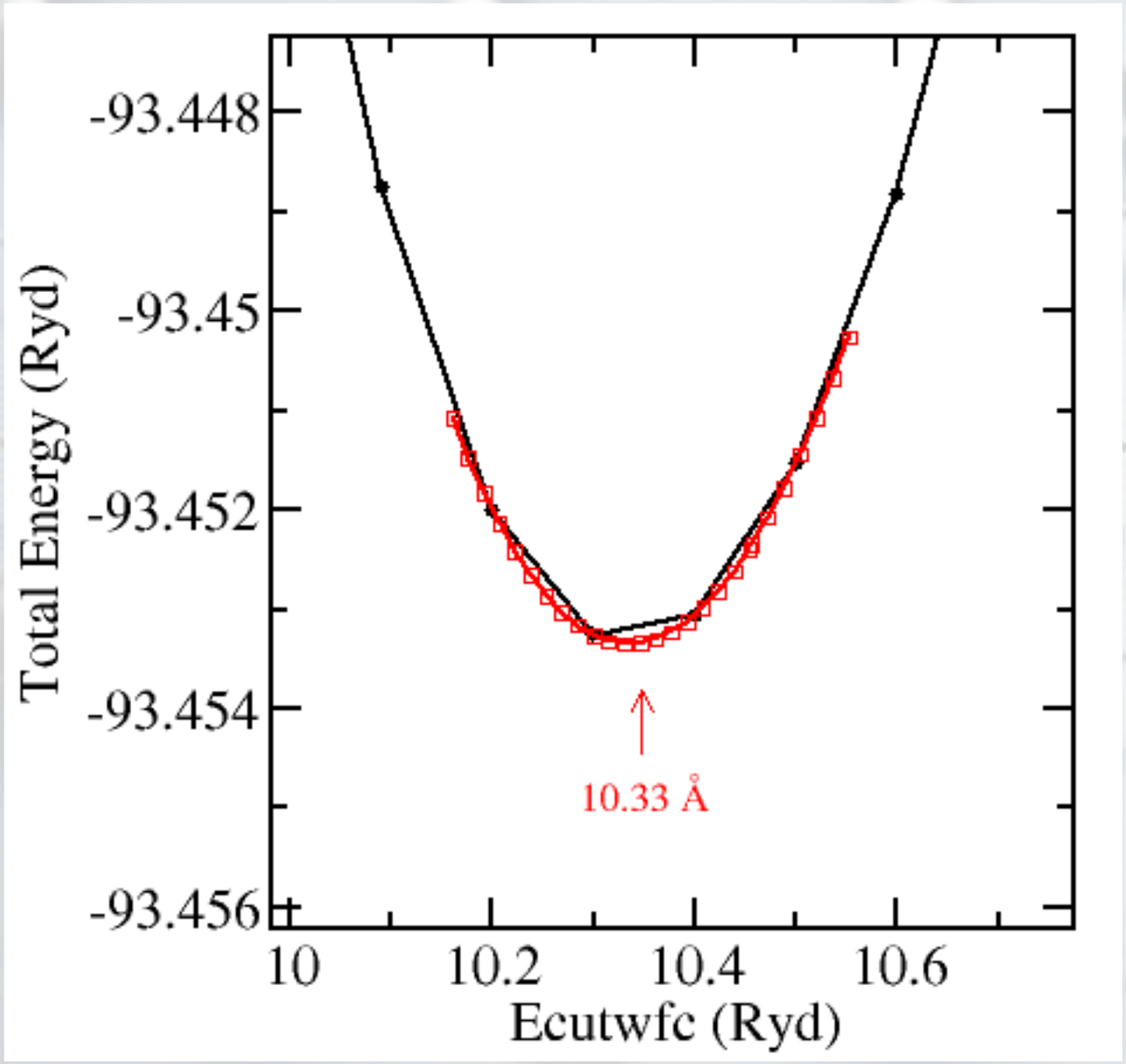


lattice parameter (Bohr)

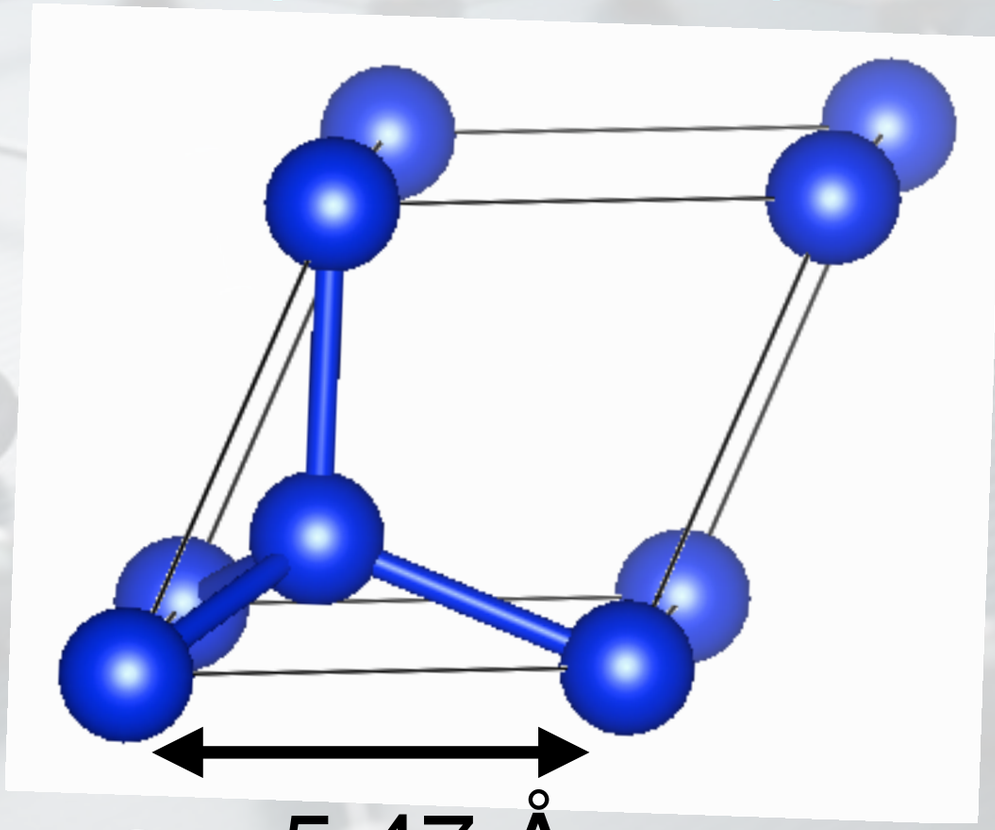


Lattice Parameter

Lattice Parameter - PAW-PBE (GGA)



lattice parameter (Bohr)



a = 5.47 Å

Lattice Parameter

Article | Open Access | Published: 12 July 2017

High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory

Kamal Choudhary ✉, Irina Kalish, Ryan Beams & Francesca Tavazza

Scientific Reports **7**, Article number: 5179 (2017) | Cite this article

We introduce a simple criterion to identify two-dimensional (2D) materials based on the comparison between experimental lattice constants and lattice constants mainly obtained from Materials-Project (MP) density functional theory (DFT) calculation repository. Specifically, if the relative difference between the two lattice constants for a specific material is greater than or equal to 5%, we predict them to be good candidates for 2D materials. We have predicted at least 1356 such 2D materials. For all the systems satisfying our criterion, we manually create single layer systems and calculate their energetics, structural, electronic, and elastic properties for both the bulk and the single layer cases. Currently the database consists of 1012 bulk and 430 single layer

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```

number of bands

Band Structure

SCF Calculation

```
 &system
    ibrav=  2,
    celldm(1) =10.20
    nat=  2,
    ntyp= 1,
    ecutwfc =32.0,
    nbnd = 8,
 /
!FCC (face-centere
K_POINTS crystal_
11
   0.0000   0.0000
   0.5000   0.0000
   0.5000   0.2500
   0.3750   0.3750
   0.0000   0.0000
   0.5000   0.5000
   0.6250   0.2500
   0.5000   0.2500
   0.5000   0.5000
   0.6250   0.2500
   0.5000   0.0000   0.5000 20  ! X
```

```
     bravais-lattice index     =            2
     lattice parameter (alat)  =      10.2000  a.u.
     unit-cell volume          =     265.3020 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            1
     number of electrons       =         8.00
     number of Kohn-Sham states=            4
     kinetic-energy cutoff     =      32.0000  Ry
     charge density cutoff     =     128.0000  Ry
     convergence threshold     =      1.0E-08
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation=  SLA  PZ   NOGX NOGC
                          (   1   1    0    0    0    0    0)

     celldm(1)=  10.200000  celldm(2)=   0.000000  celldm(3)=   0.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (  -0.500000   0.000000   0.500000 )
               a(2) = (   0.000000   0.500000   0.500000 )
               a(3) = (  -0.500000   0.500000   0.000000 )

     reciprocal axes: (cart. coord. in units 2 pi/alat)
               b(1) = ( -1.000000 -1.000000  1.000000 )
               b(2) = (  1.000000  1.000000  1.000000 )
               b(3) = ( -1.000000  1.000000 -1.000000 )
```

Band Structure

SCF Calculation

```
 &system
    ibrav=  2,
    celldm(1) =10.20
    nat=  2,
    ntyp= 1,
    ecutwfc =32.0,
    nbnd = 8,
 /
!FCC (face-centere
K_POINTS crystal_
11
   0.0000   0.0000
   0.5000   0.0000
   0.5000   0.2500
   0.3750   0.3750
   0.0000   0.0000
   0.5000   0.5000
   0.6250   0.2500
   0.5000   0.2500
   0.5000   0.5000
   0.6250   0.2500
   0.5000   0.0000   0.5000 20  ! X
```

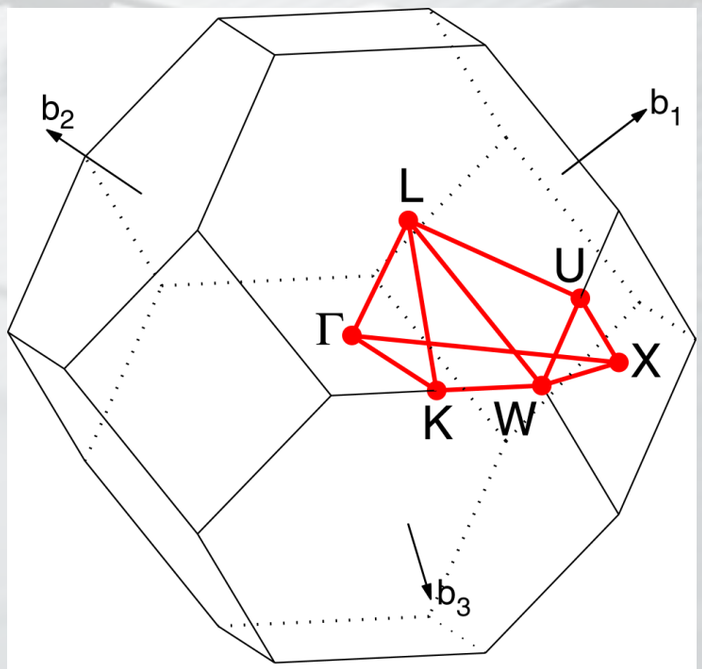
```
     bravais-lattice index     =            2
     lattice parameter (alat)  =      10.2000  a.u.
     unit-cell volume          =     265.3020 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            1
     number of electrons       =         8.00
     number of Kohn-Sham states=            4
     kinetic-energy cutoff     =      32.0000  Ry
     charge density cutoff     =     128.0000  Ry
     convergence threshold     =      1.0E-08
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation=  SLA  PZ   NOGX NOGC
                          (   1   1    0    0    0    0    0)

     celldm(1)=  10.200000  celldm(2)=   0.000000  celldm(3)=   0.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (  -0.500000   0.000000   0.500000 )
               a(2) = (   0.000000   0.500000   0.500000 )
               a(3) = (  -0.500000   0.500000   0.000000 )

     reciprocal axes: (cart. coord. in units 2 pi/alat)
               b(1) = ( -1.000000 -1.000000  1.000000 )
               b(2) = (  1.000000  1.000000  1.000000 )
               b(3) = ( -1.000000  1.000000 -1.000000 )
```

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```

← path along the BZ



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

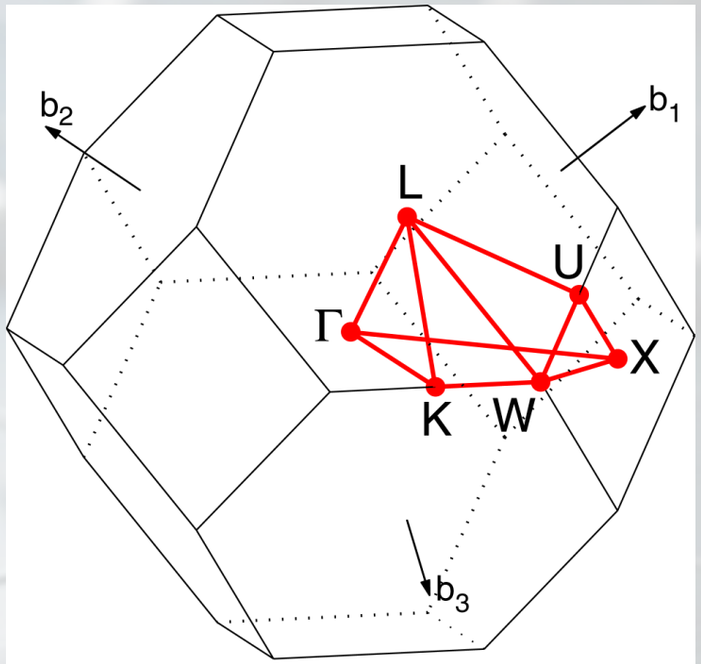
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```

number of segments



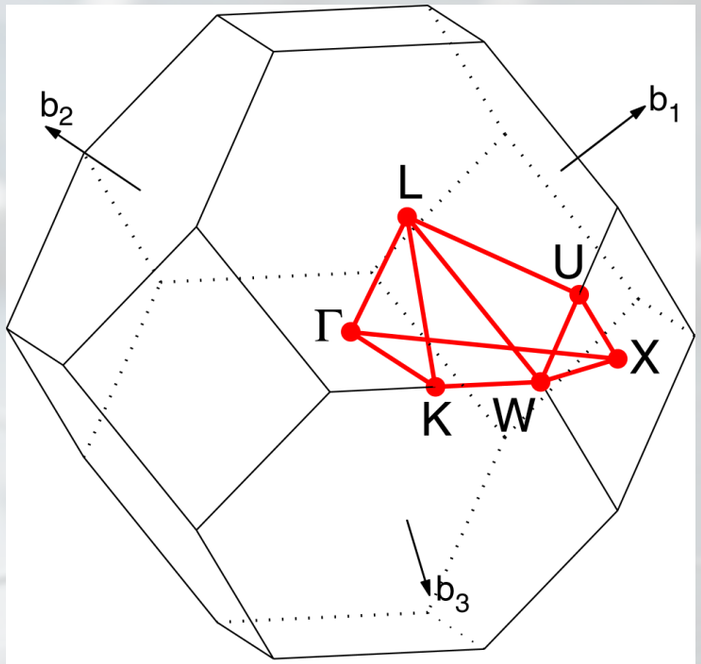
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

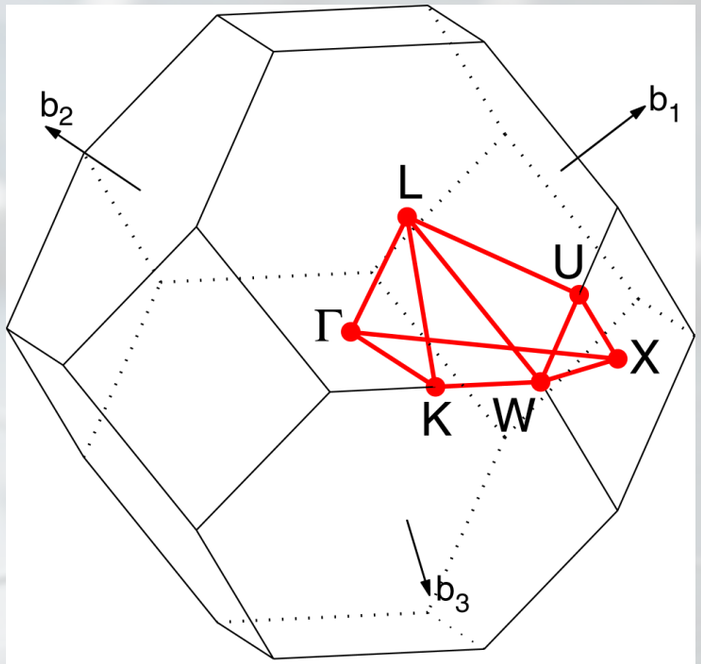
number of points

between 2 segments

Band Structure

Band structure PZ-VBC(LDA)

```
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =32.0,
   nbnd = 8,
/
!FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X
K_POINTS crystal_b
11
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.5000 20  ! X
   0.5000   0.2500   0.7500 20  ! W
   0.3750   0.3750   0.7500 20  ! K
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.2500   0.7500 20  ! W
   0.5000   0.5000   0.5000 20  ! L
   0.6250   0.2500   0.6250 20  ! U
   0.5000   0.0000   0.5000 20  ! X
```



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

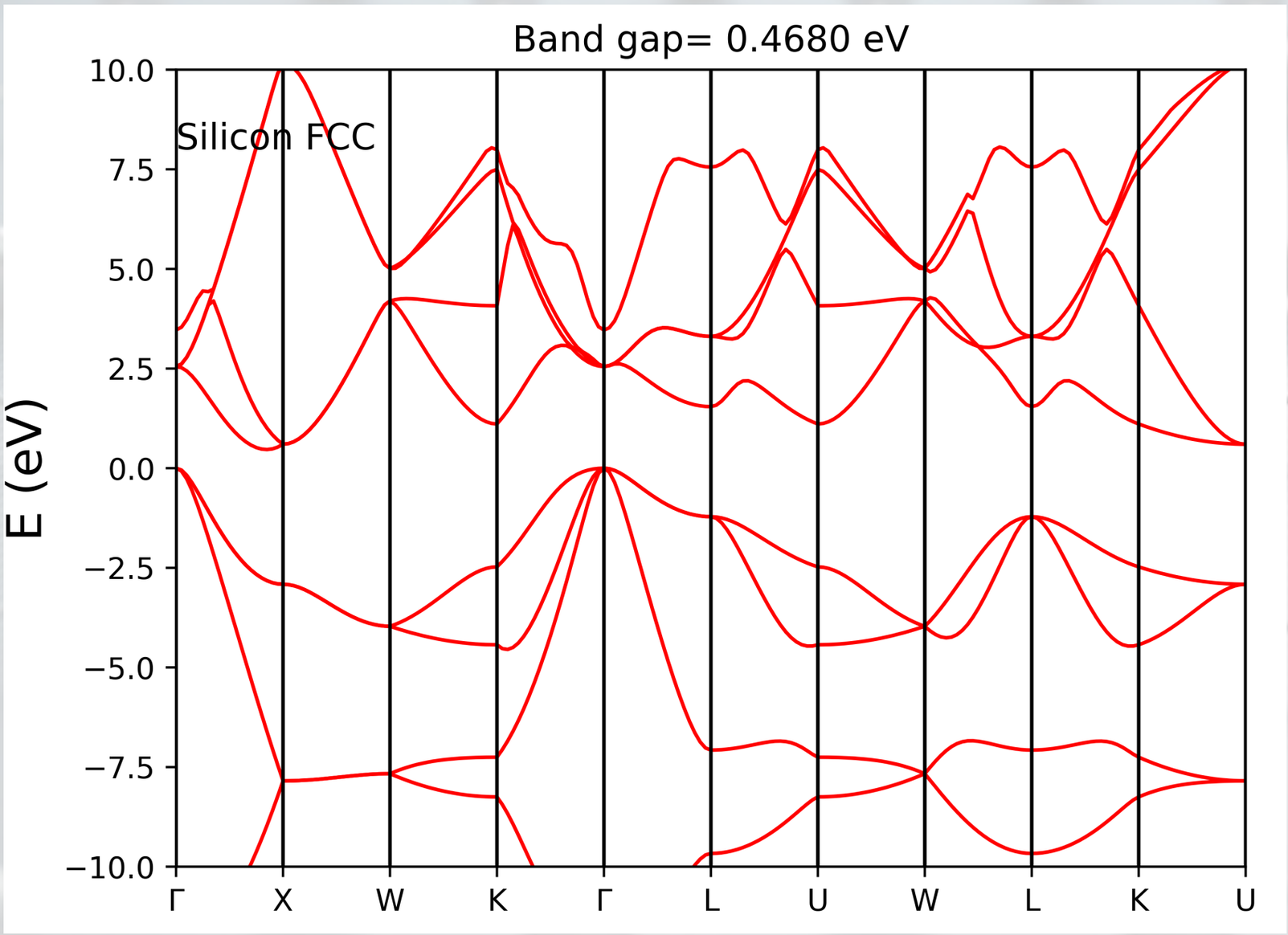
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

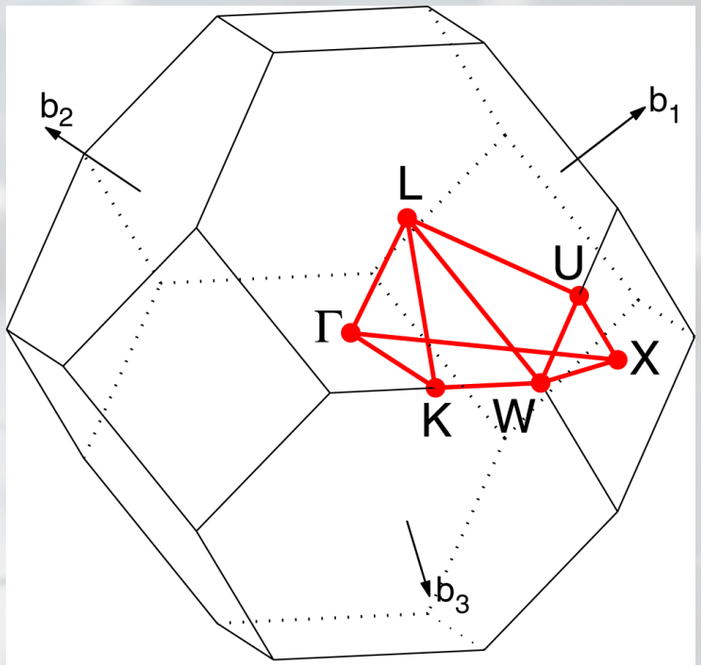
number of points

between 2 segments

Band Structure

Band structure PZ-VBC(LDA)

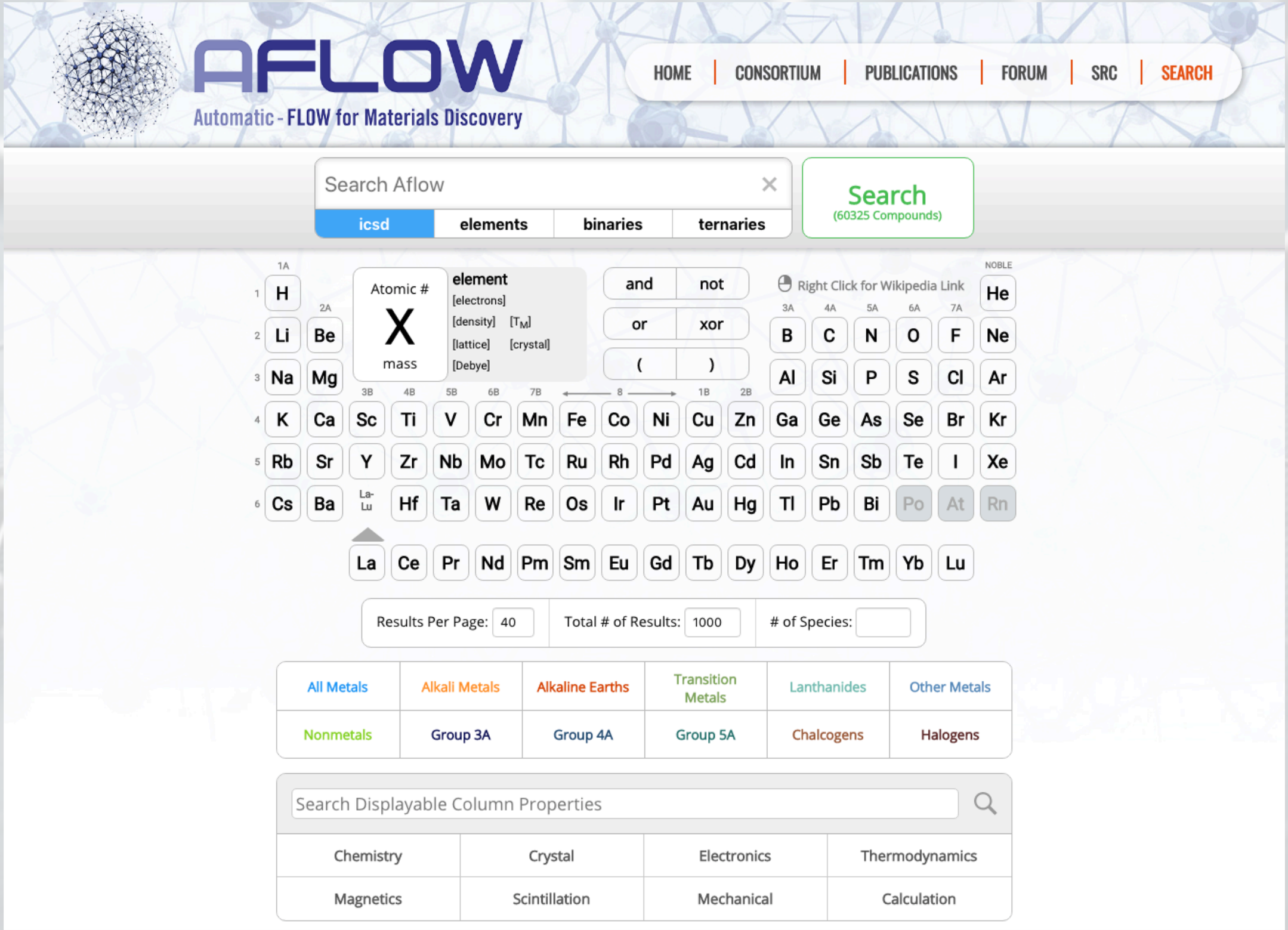




FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

DFT Databases



DFT Databases

Si_2 (ICSD# 652257)

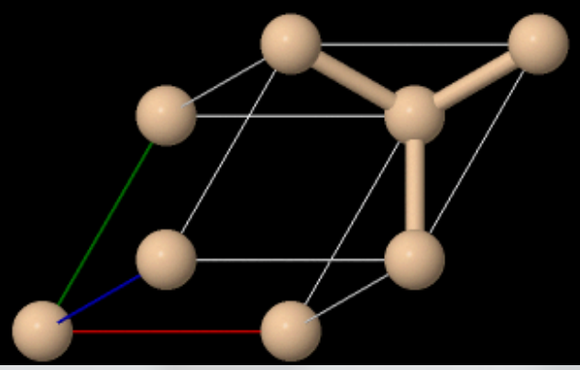
LICENSE: The data included within the aflow.org repository is free for scientific, academic and non-commercial purposes. Any other use is prohibited.

PERMANENT URL: HTTP://AFLOW.ORG/MATERIAL/?ID=AFLOW:2A2FBDFB4258EAFA

aflow.org web entry generator V3.2.3 [built=2020-05-02]

AFLOW.org consortium (AFLOW v3.1.222)
entry=Si1_ICSD_652257

Spacegroup = Fd-3m (#227)
a=3.87Å, b=3.87Å, c=3.87Å
α=60°, β=60°, γ=60°



Relaxed Structure:

As calculated
Standard conventional [info]
Standard primitive [info]

Supercell:

2 × 2 × 2 | 20Å box
2 × 2 × 2
Build
RESET

Visualization:

Ball & Stick | Spacefill
Rotation Labels Background
axis: a b c RESET

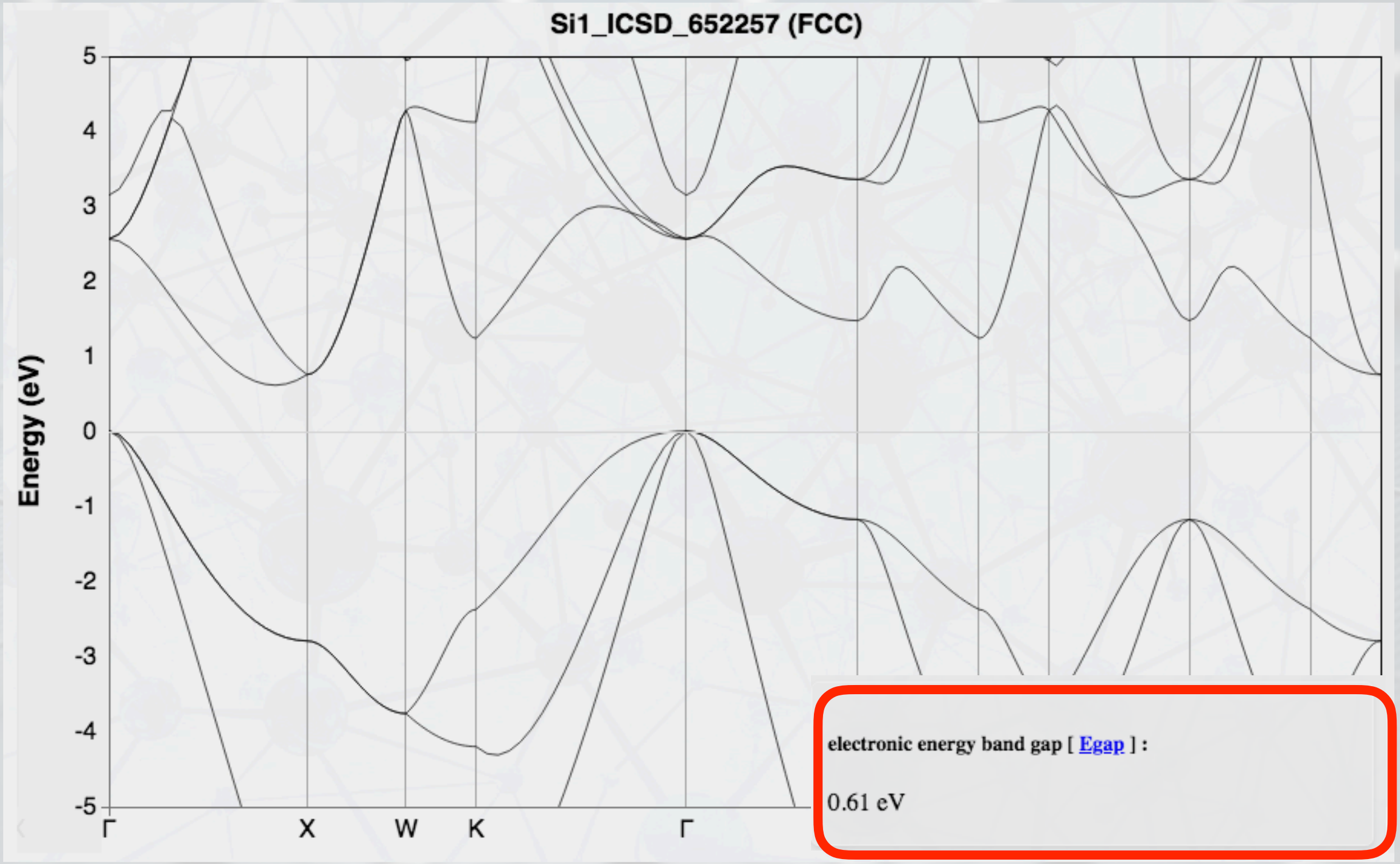
Crystallographic Planes:

h: 2 k: 2 l: 2
Show plane
RESET

Symmetry Operations:

Bader Isosurfaces:

DFT Databases

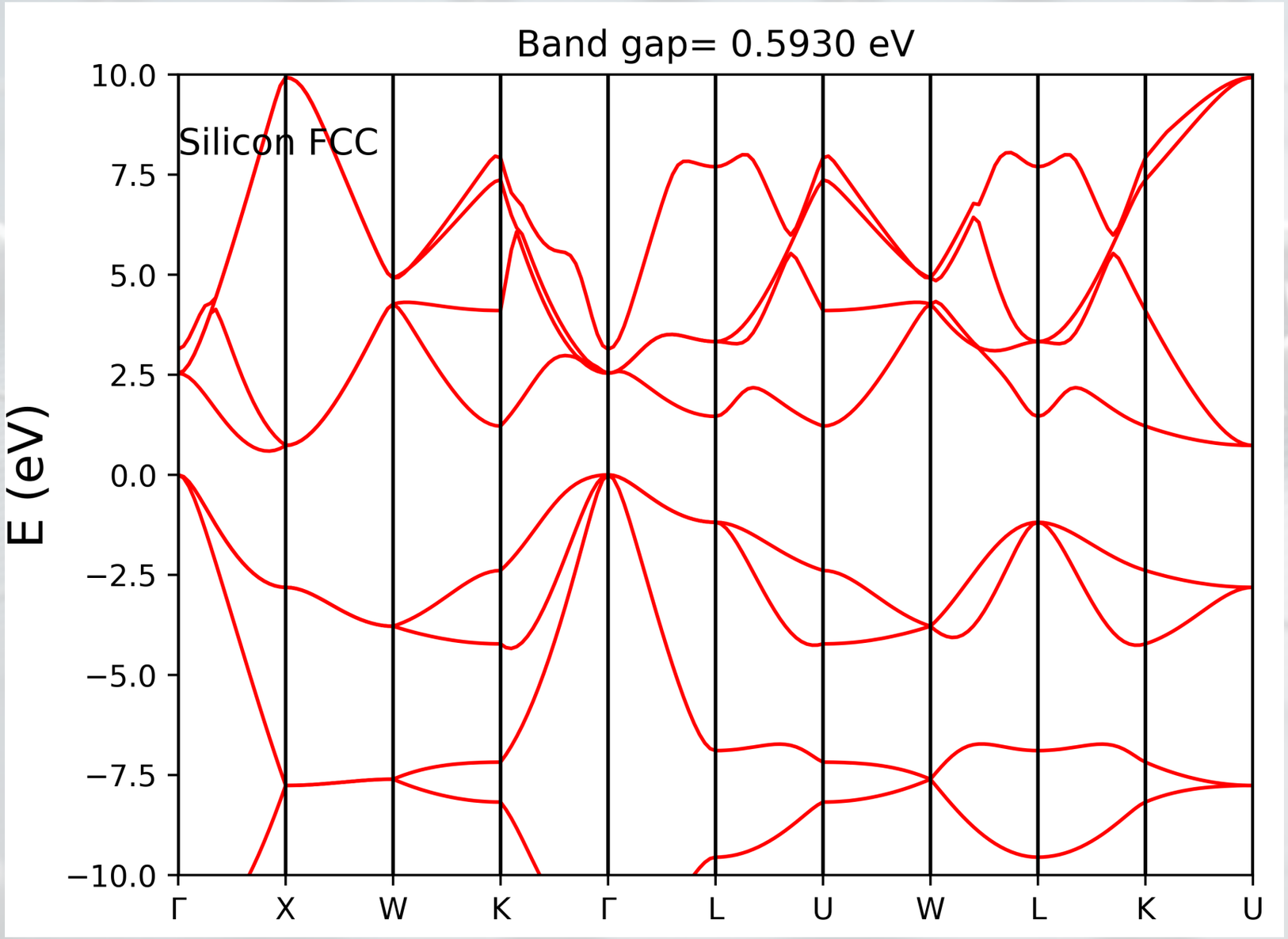


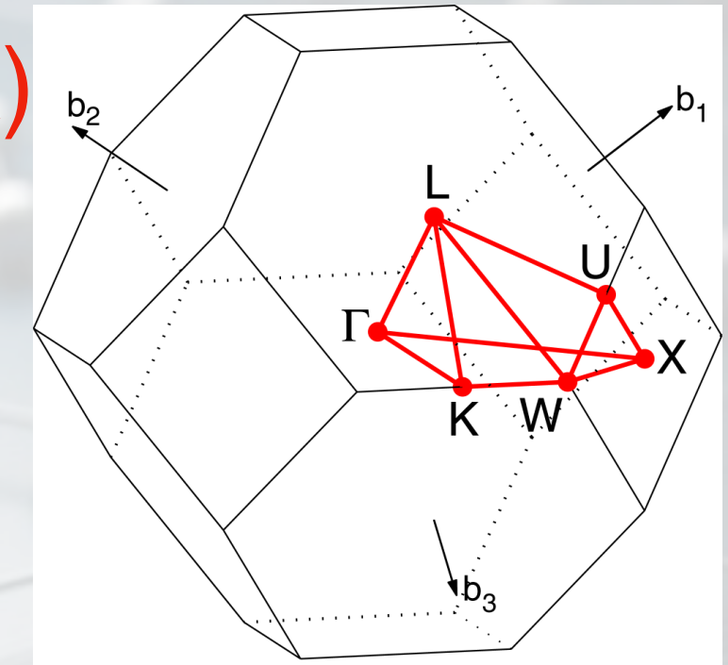
electronic energy band gap [Egap] :

0.61 eV

Band Structure

Band structure PBE-PAW(GGA)



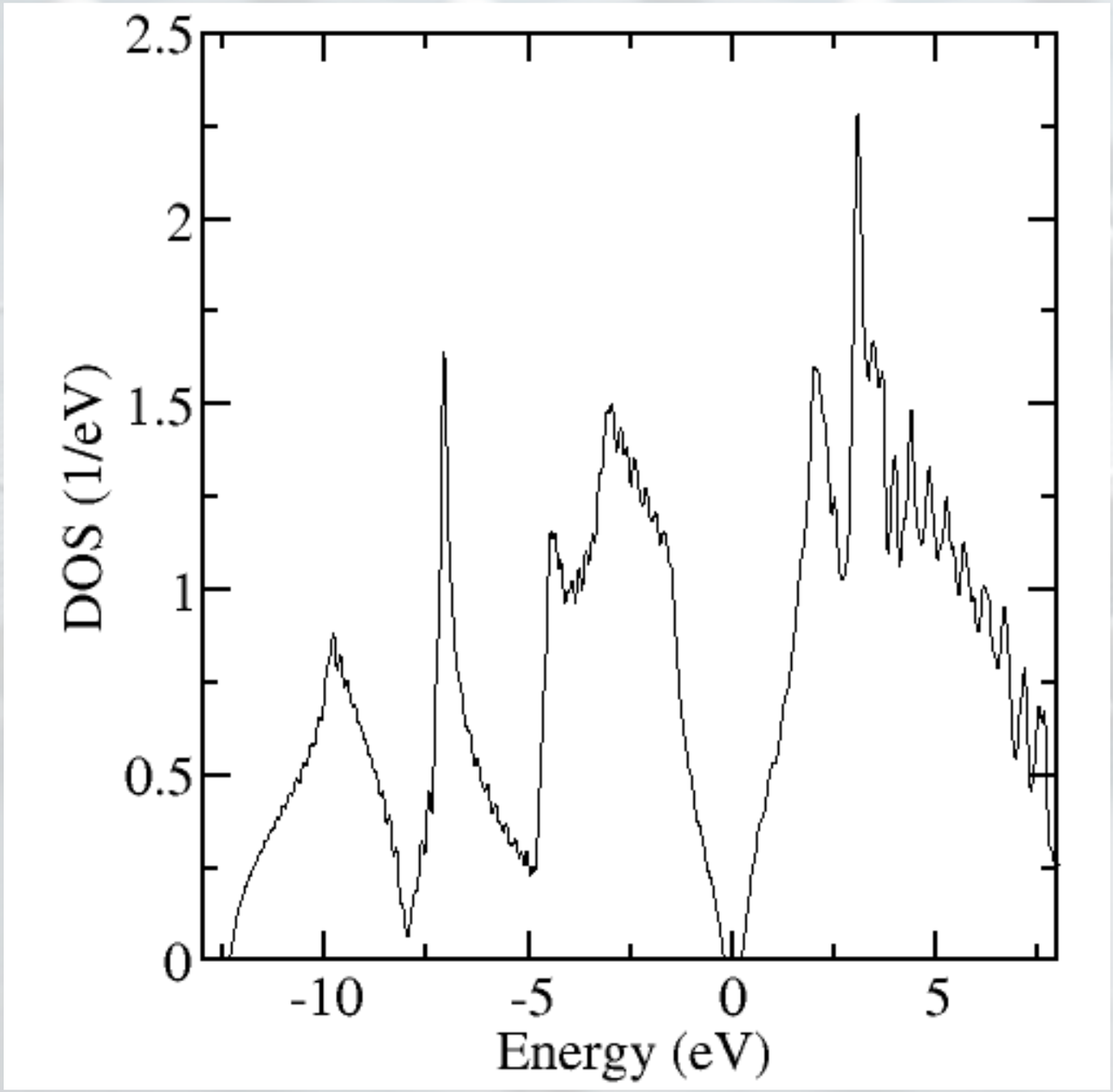


FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Density of States

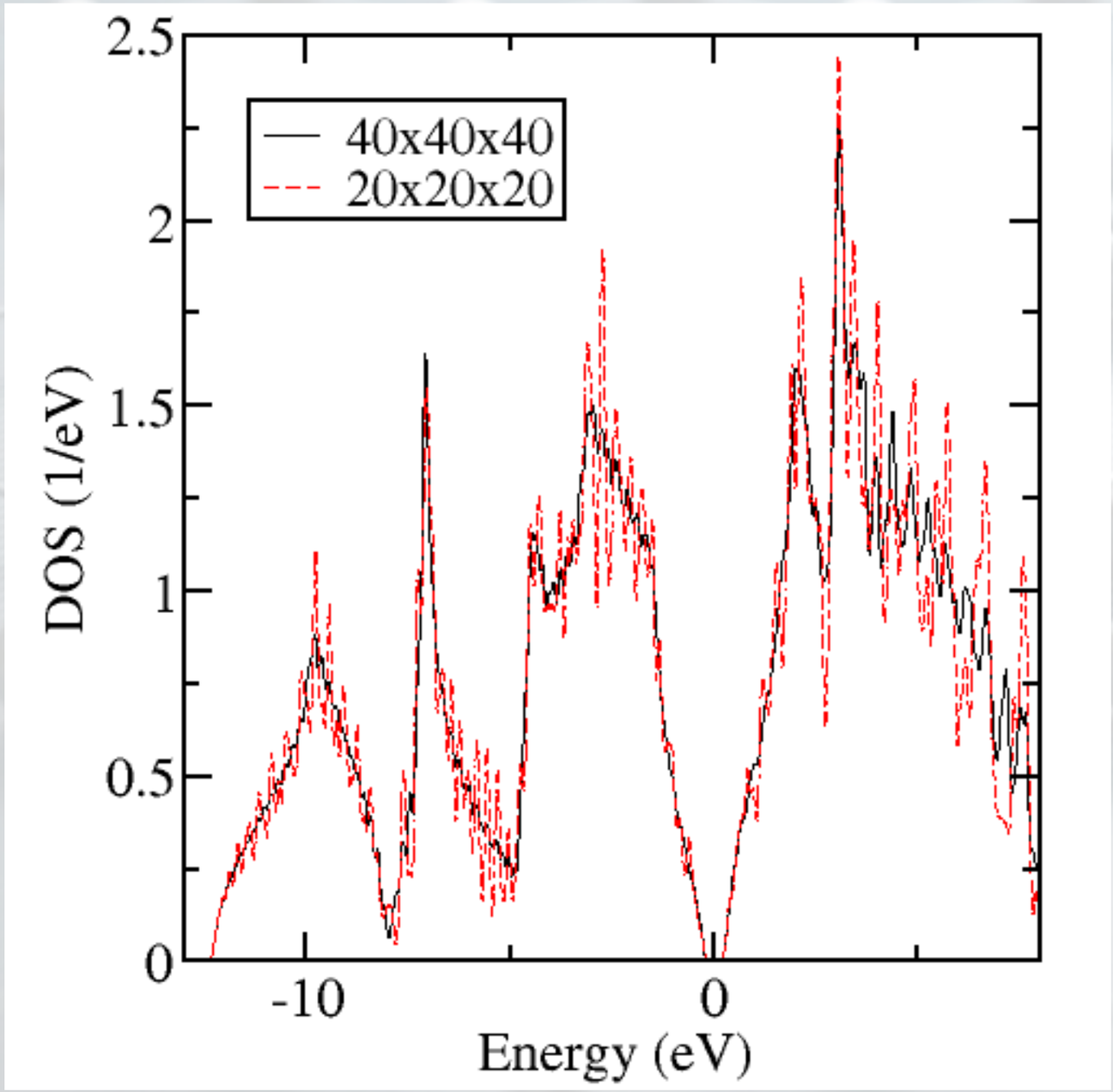
PZ-VBC(LDA)



Density of States

PZ-VBC(LDA)

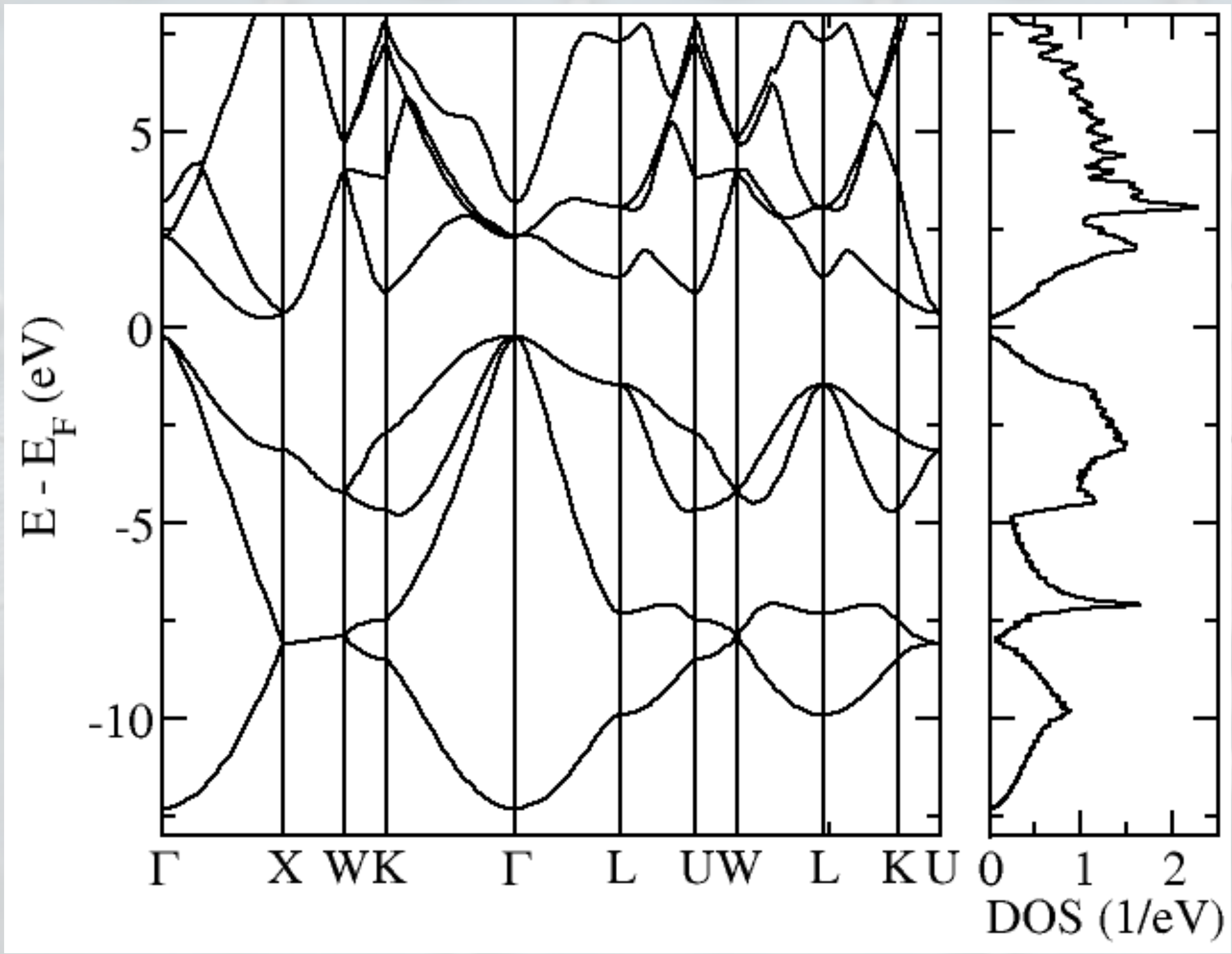
K-points density



Density of States

K-points density

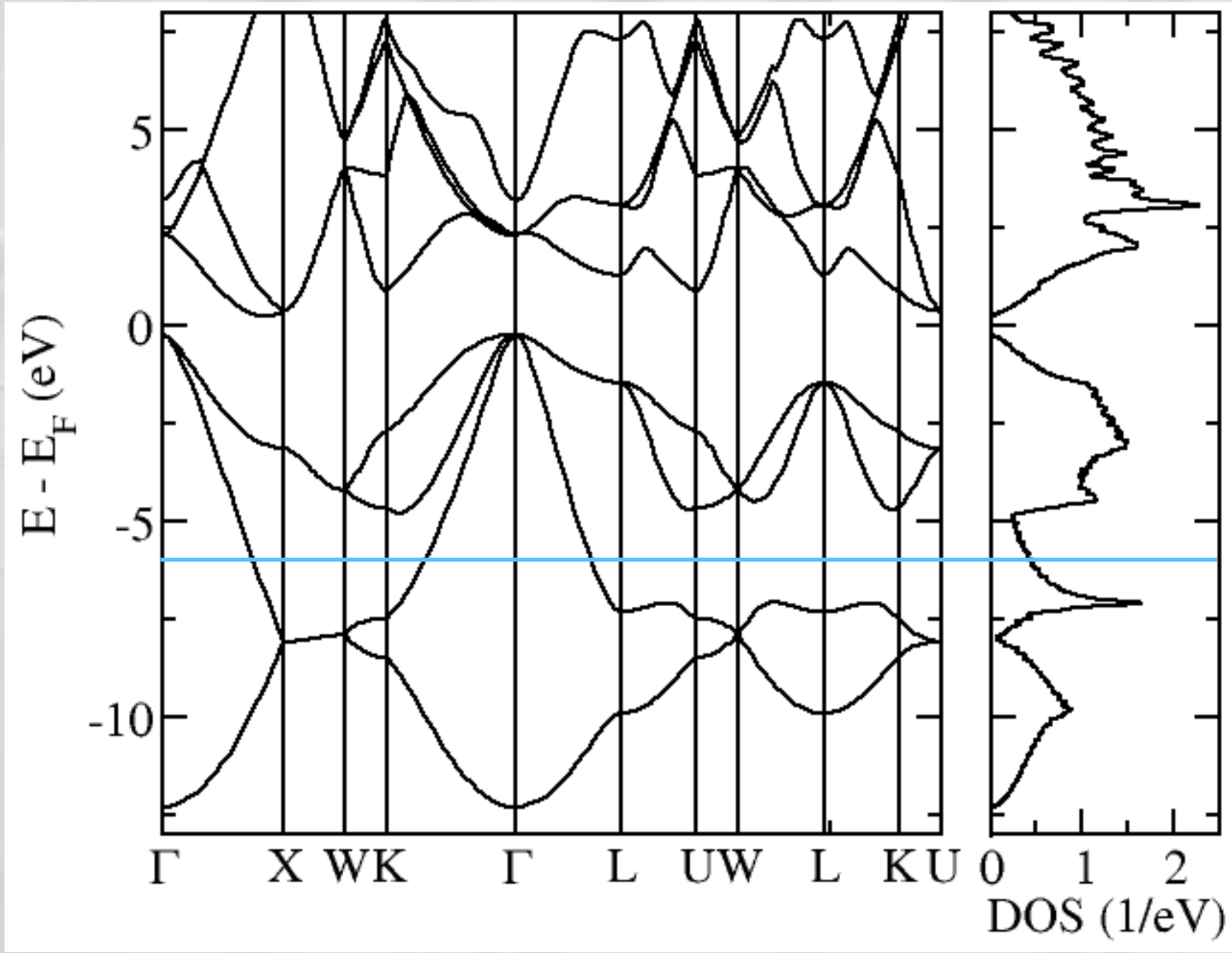
PZ-VBC(LDA)



Density of States

PZ-VBC(LDA)

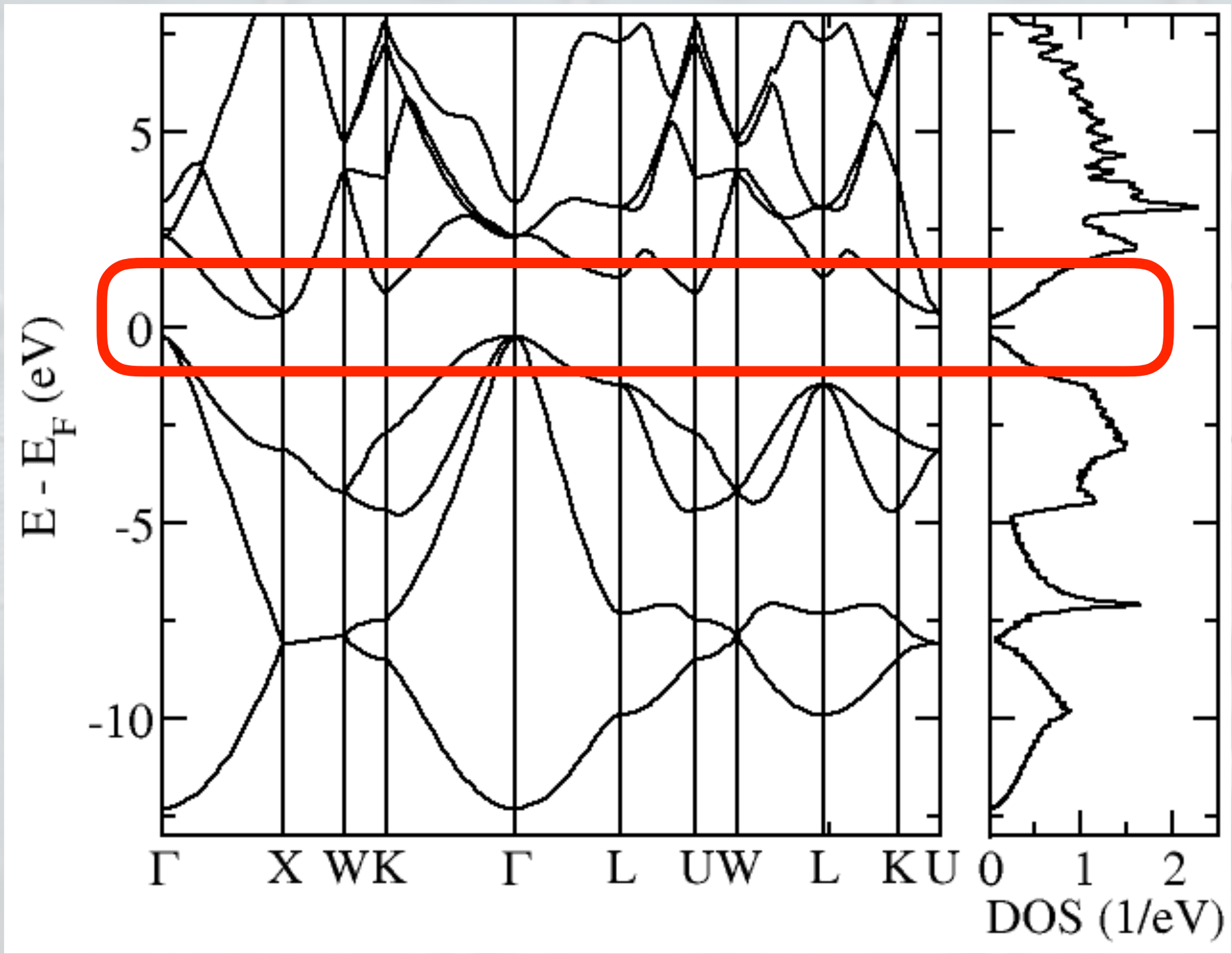
K-points density



Density of States

K-points density

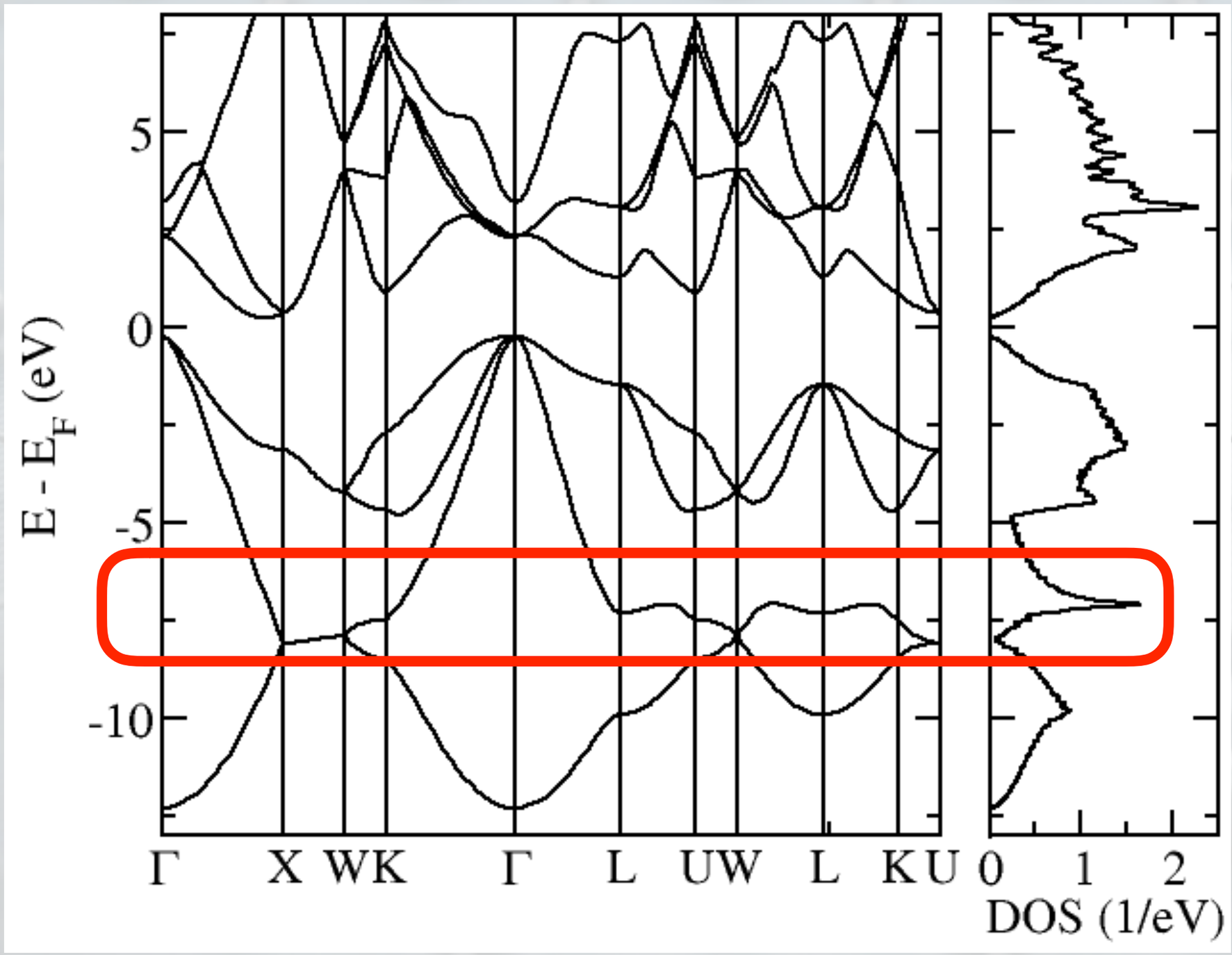
PZ-VBC(LDA)



Density of States

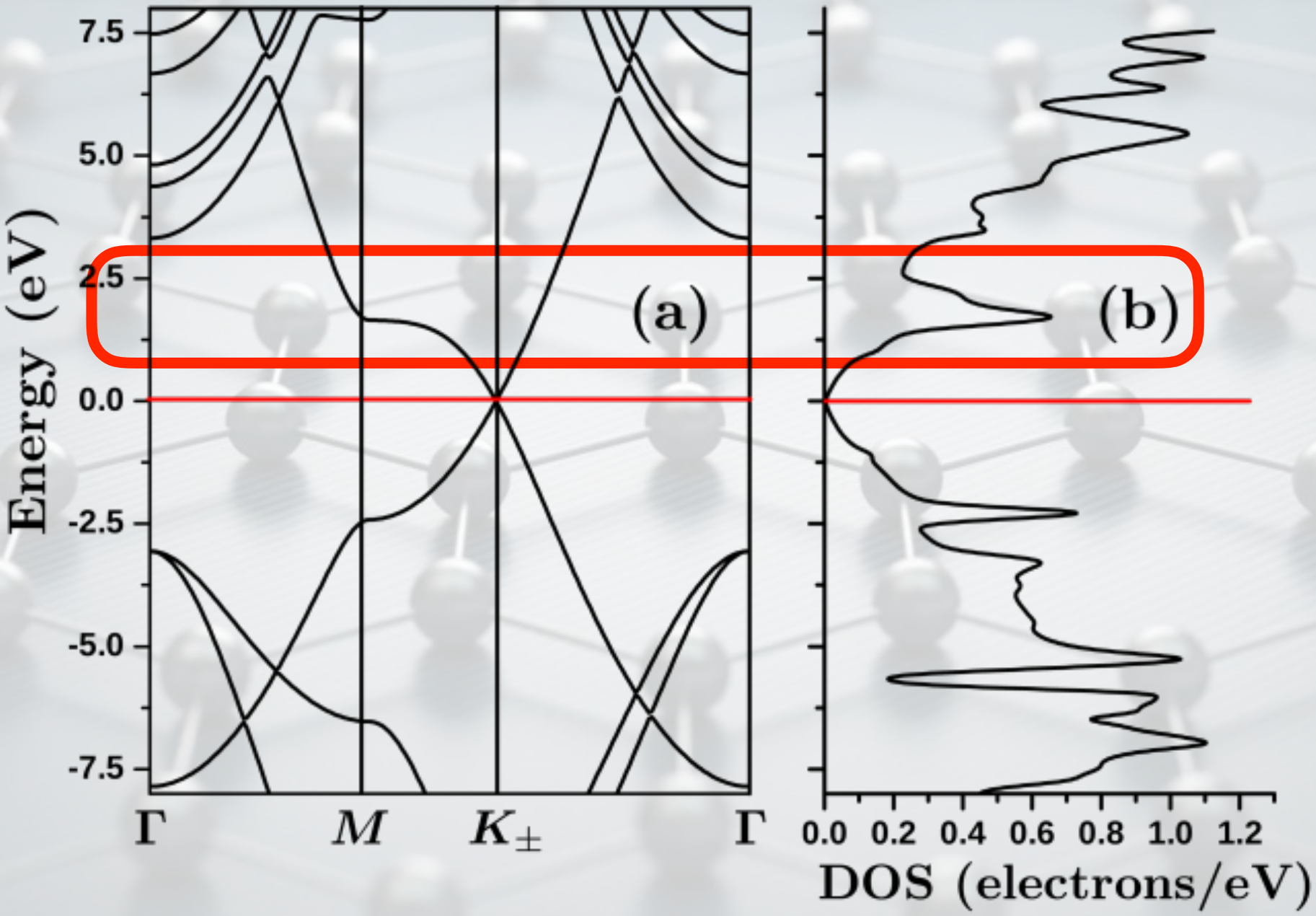
K-points density

PZ-VBC(LDA)



Density of States

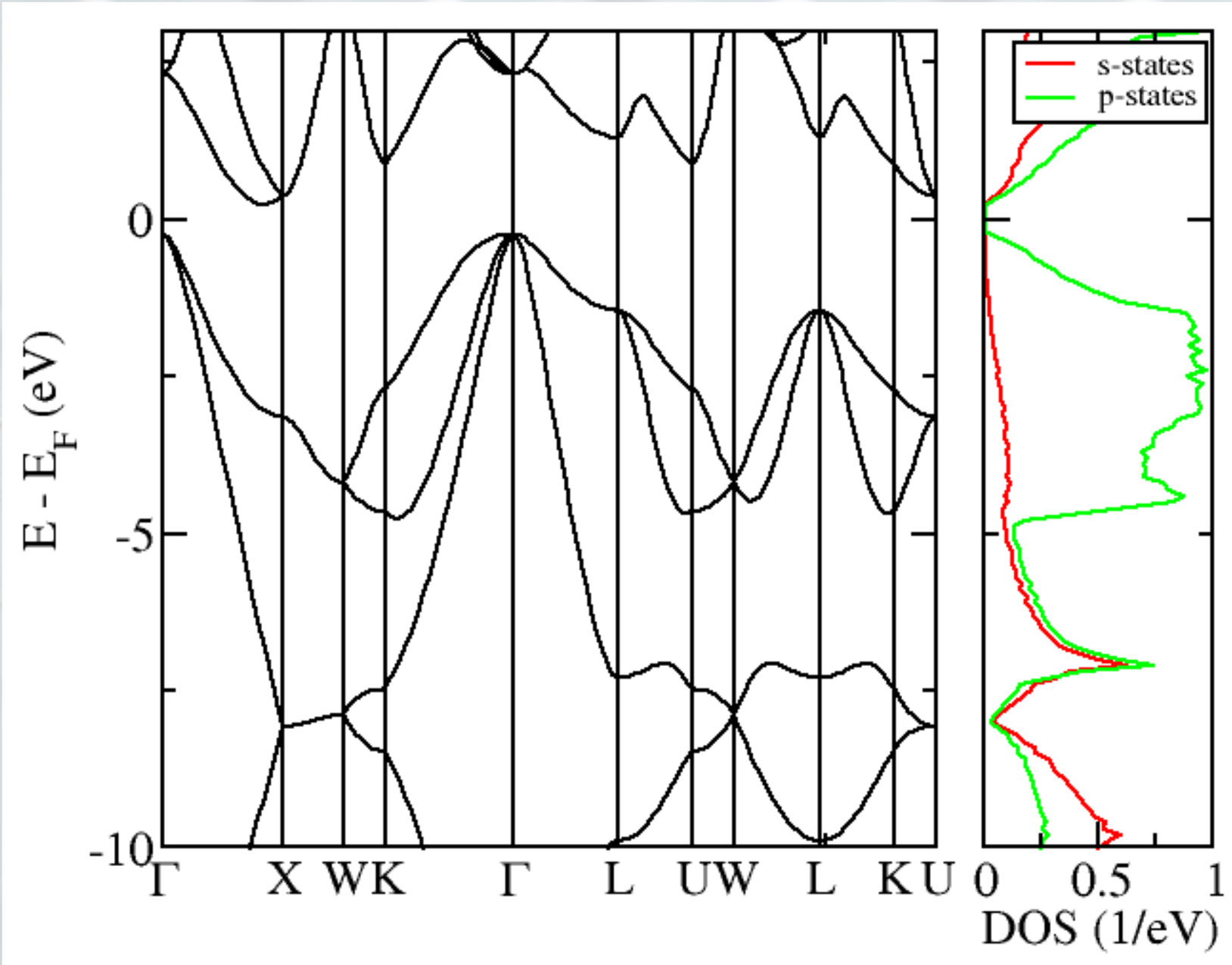
Graphene



Projected Density of States

PDOS

PZ-VBC(LDA)



Practical Part

Iron

- Non spin polarized band structure (1 atom unit cell)
- Spin polarized band structure (1 atom unit cell)
- Total and projected density of states (SP and Non SP)

Practical Part

Graphene

- Band Structure
- Total and projected density of states
- Carbon phase diagram: Diamond X Honeycomb
- Phonons