

Program PWSCF v.6.5 starts on 25Oct2023 at 19:31:32

This program is part of the open-source Quantum ESPRESSO suite  
for quantum simulation of materials; please cite

"P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);

"P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);

URL <http://www.quantum-espresso.org>,

in publications or presentations arising from this work. More details at

<http://www.quantum-espresso.org/quote>

Parallel version (MPI), running on 1 processors

MPI processes distributed on 1 nodes

Waiting for input...

Reading input from standard input

Warning: card &IONS ignored

Warning: card ION\_DYNAMICS = 'BFGS' ignored

Warning: card / ignored

Current dimensions of program PWSCF are:

Max number of different atomic species (ntypx) = 10

Max number of k-points (npk) = 40000

Max angular momentum in pseudopotentials (lmaxx) = 3

Atomic positions and unit cell read from directory:

./tmp-hetero/

A.save/

file C.pbe-rrkjus.UPF: wavefunction(s) 2S 2P renormalized

Subspace diagonalization in iterative solution of the eigenvalue problem:  
a serial algorithm will be used

G-vector sticks info

-----

sticks:	dense	smooth	PW	G-vecs:	dense	smooth	PW
Sum	673	265	85		42167	10667	1953

bravais-lattice index = 4

lattice parameter (alat) = 4.6500 a.u.

unit-cell volume = 261.2226 (a.u.)<sup>3</sup>

number of atoms/cell = 2

number of atomic types = 1

number of electrons = 8.00

number of Kohn-Sham states= 8

kinetic-energy cutoff = 45.0000 Ry

charge density cutoff = 450.0000 Ry

Exchange-correlation= SLA PW PBE PBE  
( 1 4 3 4 0 0 0)

celldm(1)= 4.650000 celldm(2)= 0.000000 celldm(3)= 3.000000

celldm(4)= 0.000000 celldm(5)= 0.000000 celldm(6)= 0.000000

crystal axes: (cart. coord. in units of alat)

a(1) = ( 1.000000 0.000000 0.000000 )

a(2) = ( -0.500000 0.866025 0.000000 )

a(3) = ( 0.000000 0.000000 3.000000 )

```

reciprocal axes: (cart. coord. in units 2 pi/alat)
b(1) = ( 1.000000 0.577350 -0.000000 )
b(2) = ( 0.000000 1.154701 0.000000 )
b(3) = ( 0.000000 -0.000000 0.333333 )

```

```

PseudoPot. # 1 for C read from file:
./pseudo/C.pbe-rrkjus.UPF
MD5 check sum: 00fb224312de0c5b6853bd333518df6f
Pseudo is Ultrasoft, Zval = 4.0
Generated by new atomic code, or converted to UPF format
Using radial grid of 627 points, 4 beta functions with:
l(1) = 0
l(2) = 0
l(3) = 1
l(4) = 1
Q(r) pseudized with 0 coefficients

```

```

atomic species  valence  mass    pseudopotential
C                4.00    12.01000  C ( 1.00)

```

```

Starting magnetic structure
atomic species  magnetization
C                0.500

```

24 Sym. Ops., with inversion, found (12 have fractional translation)

```

                                s                                frac. trans.

isym = 1      identity

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

cart.    s( 1) = ( 1.00000000 0.00000000 0.00000000 )
              ( 0.00000000 1.00000000 0.00000000 )
              ( 0.00000000 0.00000000 1.00000000 )

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

cryst.  s( 2) = (   -1          0          0      )    f=( -0.3333333 )
              (    0         -1          0      )    (  0.3333333 )
              (    0          0          1      )    (  0.0000000 )

cart.    s( 2) = ( -1.00000000 0.00000000 0.00000000 )    f=( -0.5000000 )
              ( 0.00000000 -1.00000000 0.00000000 )    (  0.2886751 )
              ( 0.00000000 0.00000000 1.00000000 )    (  0.0000000 )

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

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

cart.    s( 3) = ( -1.00000000 0.00000000 0.00000000 )
              ( 0.00000000 1.00000000 0.00000000 )
              ( 0.00000000 0.00000000 -1.00000000 )

```

```

    isym = 4      180 deg rotation - cart. axis [1,0,0]

cryst.   s( 4) = (    1          0          0      )    f =( -0.3333333 )
              (   -1          -1          0      )    (  0.3333333 )
              (    0          0         -1      )    ( -0.0000000 )

cart.    s( 4) = (  1.0000000  0.0000000  0.0000000 )    f =( -0.5000000 )
              (  0.0000000 -1.0000000  0.0000000 )    (  0.2886751 )
              (  0.0000000  0.0000000 -1.0000000 )    ( -0.0000000 )

    isym = 5      60 deg rotation - cryst. axis [0,0,1]

cryst.   s( 5) = (    1          1          0      )    f =( -0.3333333 )
              (   -1          0          0      )    (  0.3333333 )
              (    0          0          1      )    (  0.0000000 )

cart.    s( 5) = (  0.5000000 -0.8660254  0.0000000 )    f =( -0.5000000 )
              (  0.8660254  0.5000000  0.0000000 )    (  0.2886751 )
              (  0.0000000  0.0000000  1.0000000 )    (  0.0000000 )

    isym = 6      60 deg rotation - cryst. axis [0,0,-1]

cryst.   s( 6) = (    0          -1          0      )    f =( -0.3333333 )
              (    1          1          0      )    (  0.3333333 )
              (    0          0          1      )    (  0.0000000 )

cart.    s( 6) = (  0.5000000  0.8660254  0.0000000 )    f =( -0.5000000 )
              ( -0.8660254  0.5000000  0.0000000 )    (  0.2886751 )
              (  0.0000000  0.0000000  1.0000000 )    (  0.0000000 )

    isym = 7      120 deg rotation - cryst. axis [0,0,1]

cryst.   s( 7) = (    0          1          0      )
              (   -1          -1          0      )
              (    0          0          1      )

cart.    s( 7) = ( -0.5000000 -0.8660254  0.0000000 )
              (  0.8660254 -0.5000000  0.0000000 )
              (  0.0000000  0.0000000  1.0000000 )

    isym = 8      120 deg rotation - cryst. axis [0,0,-1]

cryst.   s( 8) = (   -1          -1          0      )
              (    1          0          0      )
              (    0          0          1      )

cart.    s( 8) = ( -0.5000000  0.8660254  0.0000000 )
              ( -0.8660254 -0.5000000  0.0000000 )
              (  0.0000000  0.0000000  1.0000000 )

    isym = 9      180 deg rotation - cryst. axis [1,-1,0]

cryst.   s( 9) = (    0          -1          0      )
              (   -1          0          0      )
              (    0          0         -1      )

```

```

cart.    s( 9) = (  0.5000000  -0.8660254  0.0000000 )
                ( -0.8660254  -0.5000000  0.0000000 )
                (  0.0000000  0.0000000 -1.0000000 )

```

isym = 10      180 deg rotation - cryst. axis [2,1,0]

```

cryst.    s(10) = (   1         1         0         )
                  (   0        -1         0         )
                  (   0         0        -1         )

```

```

cart.    s(10) = (  0.5000000  0.8660254  0.0000000 )
                  (  0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )

```

isym = 11      180 deg rotation - cryst. axis [0,1,0]

```

cryst.    s(11) = (  -1         -1         0         )   f =( -0.3333333 )
                  (   0         1         0         )   (  0.3333333 )
                  (   0         0        -1         )   ( -0.0000000 )

```

```

cart.    s(11) = ( -0.5000000 -0.8660254  0.0000000 )   f =( -0.5000000 )
                  ( -0.8660254  0.5000000  0.0000000 )   (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )   ( -0.0000000 )

```

isym = 12      180 deg rotation - cryst. axis [1,1,0]

```

cryst.    s(12) = (   0         1         0         )   f =( -0.3333333 )
                  (   1         0         0         )   (  0.3333333 )
                  (   0         0        -1         )   ( -0.0000000 )

```

```

cart.    s(12) = ( -0.5000000  0.8660254  0.0000000 )   f =( -0.5000000 )
                  (  0.8660254  0.5000000  0.0000000 )   (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )   ( -0.0000000 )

```

isym = 13      inversion

```

cryst.    s(13) = (  -1         0         0         )   f =( -0.3333333 )
                  (   0        -1         0         )   (  0.3333333 )
                  (   0         0        -1         )   ( -0.0000000 )

```

```

cart.    s(13) = ( -1.0000000  0.0000000  0.0000000 )   f =( -0.5000000 )
                  (  0.0000000 -1.0000000  0.0000000 )   (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )   ( -0.0000000 )

```

isym = 14      inv. 180 deg rotation - cart. axis [0,0,1]

```

cryst.    s(14) = (   1         0         0         )
                  (   0         1         0         )
                  (   0         0        -1         )

```

```

cart.    s(14) = (  1.0000000  0.0000000  0.0000000 )
                  (  0.0000000  1.0000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )

```

isym = 15      inv. 180 deg rotation - cart. axis [0,1,0]

```
cryst.  s(15) = (    1      0      0      )   f =( -0.3333333 )
              (   -1     -1      0      )   (  0.3333333 )
              (    0      0      1      )   (  0.0000000 )
```

```
cart.    s(15) = (  1.0000000  0.0000000  0.0000000 )   f =( -0.5000000 )
                  (  0.0000000 -1.0000000  0.0000000 )   (  0.2886751 )
                  (  0.0000000  0.0000000  1.0000000 )   (  0.0000000 )
```

isym = 16      inv. 180 deg rotation - cart. axis [1,0,0]

```
cryst.  s(16) = (   -1      0      0      )
                  (    1      1      0      )
                  (    0      0      1      )
```

```
cart.    s(16) = ( -1.0000000  0.0000000  0.0000000 )
                  (  0.0000000  1.0000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )
```

isym = 17      inv. 60 deg rotation - cryst. axis [0,0,1]

```
cryst.  s(17) = (   -1     -1      0      )
                  (    1      0      0      )
                  (    0      0     -1      )
```

```
cart.    s(17) = ( -0.5000000  0.8660254  0.0000000 )
                  ( -0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )
```

isym = 18      inv. 60 deg rotation - cryst. axis [0,0,-1]

```
cryst.  s(18) = (    0      1      0      )
                  (   -1     -1      0      )
                  (    0      0     -1      )
```

```
cart.    s(18) = ( -0.5000000 -0.8660254  0.0000000 )
                  (  0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )
```

isym = 19      inv. 120 deg rotation - cryst. axis [0,0,1]

```
cryst.  s(19) = (    0     -1      0      )   f =( -0.3333333 )
                  (    1      1      0      )   (  0.3333333 )
                  (    0      0     -1      )   ( -0.0000000 )
```

```
cart.    s(19) = (  0.5000000  0.8660254  0.0000000 )   f =( -0.5000000 )
                  (-0.8660254  0.5000000  0.0000000 )   (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )   ( -0.0000000 )
```

isym = 20      inv. 120 deg rotation - cryst. axis [0,0,-1]

```
cryst.  s(20) = (    1      1      0      )   f =( -0.3333333 )
                  (   -1      0      0      )   (  0.3333333 )
                  (    0      0     -1      )   ( -0.0000000 )
```

```
cart.    s(20) = (  0.5000000 -0.8660254  0.0000000 )   f =( -0.5000000 )
                  (  0.8660254  0.5000000  0.0000000 )   (  0.2886751 )
```

( 0.0000000 0.0000000 -1.0000000 ) ( -0.0000000 )

isym = 21 inv. 180 deg rotation - cryst. axis [1,-1,0]

cryst. s(21) = ( 0 1 0 ) f=( -0.3333333 )  
 ( 1 0 0 ) ( 0.3333333 )  
 ( 0 0 1 ) ( 0.0000000 )

cart. s(21) = ( -0.5000000 0.8660254 0.0000000 ) f=( -0.5000000 )  
 ( 0.8660254 0.5000000 0.0000000 ) ( 0.2886751 )  
 ( 0.0000000 0.0000000 1.0000000 ) ( 0.0000000 )

isym = 22 inv. 180 deg rotation - cryst. axis [2,1,0]

cryst. s(22) = ( -1 -1 0 ) f=( -0.3333333 )  
 ( 0 1 0 ) ( 0.3333333 )  
 ( 0 0 1 ) ( 0.0000000 )

cart. s(22) = ( -0.5000000 -0.8660254 0.0000000 ) f=( -0.5000000 )  
 ( -0.8660254 0.5000000 0.0000000 ) ( 0.2886751 )  
 ( 0.0000000 0.0000000 1.0000000 ) ( 0.0000000 )

isym = 23 inv. 180 deg rotation - cryst. axis [0,1,0]

cryst. s(23) = ( 1 1 0 )  
 ( 0 -1 0 )  
 ( 0 0 1 )

cart. s(23) = ( 0.5000000 0.8660254 0.0000000 )  
 ( 0.8660254 -0.5000000 0.0000000 )  
 ( 0.0000000 0.0000000 1.0000000 )

isym = 24 inv. 180 deg rotation - cryst. axis [1,1,0]

cryst. s(24) = ( 0 -1 0 )  
 ( -1 0 0 )  
 ( 0 0 1 )

cart. s(24) = ( 0.5000000 -0.8660254 0.0000000 )  
 ( -0.8660254 -0.5000000 0.0000000 )  
 ( 0.0000000 0.0000000 1.0000000 )

point group D<sub>6h</sub>(6/mmm)  
 there are 12 classes  
 the character table:

	E	2C <sub>6</sub>	2C <sub>3</sub>	C <sub>2</sub>	3C <sub>2</sub> '	3C <sub>2</sub> ''	i	2S <sub>3</sub>	2S <sub>6</sub>	s <sub>h</sub>	3s <sub>d</sub>	3s <sub>v</sub>
A <sub>1g</sub>	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
A <sub>2g</sub>	1.00	1.00	1.00	1.00	-1.00	-1.00	1.00	1.00	1.00	1.00	-1.00	-1.00
B <sub>1g</sub>	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00
B <sub>2g</sub>	1.00	-1.00	1.00	-1.00	-1.00	1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00
E <sub>1g</sub>	2.00	1.00	-1.00	-2.00	0.00	0.00	2.00	1.00	-1.00	-2.00	0.00	0.00
E <sub>2g</sub>	2.00	-1.00	-1.00	2.00	0.00	0.00	2.00	-1.00	-1.00	2.00	0.00	0.00
A <sub>1u</sub>	1.00	1.00	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00
A <sub>2u</sub>	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	1.00	1.00
B <sub>1u</sub>	1.00	-1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00
B <sub>2u</sub>	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	1.00	-1.00

```

E_1u  2.00  1.00 -1.00 -2.00  0.00  0.00 -2.00 -1.00  1.00  2.00  0.00  0.00
E_2u  2.00 -1.00 -1.00  2.00  0.00  0.00 -2.00  1.00  1.00 -2.00  0.00  0.00

```

the symmetry operations in each class and the name of the first element:

```

E      1
      identity
2C6    5   6
      60 deg rotation - cryst. axis [0,0,1]
2C3    7   8
      120 deg rotation - cryst. axis [0,0,1]
C2     2
      180 deg rotation - cart. axis [0,0,1]
3C2'   4  12  11
      180 deg rotation - cart. axis [1,0,0]
3C2''  3   9  10
      180 deg rotation - cart. axis [0,1,0]
i      13
      inversion
2S3    17  18
      inv. 60 deg rotation - cryst. axis [0,0,1]
2S6    19  20
      inv. 120 deg rotation - cryst. axis [0,0,1]
s_h    14
      inv. 180 deg rotation - cart. axis [0,0,1]
3s_d   16  24  23
      inv. 180 deg rotation - cart. axis [1,0,0]
3s_v   15  21  22
      inv. 180 deg rotation - cart. axis [0,1,0]

```

Cartesian axes

```

site n.    atom      positions (alat units)
  1         C   tau(  1) = (  0.0000000  0.0000000  1.5000000 )
  2         C   tau(  2) = ( -0.0000000  0.5773503  1.5000000 )

```

Crystallographic axes

```

site n.    atom      positions (cryst. coord.)
  1         C   tau(  1) = (  0.0000000  0.0000000  0.5000000 )
  2         C   tau(  2) = (  0.3333333  0.6666667  0.5000000 )

```

number of k points= 400 Marzari-Vanderbilt smearing, width (Ry)= 0.0010

```

      cart. coord. in units 2pi/alat
k(  1) = (  0.0000000  0.0000000  0.0000000), wk =  0.0025000
k(  2) = (  0.0034247  0.0019772  0.0000000), wk =  0.0025000
k(  3) = (  0.0068493  0.0039545  0.0000000), wk =  0.0025000
k(  4) = (  0.0102740  0.0059317  0.0000000), wk =  0.0025000
k(  5) = (  0.0136986  0.0079089  0.0000000), wk =  0.0025000
k(  6) = (  0.0171233  0.0098861  0.0000000), wk =  0.0025000
k(  7) = (  0.0205479  0.0118634  0.0000000), wk =  0.0025000
k(  8) = (  0.0239726  0.0138406  0.0000000), wk =  0.0025000
k(  9) = (  0.0273973  0.0158178  0.0000000), wk =  0.0025000
k( 10) = (  0.0308219  0.0177950  0.0000000), wk =  0.0025000
k( 11) = (  0.0342466  0.0197723  0.0000000), wk =  0.0025000
k( 12) = (  0.0376712  0.0217495  0.0000000), wk =  0.0025000
k( 13) = (  0.0410959  0.0237267  0.0000000), wk =  0.0025000
k( 14) = (  0.0445205  0.0257040  0.0000000), wk =  0.0025000
k( 15) = (  0.0479452  0.0276812  0.0000000), wk =  0.0025000
k( 16) = (  0.0513699  0.0296584  0.0000000), wk =  0.0025000
k( 17) = (  0.0547945  0.0316356  0.0000000), wk =  0.0025000
k( 18) = (  0.0582192  0.0336129  0.0000000), wk =  0.0025000

```

```
k( 19) = ( 0.0616438 0.0355901 0.0000000), wk = 0.0025000
k( 20) = ( 0.0650685 0.0375673 0.0000000), wk = 0.0025000
k( 21) = ( 0.0684932 0.0395445 0.0000000), wk = 0.0025000
k( 22) = ( 0.0719178 0.0415218 0.0000000), wk = 0.0025000
k( 23) = ( 0.0753425 0.0434990 0.0000000), wk = 0.0025000
k( 24) = ( 0.0787671 0.0454762 0.0000000), wk = 0.0025000
k( 25) = ( 0.0821918 0.0474534 0.0000000), wk = 0.0025000
k( 26) = ( 0.0856164 0.0494307 0.0000000), wk = 0.0025000
k( 27) = ( 0.0890411 0.0514079 0.0000000), wk = 0.0025000
k( 28) = ( 0.0924658 0.0533851 0.0000000), wk = 0.0025000
k( 29) = ( 0.0958904 0.0553624 0.0000000), wk = 0.0025000
k( 30) = ( 0.0993151 0.0573396 0.0000000), wk = 0.0025000
k( 31) = ( 0.1027397 0.0593168 0.0000000), wk = 0.0025000
k( 32) = ( 0.1061644 0.0612940 0.0000000), wk = 0.0025000
k( 33) = ( 0.1095890 0.0632713 0.0000000), wk = 0.0025000
k( 34) = ( 0.1130137 0.0652485 0.0000000), wk = 0.0025000
k( 35) = ( 0.1164384 0.0672257 0.0000000), wk = 0.0025000
k( 36) = ( 0.1198630 0.0692029 0.0000000), wk = 0.0025000
k( 37) = ( 0.1232877 0.0711802 0.0000000), wk = 0.0025000
k( 38) = ( 0.1267123 0.0731574 0.0000000), wk = 0.0025000
k( 39) = ( 0.1301370 0.0751346 0.0000000), wk = 0.0025000
k( 40) = ( 0.1335616 0.0771119 0.0000000), wk = 0.0025000
k( 41) = ( 0.1369863 0.0790891 0.0000000), wk = 0.0025000
k( 42) = ( 0.1404110 0.0810663 0.0000000), wk = 0.0025000
k( 43) = ( 0.1438356 0.0830435 0.0000000), wk = 0.0025000
k( 44) = ( 0.1472603 0.0850208 0.0000000), wk = 0.0025000
k( 45) = ( 0.1506849 0.0869980 0.0000000), wk = 0.0025000
k( 46) = ( 0.1541096 0.0889752 0.0000000), wk = 0.0025000
k( 47) = ( 0.1575342 0.0909524 0.0000000), wk = 0.0025000
k( 48) = ( 0.1609589 0.0929297 0.0000000), wk = 0.0025000
k( 49) = ( 0.1643836 0.0949069 0.0000000), wk = 0.0025000
k( 50) = ( 0.1678082 0.0968841 0.0000000), wk = 0.0025000
k( 51) = ( 0.1712329 0.0988613 0.0000000), wk = 0.0025000
k( 52) = ( 0.1746575 0.1008386 0.0000000), wk = 0.0025000
k( 53) = ( 0.1780822 0.1028158 0.0000000), wk = 0.0025000
k( 54) = ( 0.1815068 0.1047930 0.0000000), wk = 0.0025000
k( 55) = ( 0.1849315 0.1067703 0.0000000), wk = 0.0025000
k( 56) = ( 0.1883562 0.1087475 0.0000000), wk = 0.0025000
k( 57) = ( 0.1917808 0.1107247 0.0000000), wk = 0.0025000
k( 58) = ( 0.1952055 0.1127019 0.0000000), wk = 0.0025000
k( 59) = ( 0.1986301 0.1146792 0.0000000), wk = 0.0025000
k( 60) = ( 0.2020548 0.1166564 0.0000000), wk = 0.0025000
k( 61) = ( 0.2054795 0.1186336 0.0000000), wk = 0.0025000
k( 62) = ( 0.2089041 0.1206108 0.0000000), wk = 0.0025000
k( 63) = ( 0.2123288 0.1225881 0.0000000), wk = 0.0025000
k( 64) = ( 0.2157534 0.1245653 0.0000000), wk = 0.0025000
k( 65) = ( 0.2191781 0.1265425 0.0000000), wk = 0.0025000
k( 66) = ( 0.2226027 0.1285198 0.0000000), wk = 0.0025000
k( 67) = ( 0.2260274 0.1304970 0.0000000), wk = 0.0025000
k( 68) = ( 0.2294521 0.1324742 0.0000000), wk = 0.0025000
k( 69) = ( 0.2328767 0.1344514 0.0000000), wk = 0.0025000
k( 70) = ( 0.2363014 0.1364287 0.0000000), wk = 0.0025000
k( 71) = ( 0.2397260 0.1384059 0.0000000), wk = 0.0025000
k( 72) = ( 0.2431507 0.1403831 0.0000000), wk = 0.0025000
k( 73) = ( 0.2465753 0.1423603 0.0000000), wk = 0.0025000
k( 74) = ( 0.2500000 0.1443376 0.0000000), wk = 0.0025000
k( 75) = ( 0.2534247 0.1463148 0.0000000), wk = 0.0025000
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k( 78) = ( 0.2636986 0.1522465 0.0000000), wk = 0.0025000
k( 79) = ( 0.2671233 0.1542237 0.0000000), wk = 0.0025000
k( 80) = ( 0.2705479 0.1562009 0.0000000), wk = 0.0025000
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k( 84) = (	0.2842466	0.1641098	0.0000000), wk =	0.0025000
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k( 86) = (	0.2910959	0.1680643	0.0000000), wk =	0.0025000
k( 87) = (	0.2945205	0.1700415	0.0000000), wk =	0.0025000
k( 88) = (	0.2979452	0.1720187	0.0000000), wk =	0.0025000
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k( 90) = (	0.3047945	0.1759732	0.0000000), wk =	0.0025000
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k( 94) = (	0.3184932	0.1838821	0.0000000), wk =	0.0025000
k( 95) = (	0.3219178	0.1858593	0.0000000), wk =	0.0025000
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k( 103) = (	0.3493151	0.2016771	0.0000000), wk =	0.0025000
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k( 119) = (	0.4041096	0.2333128	0.0000000), wk =	0.0025000
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k( 140) = (	0.4760274	0.2748345	0.0000000), wk =	0.0025000
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k( 151) = (	0.4920633	0.3024213	0.0000000), wk =	0.0025000
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k( 153) = (	0.4880950	0.3092944	0.0000000), wk =	0.0025000
k( 154) = (	0.4861108	0.3127309	0.0000000), wk =	0.0025000
k( 155) = (	0.4841267	0.3161675	0.0000000), wk =	0.0025000
k( 156) = (	0.4821425	0.3196040	0.0000000), wk =	0.0025000
k( 157) = (	0.4801583	0.3230405	0.0000000), wk =	0.0025000
k( 158) = (	0.4781742	0.3264771	0.0000000), wk =	0.0025000
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k( 161) = (	0.4722217	0.3367867	0.0000000), wk =	0.0025000
k( 162) = (	0.4702375	0.3402232	0.0000000), wk =	0.0025000
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k( 165) = (	0.4642850	0.3505329	0.0000000), wk =	0.0025000
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k( 168) = (	0.4583325	0.3608425	0.0000000), wk =	0.0025000
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k( 170) = (	0.4543642	0.3677156	0.0000000), wk =	0.0025000
k( 171) = (	0.4523800	0.3711521	0.0000000), wk =	0.0025000
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k( 180) = (	0.4345225	0.4020810	0.0000000), wk =	0.0025000
k( 181) = (	0.4325383	0.4055175	0.0000000), wk =	0.0025000
k( 182) = (	0.4305542	0.4089540	0.0000000), wk =	0.0025000
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k( 189) = (	0.4166650	0.4330098	0.0000000), wk =	0.0025000
k( 190) = (	0.4146808	0.4364464	0.0000000), wk =	0.0025000
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k( 192) = (	0.4107125	0.4433194	0.0000000), wk =	0.0025000
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k( 201) = (	0.3928550	0.4742483	0.0000000), wk =	0.0025000
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k( 206) = (	0.3829342	0.4914310	0.0000000), wk =	0.0025000
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k( 265) = (	0.2662695	0.4611923	0.0000000), wk =	0.0025000
k( 266) = (	0.2642972	0.4577761	0.0000000), wk =	0.0025000

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k( 278) = (	0.2406288	0.4167812	0.0000000), wk =	0.0025000
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k( 235) = ( 0.3254405 0.3254405 0.0000000), wk = 0.0025000
k( 236) = ( 0.3234682 0.3234682 0.0000000), wk = 0.0025000
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k( 322) = ( 0.1538446 0.1538446 0.0000000), wk = 0.0025000
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k( 360) = ( 0.0788947 0.0788947 0.0000000), wk = 0.0025000
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k( 362) = ( 0.0749499 0.0749499 0.0000000), wk = 0.0025000
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k( 399) = ( 0.0019724 0.0019724 0.0000000), wk = 0.0025000
k( 400) = ( 0.0000000 0.0000000 0.0000000), wk = 0.0025000

```

Dense grid: 42167 G-vectors FFT dimensions: ( 36, 36, 96)

Smooth grid: 10667 G-vectors FFT dimensions: ( 24, 24, 60)

Dynamical RAM for wfc: 0.16 MB

Dynamical RAM for wfc (w. buffer): 0.16 MB

Dynamical RAM for str. fact: 0.64 MB

Dynamical RAM for local pot: 0.00 MB

Dynamical RAM for nlocal pot: 0.33 MB

Dynamical RAM for grad: 0.36 MB

Dynamical RAM for rho,v,vnew: 9.56 MB

Dynamical RAM for G-vectors: 2.49 MB

Dynamical RAM for h,s,v(r/c): 0.05 MB

Dynamical RAM for <psi|beta>: 0.00 MB  
Dynamical RAM for psi: 0.65 MB  
Dynamical RAM for hpsi: 0.65 MB  
Dynamical RAM for spsi: 0.65 MB  
Dynamical RAM for wfcinit/wfcrot: 0.33 MB  
Dynamical RAM for addusdens: 29.60 MB  
Estimated static dynamical RAM per process > 20.52 MB  
Estimated max dynamical RAM per process > 50.12 MB  
Generating pointlists ...  
new r\_m : 0.2382 (alat units) 1.1074 (a.u.) for type 1  
  
The potential is recalculated from file :  
./tmp-hetero/A.save/charge-density  
  
Starting wfcs are 8 randomized atomic wfcs  
  
Band Structure Calculation  
Davidson diagonalization with overlap  
  
Computing kpt #: 1 of 800  
total cpu time spent up to now is 2.0 secs  
  
Computing kpt #: 2 of 800  
total cpu time spent up to now is 2.3 secs  
  
Computing kpt #: 3 of 800  
total cpu time spent up to now is 2.5 secs  
  
Computing kpt #: 4 of 800  
total cpu time spent up to now is 2.9 secs  
  
Computing kpt #: 5 of 800  
total cpu time spent up to now is 3.2 secs  
  
Computing kpt #: 6 of 800  
total cpu time spent up to now is 3.5 secs  
  
Computing kpt #: 7 of 800  
total cpu time spent up to now is 3.8 secs  
  
Computing kpt #: 8 of 800  
total cpu time spent up to now is 4.1 secs  
  
Computing kpt #: 9 of 800  
total cpu time spent up to now is 4.4 secs  
  
Computing kpt #: 10 of 800  
total cpu time spent up to now is 4.8 secs  
  
Computing kpt #: 11 of 800  
total cpu time spent up to now is 5.1 secs  
  
Computing kpt #: 12 of 800  
total cpu time spent up to now is 5.4 secs

Computing kpt #:	13	of	800	
total cpu time spent up to now is				5.7 secs
Computing kpt #:	14	of	800	
total cpu time spent up to now is				6.0 secs
Computing kpt #:	15	of	800	
total cpu time spent up to now is				6.3 secs
Computing kpt #:	16	of	800	
total cpu time spent up to now is				6.6 secs
Computing kpt #:	17	of	800	
total cpu time spent up to now is				6.9 secs
Computing kpt #:	18	of	800	
total cpu time spent up to now is				7.1 secs
Computing kpt #:	19	of	800	
total cpu time spent up to now is				7.3 secs
Computing kpt #:	20	of	800	
total cpu time spent up to now is				7.6 secs
Computing kpt #:	21	of	800	
total cpu time spent up to now is				7.9 secs
Computing kpt #:	22	of	800	
total cpu time spent up to now is				8.2 secs
Computing kpt #:	23	of	800	
total cpu time spent up to now is				8.5 secs
Computing kpt #:	24	of	800	
total cpu time spent up to now is				8.7 secs
Computing kpt #:	25	of	800	
total cpu time spent up to now is				9.1 secs
Computing kpt #:	26	of	800	
total cpu time spent up to now is				9.3 secs
Computing kpt #:	27	of	800	
total cpu time spent up to now is				9.6 secs
Computing kpt #:	28	of	800	
total cpu time spent up to now is				9.9 secs
Computing kpt #:	29	of	800	
total cpu time spent up to now is				10.1 secs
Computing kpt #:	30	of	800	
total cpu time spent up to now is				10.4 secs
Computing kpt #:	31	of	800	
total cpu time spent up to now is				10.6 secs
Computing kpt #:	32	of	800	
total cpu time spent up to now is				10.8 secs
Computing kpt #:	33	of	800	

---

total cpu time spent up to now is	11.1 secs
Computing kpt #: 34 of 800	
total cpu time spent up to now is	11.3 secs
Computing kpt #: 35 of 800	
total cpu time spent up to now is	11.5 secs
Computing kpt #: 36 of 800	
total cpu time spent up to now is	11.8 secs
Computing kpt #: 37 of 800	
total cpu time spent up to now is	12.0 secs
Computing kpt #: 38 of 800	
total cpu time spent up to now is	12.3 secs
Computing kpt #: 39 of 800	
total cpu time spent up to now is	12.6 secs
Computing kpt #: 40 of 800	
total cpu time spent up to now is	12.8 secs
Computing kpt #: 41 of 800	
total cpu time spent up to now is	13.1 secs
Computing kpt #: 42 of 800	
total cpu time spent up to now is	13.3 secs
Computing kpt #: 43 of 800	
total cpu time spent up to now is	13.6 secs
Computing kpt #: 44 of 800	
total cpu time spent up to now is	13.8 secs
Computing kpt #: 45 of 800	
total cpu time spent up to now is	14.2 secs
Computing kpt #: 46 of 800	
total cpu time spent up to now is	14.5 secs
Computing kpt #: 47 of 800	
total cpu time spent up to now is	14.8 secs
Computing kpt #: 48 of 800	
total cpu time spent up to now is	15.1 secs
Computing kpt #: 49 of 800	
total cpu time spent up to now is	15.4 secs
Computing kpt #: 50 of 800	
total cpu time spent up to now is	15.6 secs
Computing kpt #: 51 of 800	
total cpu time spent up to now is	15.9 secs
Computing kpt #: 52 of 800	
total cpu time spent up to now is	16.1 secs
Computing kpt #: 53 of 800	
total cpu time spent up to now is	16.4 secs

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Computing kpt #: 54 of 800	
total cpu time spent up to now is	16.6 secs
Computing kpt #: 55 of 800	
total cpu time spent up to now is	16.9 secs
Computing kpt #: 56 of 800	
total cpu time spent up to now is	17.2 secs
Computing kpt #: 57 of 800	
total cpu time spent up to now is	17.4 secs
Computing kpt #: 58 of 800	
total cpu time spent up to now is	17.7 secs
Computing kpt #: 59 of 800	
total cpu time spent up to now is	17.9 secs
Computing kpt #: 60 of 800	
total cpu time spent up to now is	18.2 secs
Computing kpt #: 61 of 800	
total cpu time spent up to now is	18.4 secs
Computing kpt #: 62 of 800	
total cpu time spent up to now is	18.7 secs
Computing kpt #: 63 of 800	
total cpu time spent up to now is	18.9 secs
Computing kpt #: 64 of 800	
total cpu time spent up to now is	19.1 secs
Computing kpt #: 65 of 800	
total cpu time spent up to now is	19.4 secs
Computing kpt #: 66 of 800	
total cpu time spent up to now is	19.6 secs
Computing kpt #: 67 of 800	
total cpu time spent up to now is	19.9 secs
Computing kpt #: 68 of 800	
total cpu time spent up to now is	20.1 secs
Computing kpt #: 69 of 800	
total cpu time spent up to now is	20.4 secs
Computing kpt #: 70 of 800	
total cpu time spent up to now is	20.6 secs
Computing kpt #: 71 of 800	
total cpu time spent up to now is	20.9 secs
Computing kpt #: 72 of 800	
total cpu time spent up to now is	21.1 secs
Computing kpt #: 73 of 800	
total cpu time spent up to now is	21.4 secs
Computing kpt #: 74 of 800	
total cpu time spent up to now is	21.6 secs



Computing kpt #: 75 of 800	
total cpu time spent up to now is	21.9 secs
Computing kpt #: 76 of 800	
total cpu time spent up to now is	22.1 secs
Computing kpt #: 77 of 800	
total cpu time spent up to now is	22.3 secs
Computing kpt #: 78 of 800	
total cpu time spent up to now is	22.5 secs
Computing kpt #: 79 of 800	
total cpu time spent up to now is	22.8 secs
Computing kpt #: 80 of 800	
total cpu time spent up to now is	23.0 secs
Computing kpt #: 81 of 800	
total cpu time spent up to now is	23.3 secs
Computing kpt #: 82 of 800	
total cpu time spent up to now is	23.5 secs
Computing kpt #: 83 of 800	
total cpu time spent up to now is	23.7 secs
Computing kpt #: 84 of 800	
total cpu time spent up to now is	24.0 secs
Computing kpt #: 85 of 800	
total cpu time spent up to now is	24.3 secs
Computing kpt #: 86 of 800	
total cpu time spent up to now is	24.5 secs
Computing kpt #: 87 of 800	
total cpu time spent up to now is	24.8 secs
Computing kpt #: 88 of 800	
total cpu time spent up to now is	25.0 secs
Computing kpt #: 89 of 800	
total cpu time spent up to now is	25.3 secs
Computing kpt #: 90 of 800	
total cpu time spent up to now is	25.5 secs
Computing kpt #: 91 of 800	
total cpu time spent up to now is	25.8 secs
Computing kpt #: 92 of 800	
total cpu time spent up to now is	26.0 secs
Computing kpt #: 93 of 800	
total cpu time spent up to now is	26.3 secs
Computing kpt #: 94 of 800	
total cpu time spent up to now is	26.5 secs
Computing kpt #: 95 of 800	

total cpu time spent up to now is	26.7 secs
Computing kpt #: 96 of 800	
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Computing kpt #: 116 of 800 total cpu time spent up to now is	32.1 secs
Computing kpt #: 117 of 800 total cpu time spent up to now is	32.3 secs
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Computing kpt #: 302 of 800 total cpu time spent up to now is	89.4 secs
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total cpu time spent up to now is	117.5 secs
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Computing kpt #: 407 of 800	
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Computing kpt #: 695 of 800	
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total cpu time spent up to now is	209.0 secs
Computing kpt #: 726 of 800	
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total cpu time spent up to now is	210.6 secs
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Computing kpt #: 736 of 800 total cpu time spent up to now is	211.9 secs
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total cpu time spent up to now is	223.0 secs
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total cpu time spent up to now is	227.8 secs
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total cpu time spent up to now is	228.4 secs
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total cpu time spent up to now is	229.0 secs

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total cpu time spent up to now is 229.2 secs

Computing kpt #: 799 of 800  
total cpu time spent up to now is 229.4 secs

Computing kpt #: 800 of 800  
total cpu time spent up to now is 229.7 secs

ethr = 1.25E-10, avg # of iterations = 18.7

total cpu time spent up to now is 229.7 secs

End of band structure calculation

----- SPIN UP -----

k = 0.0000 0.0000 0.0000 ( 1301 PWs)	bands (ev):
-18.6337 -6.7492 -2.1631 -2.1631 3.7766	7.1287 9.2231 9.2231
k = 0.0034 0.0020 0.0000 ( 1301 PWs)	bands (ev):
-18.6334 -6.7488 -2.1642 -2.1637 3.7770	7.1291 9.2231 9.2243
k = 0.0068 0.0040 0.0000 ( 1301 PWs)	bands (ev):
-18.6326 -6.7478 -2.1677 -2.1655 3.7781	7.1302 9.2232 9.2279
k = 0.0103 0.0059 0.0000 ( 1301 PWs)	bands (ev):
-18.6312 -6.7462 -2.1735 -2.1686 3.7800	7.1320 9.2234 9.2340
k = 0.0137 0.0079 0.0000 ( 1301 PWs)	bands (ev):
-18.6292 -6.7438 -2.1815 -2.1729 3.7827	7.1345 9.2236 9.2426
k = 0.0171 0.0099 0.0000 ( 1301 PWs)	bands (ev):
-18.6267 -6.7408 -2.1918 -2.1784 3.7861	7.1378 9.2240 9.2535
k = 0.0205 0.0119 0.0000 ( 1301 PWs)	bands (ev):
-18.6237 -6.7372 -2.2044 -2.1851 3.7902	7.1418 9.2244 9.2669
k = 0.0240 0.0138 0.0000 ( 1297 PWs)	bands (ev):
-18.6201 -6.7328 -2.2193 -2.1931 3.7952	7.1465 9.2250 9.2827
k = 0.0274 0.0158 0.0000 ( 1297 PWs)	bands (ev):
-18.6159 -6.7279 -2.2364 -2.2022 3.8008	7.1519 9.2256 9.3009
k = 0.0308 0.0178 0.0000 ( 1293 PWs)	bands (ev):
-18.6112 -6.7222 -2.2557 -2.2124 3.8073	7.1581 9.2265 9.3214
k = 0.0342 0.0198 0.0000 ( 1293 PWs)	bands (ev):
-18.6059 -6.7159 -2.2772 -2.2238 3.8144	7.1650 9.2274 9.3443

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k = 0.0377 0.0217 0.0000 ( 1293 PWs)	bands (ev):
-18.6001 -6.7089 -2.3010 -2.2364 3.8224	7.1726 9.2285 9.3696
k = 0.0411 0.0237 0.0000 ( 1293 PWs)	bands (ev):
-18.5937 -6.7012 -2.3268 -2.2501 3.8311	7.1809 9.2297 9.3972
k = 0.0445 0.0257 0.0000 ( 1297 PWs)	bands (ev):
-18.5867 -6.6929 -2.3548 -2.2649 3.8405	7.1900 9.2311 9.4271
k = 0.0479 0.0277 0.0000 ( 1297 PWs)	bands (ev):
-18.5793 -6.6840 -2.3850 -2.2808 3.8508	7.1997 9.2326 9.4593
k = 0.0514 0.0297 0.0000 ( 1295 PWs)	bands (ev):
-18.5712 -6.6743 -2.4171 -2.2977 3.8617	7.2102 9.2343 9.4937
k = 0.0548 0.0316 0.0000 ( 1295 PWs)	bands (ev):
-18.5626 -6.6640 -2.4513 -2.3157 3.8735	7.2215 9.2361 9.5304
k = 0.0582 0.0336 0.0000 ( 1295 PWs)	bands (ev):
-18.5534 -6.6531 -2.4875 -2.3347 3.8859	7.2334 9.2380 9.5692
k = 0.0616 0.0356 0.0000 ( 1295 PWs)	bands (ev):
-18.5437 -6.6414 -2.5257 -2.3546 3.8992	7.2461 9.2400 9.5986
k = 0.0651 0.0376 0.0000 ( 1299 PWs)	bands (ev):
-18.5335 -6.6292 -2.5659 -2.3756 3.9132	7.2595 9.2420 9.6144
k = 0.0685 0.0395 0.0000 ( 1299 PWs)	bands (ev):
-18.5227 -6.6162 -2.6079 -2.3974 3.9279	7.2736 9.2441 9.6308
k = 0.0719 0.0415 0.0000 ( 1299 PWs)	bands (ev):
-18.5113 -6.6026 -2.6518 -2.4202 3.9434	7.2884 9.2463 9.6478
k = 0.0753 0.0435 0.0000 ( 1297 PWs)	bands (ev):
-18.4994 -6.5883 -2.6975 -2.4439 3.9597	7.3039 9.2484 9.6654
k = 0.0788 0.0455 0.0000 ( 1301 PWs)	bands (ev):
-18.4869 -6.5734 -2.7451 -2.4684 3.9767	7.3202 9.2505 9.6837
k = 0.0822 0.0475 0.0000 ( 1301 PWs)	bands (ev):
-18.4739 -6.5578 -2.7943 -2.4937 3.9945	7.3372 9.2526 9.7025
k = 0.0856 0.0494 0.0000 ( 1301 PWs)	bands (ev):
-18.4603 -6.5416 -2.8452 -2.5198 4.0130	7.3549 9.2546 9.7219
k = 0.0890 0.0514 0.0000 ( 1305 PWs)	bands (ev):

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-18.4461	-6.5247	-2.8978	-2.5468	4.0323	7.3733	9.2565	9.7419
k = 0.0925 0.0534 0.0000 ( 1305 PWs)					bands (ev):		
-18.4314	-6.5071	-2.9520	-2.5744	4.0524	7.3924	9.2583	9.7624
k = 0.0959 0.0554 0.0000 ( 1305 PWs)					bands (ev):		
-18.4162	-6.4889	-3.0078	-2.6027	4.0732	7.4123	9.2600	9.7836
k = 0.0993 0.0573 0.0000 ( 1299 PWs)					bands (ev):		
-18.4004	-6.4701	-3.0650	-2.6317	4.0948	7.4328	9.2614	9.8053
k = 0.1027 0.0593 0.0000 ( 1301 PWs)					bands (ev):		
-18.3841	-6.4506	-3.1238	-2.6613	4.1171	7.4541	9.2627	9.8276
k = 0.1062 0.0613 0.0000 ( 1305 PWs)					bands (ev):		
-18.3672	-6.4304	-3.1841	-2.6915	4.1402	7.4761	9.2637	9.8505
k = 0.1096 0.0633 0.0000 ( 1309 PWs)					bands (ev):		
-18.3497	-6.4096	-3.2458	-2.7224	4.1640	7.4987	9.2644	9.8739
k = 0.1130 0.0652 0.0000 ( 1309 PWs)					bands (ev):		
-18.3317	-6.3881	-3.3088	-2.7538	4.1886	7.5221	9.2649	9.8980
k = 0.1164 0.0672 0.0000 ( 1309 PWs)					bands (ev):		
-18.3132	-6.3660	-3.3732	-2.7857	4.2139	7.5462	9.2650	9.9227
k = 0.1199 0.0692 0.0000 ( 1309 PWs)					bands (ev):		
-18.2941	-6.3432	-3.4388	-2.8181	4.2400	7.5710	9.2649	9.9480
k = 0.1233 0.0712 0.0000 ( 1309 PWs)					bands (ev):		
-18.2745	-6.3198	-3.5057	-2.8510	4.2669	7.5965	9.2644	9.9739
k = 0.1267 0.0732 0.0000 ( 1313 PWs)					bands (ev):		
-18.2543	-6.2958	-3.5738	-2.8844	4.2945	7.6227	9.2635	10.0004
k = 0.1301 0.0751 0.0000 ( 1313 PWs)					bands (ev):		
-18.2335	-6.2711	-3.6430	-2.9181	4.3229	7.6496	9.2623	10.0276
k = 0.1336 0.0771 0.0000 ( 1321 PWs)					bands (ev):		
-18.2123	-6.2457	-3.7134	-2.9523	4.3520	7.6771	9.2606	10.0554
k = 0.1370 0.0791 0.0000 ( 1321 PWs)					bands (ev):		
-18.1904	-6.2197	-3.7848	-2.9868	4.3819	7.7054	9.2586	10.0838
k = 0.1404 0.0811 0.0000 ( 1321 PWs)					bands (ev):		
-18.1680	-6.1931	-3.8574	-3.0216	4.4126	7.7343	9.2561	10.1129

k = 0.1438 0.0830 0.0000 ( 1319 PWs) bands (ev):  
-18.1451 -6.1658 -3.9309 -3.0567 4.4440 7.7639 9.2533 10.1426

k = 0.1473 0.0850 0.0000 ( 1319 PWs) bands (ev):  
-18.1216 -6.1379 -4.0053 -3.0921 4.4761 7.7942 9.2500 10.1730

k = 0.1507 0.0870 0.0000 ( 1319 PWs) bands (ev):  
-18.0976 -6.1094 -4.0808 -3.1278 4.5090 7.8252 9.2463 10.2041

k = 0.1541 0.0890 0.0000 ( 1319 PWs) bands (ev):  
-18.0731 -6.0802 -4.1571 -3.1637 4.5427 7.8568 9.2422 10.2358

k = 0.1575 0.0910 0.0000 ( 1319 PWs) bands (ev):  
-18.0479 -6.0504 -4.2343 -3.1998 4.5771 7.8891 9.2376 10.2682

k = 0.1610 0.0929 0.0000 ( 1319 PWs) bands (ev):  
-18.0223 -6.0199 -4.3124 -3.2360 4.6123 7.9220 9.2326 10.3013

k = 0.1644 0.0949 0.0000 ( 1323 PWs) bands (ev):  
-17.9961 -5.9889 -4.3913 -3.2725 4.6482 7.9555 9.2272 10.3351

k = 0.1678 0.0969 0.0000 ( 1323 PWs) bands (ev):  
-17.9693 -5.9572 -4.4709 -3.3090 4.6849 7.9897 9.2214 10.2665

k = 0.1712 0.0989 0.0000 ( 1323 PWs) bands (ev):  
-17.9421 -5.9248 -4.5513 -3.3457 4.7223 8.0244 9.2152 10.1897

k = 0.1747 0.1008 0.0000 ( 1323 PWs) bands (ev):  
-17.9142 -5.8919 -4.6324 -3.3825 4.7605 8.0598 9.2085 10.1120

k = 0.1781 0.1028 0.0000 ( 1323 PWs) bands (ev):  
-17.8859 -5.8583 -4.7141 -3.4193 4.7995 8.0956 9.2015 10.0336

k = 0.1815 0.1048 0.0000 ( 1323 PWs) bands (ev):  
-17.8570 -5.8241 -4.7965 -3.4563 4.8392 8.1320 9.1941 9.9544

k = 0.1849 0.1068 0.0000 ( 1319 PWs) bands (ev):  
-17.8275 -5.7893 -4.8795 -3.4932 4.8796 8.1689 9.1863 9.8746

k = 0.1884 0.1087 0.0000 ( 1321 PWs) bands (ev):  
-17.7975 -5.7538 -4.9632 -3.5302 4.9208 8.2062 9.1781 9.7942

k = 0.1918 0.1107 0.0000 ( 1321 PWs) bands (ev):  
-17.7670 -5.7178 -5.0473 -3.5671 4.9628 8.2438 9.1696 9.7134

k = 0.1952 0.1127 0.0000 ( 1317 PWs) bands (ev):

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-17.7359	-5.6811	-5.1320	-3.6041	5.0055	8.2816	9.1608	9.6323
k = 0.1986 0.1147 0.0000 ( 1317 PWs)					bands (ev):		
-17.7043	-5.6439	-5.2172	-3.6410	5.0489	8.3195	9.1516	9.5510
k = 0.2021 0.1167 0.0000 ( 1317 PWs)					bands (ev):		
-17.6721	-5.6060	-5.3029	-3.6778	5.0932	8.3573	9.1421	9.4698
k = 0.2055 0.1186 0.0000 ( 1319 PWs)					bands (ev):		
-17.6395	-5.5676	-5.3891	-3.7145	5.1381	8.3946	9.1323	9.3891
k = 0.2089 0.1206 0.0000 ( 1319 PWs)					bands (ev):		
-17.6062	-5.5285	-5.4756	-3.7512	5.1838	8.4310	9.1223	9.3093
k = 0.2123 0.1226 0.0000 ( 1317 PWs)					bands (ev):		
-17.5725	-5.5626	-5.4889	-3.7877	5.2303	8.4656	9.1119	9.2312
k = 0.2158 0.1246 0.0000 ( 1321 PWs)					bands (ev):		
-17.5382	-5.6499	-5.4486	-3.8242	5.2775	8.4973	9.1014	9.1563
k = 0.2192 0.1265 0.0000 ( 1321 PWs)					bands (ev):		
-17.5034	-5.7377	-5.4078	-3.8605	5.3255	8.5236	9.0866	9.0905
k = 0.2226 0.1285 0.0000 ( 1321 PWs)					bands (ev):		
-17.4681	-5.8257	-5.3664	-3.8966	5.3742	8.5410	9.0261	9.0795
k = 0.2260 0.1305 0.0000 ( 1321 PWs)					bands (ev):		
-17.4322	-5.9141	-5.3243	-3.9326	5.4237	8.5439	8.9801	9.0682
k = 0.2295 0.1325 0.0000 ( 1321 PWs)					bands (ev):		
-17.3958	-6.0028	-5.2818	-3.9684	5.4739	8.5268	8.9544	9.0567
k = 0.2329 0.1345 0.0000 ( 1321 PWs)					bands (ev):		
-17.3588	-6.0917	-5.2386	-4.0040	5.5248	8.4878	8.9506	9.0451
k = 0.2363 0.1364 0.0000 ( 1321 PWs)					bands (ev):		
-17.3214	-6.1809	-5.1949	-4.0394	5.5766	8.4310	8.9649	9.0333
k = 0.2397 0.1384 0.0000 ( 1325 PWs)					bands (ev):		
-17.2834	-6.2704	-5.1506	-4.0746	5.6290	8.3619	8.9917	9.0213
k = 0.2432 0.1404 0.0000 ( 1325 PWs)					bands (ev):		
-17.2448	-6.3601	-5.1057	-4.1095	5.6822	8.2850	9.0092	9.0265
k = 0.2466 0.1424 0.0000 ( 1325 PWs)					bands (ev):		
-17.2058	-6.4499	-5.0603	-4.1442	5.7362	8.2031	8.9969	9.0666



k = 0.2500 0.1443 0.0000 ( 1325 PWs)	bands (ev):
-17.1662 -6.5399 -5.0143 -4.1787 5.7909	8.1179 8.9846 9.1102
k = 0.2534 0.1463 0.0000 ( 1325 PWs)	bands (ev):
-17.1261 -6.6301 -4.9678 -4.2129 5.8463	8.0304 8.9722 9.1565
k = 0.2568 0.1483 0.0000 ( 1325 PWs)	bands (ev):
-17.0855 -6.7204 -4.9207 -4.2468 5.9025	7.9412 8.9597 9.2048
k = 0.2603 0.1503 0.0000 ( 1325 PWs)	bands (ev):
-17.0444 -6.8109 -4.8731 -4.2804 5.9594	7.8507 8.9471 9.2547
k = 0.2637 0.1522 0.0000 ( 1323 PWs)	bands (ev):
-17.0027 -6.9014 -4.8249 -4.3137 6.0171	7.7593 8.9345 9.3060
k = 0.2671 0.1542 0.0000 ( 1315 PWs)	bands (ev):
-16.9605 -6.9921 -4.7762 -4.3467 6.0755	7.6670 8.9218 9.3585
k = 0.2705 0.1562 0.0000 ( 1315 PWs)	bands (ev):
-16.9178 -7.0828 -4.7270 -4.3794 6.1347	7.5740 8.9091 9.4121
k = 0.2740 0.1582 0.0000 ( 1315 PWs)	bands (ev):
-16.8746 -7.1736 -4.6773 -4.4118 6.1946	7.4805 8.8963 9.4666
k = 0.2774 0.1602 0.0000 ( 1319 PWs)	bands (ev):
-16.8309 -7.2644 -4.6271 -4.4439 6.2552	7.3866 8.8836 9.5221
k = 0.2808 0.1621 0.0000 ( 1319 PWs)	bands (ev):
-16.7866 -7.3553 -4.5764 -4.4756 6.3165	7.2923 8.8709 9.5784
k = 0.2842 0.1641 0.0000 ( 1319 PWs)	bands (ev):
-16.7419 -7.4462 -4.5252 -4.5070 6.3786	7.1976 8.8582 9.6356
k = 0.2877 0.1661 0.0000 ( 1319 PWs)	bands (ev):
-16.6966 -7.5371 -4.5380 -4.4735 6.4415	7.1027 8.8455 9.6936
k = 0.2911 0.1681 0.0000 ( 1319 PWs)	bands (ev):
-16.6509 -7.6279 -4.5686 -4.4213 6.5050	7.0076 8.8328 9.7523
k = 0.2945 0.1700 0.0000 ( 1319 PWs)	bands (ev):
-16.6046 -7.7188 -4.5989 -4.3687 6.5693	6.9123 8.8203 9.8118
k = 0.2979 0.1720 0.0000 ( 1319 PWs)	bands (ev):
-16.5578 -7.8096 -4.6288 -4.3156 6.6344	6.8168 8.8077 9.8720
k = 0.3014 0.1740 0.0000 ( 1322 PWs)	bands (ev):

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-16.5105	-7.9004	-4.6583	-4.2620	6.7001	6.7213	8.7953	9.9329
k = 0.3048 0.1760 0.0000 ( 1322 PWs)				bands (ev):			
-16.4627	-7.9911	-4.6874	-4.2080	6.6257	6.7666	8.7829	9.9945
k = 0.3082 0.1780 0.0000 ( 1322 PWs)				bands (ev):			
-16.4144	-8.0817	-4.7161	-4.1536	6.5300	6.8338	8.7707	10.0568
k = 0.3116 0.1799 0.0000 ( 1322 PWs)				bands (ev):			
-16.3656	-8.1722	-4.7444	-4.0987	6.4344	6.9017	8.7585	10.1198
k = 0.3151 0.1819 0.0000 ( 1322 PWs)				bands (ev):			
-16.3163	-8.2627	-4.7722	-4.0435	6.3388	6.9703	8.7465	10.1834
k = 0.3185 0.1839 0.0000 ( 1326 PWs)				bands (ev):			
-16.2666	-8.3530	-4.7997	-3.9879	6.2432	7.0396	8.7346	10.2477
k = 0.3219 0.1859 0.0000 ( 1326 PWs)				bands (ev):			
-16.2163	-8.4432	-4.8267	-3.9318	6.1478	7.1096	8.7228	10.3126
k = 0.3253 0.1878 0.0000 ( 1322 PWs)				bands (ev):			
-16.1655	-8.5332	-4.8533	-3.8754	6.0525	7.1803	8.7113	10.3782
k = 0.3288 0.1898 0.0000 ( 1330 PWs)				bands (ev):			
-16.1143	-8.6232	-4.8795	-3.8187	5.9573	7.2517	8.6999	10.4444
k = 0.3322 0.1918 0.0000 ( 1330 PWs)				bands (ev):			
-16.0626	-8.7129	-4.9052	-3.7616	5.8624	7.3238	8.6887	10.5113
k = 0.3356 0.1938 0.0000 ( 1330 PWs)				bands (ev):			
-16.0104	-8.8025	-4.9305	-3.7041	5.7676	7.3965	8.6777	10.5787
k = 0.3390 0.1957 0.0000 ( 1326 PWs)				bands (ev):			
-15.9577	-8.8919	-4.9553	-3.6464	5.6732	7.4699	8.6669	10.6468
k = 0.3425 0.1977 0.0000 ( 1330 PWs)				bands (ev):			
-15.9045	-8.9812	-4.9797	-3.5884	5.5789	7.5439	8.6565	10.7154
k = 0.3459 0.1997 0.0000 ( 1326 PWs)				bands (ev):			
-15.8509	-9.0702	-5.0036	-3.5301	5.4851	7.6184	8.6463	10.7847
k = 0.3493 0.2017 0.0000 ( 1326 PWs)				bands (ev):			
-15.7968	-9.1590	-5.0270	-3.4715	5.3915	7.6935	8.6365	10.8545
k = 0.3527 0.2037 0.0000 ( 1326 PWs)				bands (ev):			
-15.7422	-9.2476	-5.0499	-3.4128	5.2984	7.7691	8.6271	10.9249

k = 0.3562 0.2056 0.0000 ( 1326 PWs) bands (ev):  
-15.6872 -9.3360 -5.0724 -3.3538 5.2057 7.8451 8.6183 10.9959

k = 0.3596 0.2076 0.0000 ( 1326 PWs) bands (ev):  
-15.6317 -9.4241 -5.0944 -3.2947 5.1135 7.9213 8.6100 11.0674

k = 0.3630 0.2096 0.0000 ( 1326 PWs) bands (ev):  
-15.5757 -9.5119 -5.1160 -3.2354 5.0217 7.9976 8.6027 11.1395

k = 0.3664 0.2116 0.0000 ( 1326 PWs) bands (ev):  
-15.5194 -9.5995 -5.1370 -3.1760 4.9305 8.0736 8.5965 11.2121

k = 0.3699 0.2135 0.0000 ( 1326 PWs) bands (ev):  
-15.4625 -9.6868 -5.1576 -3.1165 4.8399 8.1488 8.5921 11.2853

k = 0.3733 0.2155 0.0000 ( 1326 PWs) bands (ev):  
-15.4053 -9.7738 -5.1776 -3.0569 4.7499 8.2222 8.5904 11.3590

k = 0.3767 0.2175 0.0000 ( 1324 PWs) bands (ev):  
-15.3476 -9.8605 -5.1972 -2.9973 4.6605 8.2916 8.5936 11.4332

k = 0.3801 0.2195 0.0000 ( 1328 PWs) bands (ev):  
-15.2895 -9.9470 -5.2162 -2.9377 4.5719 8.3534 8.6053 11.5079

k = 0.3836 0.2214 0.0000 ( 1328 PWs) bands (ev):  
-15.2309 -10.0330 -5.2348 -2.8782 4.4841 8.4019 8.6314 11.5830

k = 0.3870 0.2234 0.0000 ( 1328 PWs) bands (ev):  
-15.1720 -10.1188 -5.2528 -2.8188 4.3971 8.4328 8.6759 11.6587

k = 0.3904 0.2254 0.0000 ( 1328 PWs) bands (ev):  
-15.1127 -10.2041 -5.2704 -2.7595 4.3109 8.4484 8.7366 11.7348

k = 0.3938 0.2274 0.0000 ( 1332 PWs) bands (ev):  
-15.0530 -10.2892 -5.2874 -2.7004 4.2257 8.4546 8.8078 11.8114

k = 0.3973 0.2294 0.0000 ( 1328 PWs) bands (ev):  
-14.9929 -10.3738 -5.3039 -2.6415 4.1415 8.4555 8.8851 11.8884

k = 0.4007 0.2313 0.0000 ( 1328 PWs) bands (ev):  
-14.9324 -10.4580 -5.3199 -2.5830 4.0583 8.4537 8.9662 11.9658

k = 0.4041 0.2333 0.0000 ( 1328 PWs) bands (ev):  
-14.8716 -10.5418 -5.3354 -2.5248 3.9763 8.4502 9.0497 12.0436

k = 0.4075 0.2353 0.0000 ( 1328 PWs) bands (ev):

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-14.8104	-10.6252	-5.3503	-2.4671	3.8954	8.4460	9.1351	12.1217
k = 0.4110 0.2373 0.0000 ( 1324 PWs)					bands (ev):		
-14.7489	-10.7081	-5.3647	-2.4097	3.8159	8.4412	9.2219	12.2003
k = 0.4144 0.2392 0.0000 ( 1324 PWs)					bands (ev):		
-14.6872	-10.7905	-5.3786	-2.3531	3.7377	8.4361	9.3099	12.2791
k = 0.4178 0.2412 0.0000 ( 1324 PWs)					bands (ev):		
-14.6251	-10.8725	-5.3920	-2.2971	3.6610	8.4309	9.3990	12.3583
k = 0.4212 0.2432 0.0000 ( 1324 PWs)					bands (ev):		
-14.5628	-10.9539	-5.4048	-2.2418	3.5858	8.4257	9.4891	12.4377
k = 0.4247 0.2452 0.0000 ( 1324 PWs)					bands (ev):		
-14.5003	-11.0347	-5.4171	-2.1874	3.5122	8.4206	9.5800	12.5174
k = 0.4281 0.2472 0.0000 ( 1322 PWs)					bands (ev):		
-14.4376	-11.1149	-5.4289	-2.1339	3.4404	8.4156	9.6718	12.5973
k = 0.4315 0.2491 0.0000 ( 1322 PWs)					bands (ev):		
-14.3747	-11.1945	-5.4401	-2.0815	3.3705	8.4106	9.7644	12.6773
k = 0.4349 0.2511 0.0000 ( 1326 PWs)					bands (ev):		
-14.3118	-11.2734	-5.4508	-2.0302	3.3025	8.4059	9.8578	12.7575
k = 0.4384 0.2531 0.0000 ( 1326 PWs)					bands (ev):		
-14.2488	-11.3515	-5.4610	-1.9802	3.2367	8.4013	9.9520	12.8377
k = 0.4418 0.2551 0.0000 ( 1326 PWs)					bands (ev):		
-14.1858	-11.4288	-5.4706	-1.9316	3.1731	8.3969	10.0469	12.9178
k = 0.4452 0.2570 0.0000 ( 1326 PWs)					bands (ev):		
-14.1229	-11.5052	-5.4797	-1.8846	3.1119	8.3927	10.1425	12.9979
k = 0.4486 0.2590 0.0000 ( 1326 PWs)					bands (ev):		
-14.0602	-11.5806	-5.4882	-1.8393	3.0533	8.3888	10.2388	13.0778
k = 0.4521 0.2610 0.0000 ( 1334 PWs)					bands (ev):		
-13.9978	-11.6549	-5.4962	-1.7959	2.9973	8.3850	10.3359	13.1574
k = 0.4555 0.2630 0.0000 ( 1338 PWs)					bands (ev):		
-13.9359	-11.7279	-5.5037	-1.7544	2.9442	8.3815	10.4336	13.1947
k = 0.4589 0.2649 0.0000 ( 1330 PWs)					bands (ev):		
-13.8746	-11.7995	-5.5106	-1.7151	2.8941	8.3782	10.5319	13.0827

k = 0.4623 0.2669 0.0000 ( 1330 PWs) bands (ev):  
-13.8141 -11.8693 -5.5169 -1.6781 2.8471 8.3752 10.6309 12.9710

k = 0.4658 0.2689 0.0000 ( 1330 PWs) bands (ev):  
-13.7549 -11.9372 -5.5227 -1.6436 2.8036 8.3725 10.7306 12.8598

k = 0.4692 0.2709 0.0000 ( 1332 PWs) bands (ev):  
-13.6971 -12.0029 -5.5279 -1.6118 2.7635 8.3700 10.8308 12.7489

k = 0.4726 0.2729 0.0000 ( 1336 PWs) bands (ev):  
-13.6413 -12.0657 -5.5327 -1.5828 2.7271 8.3677 10.9317 12.6386

k = 0.4760 0.2748 0.0000 ( 1336 PWs) bands (ev):  
-13.5881 -12.1251 -5.5368 -1.5568 2.6946 8.3657 11.0331 12.5288

k = 0.4795 0.2768 0.0000 ( 1336 PWs) bands (ev):  
-13.5381 -12.1804 -5.5404 -1.5339 2.6660 8.3640 11.1350 12.4196

k = 0.4829 0.2788 0.0000 ( 1332 PWs) bands (ev):  
-13.4925 -12.2306 -5.5434 -1.5142 2.6416 8.3625 11.2372 12.3111

k = 0.4863 0.2808 0.0000 ( 1332 PWs) bands (ev):  
-13.4522 -12.2746 -5.5459 -1.4980 2.6214 8.3613 11.3397 12.2035

k = 0.4897 0.2827 0.0000 ( 1332 PWs) bands (ev):  
-13.4186 -12.3110 -5.5478 -1.4852 2.6056 8.3604 11.4420 12.0973

k = 0.4932 0.2847 0.0000 ( 1332 PWs) bands (ev):  
-13.3933 -12.3384 -5.5492 -1.4761 2.5943 8.3597 11.5429 11.9936

k = 0.4966 0.2867 0.0000 ( 1332 PWs) bands (ev):  
-13.3774 -12.3556 -5.5500 -1.4705 2.5874 8.3593 11.6377 11.8970

k = 0.5000 0.2887 0.0000 ( 1332 PWs) bands (ev):  
-13.3719 -12.3614 -5.5503 -1.4687 2.5852 8.3592 11.6929 11.8412

k = 0.4980 0.2921 0.0000 ( 1332 PWs) bands (ev):  
-13.3717 -12.3612 -5.5516 -1.4684 2.5851 8.3609 11.6933 11.8416

k = 0.4960 0.2955 0.0000 ( 1332 PWs) bands (ev):  
-13.3710 -12.3604 -5.5554 -1.4673 2.5848 8.3660 11.6943 11.8426

k = 0.4940 0.2990 0.0000 ( 1332 PWs) bands (ev):  
-13.3698 -12.3592 -5.5616 -1.4656 2.5845 8.3744 11.6960 11.8444

k = 0.4921 0.3024 0.0000 ( 1332 PWs) bands (ev):

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-13.3681	-12.3576	-5.5704	-1.4632	2.5839	8.3863	11.6983	11.8469
k = 0.4901 0.3059 0.0000 ( 1336 PWs)					bands (ev):		
-13.3660	-12.3554	-5.5817	-1.4602	2.5832	8.4015	11.7014	11.8501
k = 0.4881 0.3093 0.0000 ( 1336 PWs)					bands (ev):		
-13.3633	-12.3528	-5.5955	-1.4564	2.5823	8.4200	11.7051	11.8540
k = 0.4861 0.3127 0.0000 ( 1328 PWs)					bands (ev):		
-13.3602	-12.3497	-5.6116	-1.4520	2.5813	8.4420	11.7095	11.8587
k = 0.4841 0.3162 0.0000 ( 1328 PWs)					bands (ev):		
-13.3567	-12.3461	-5.6302	-1.4469	2.5800	8.4671	11.7146	11.8640
k = 0.4821 0.3196 0.0000 ( 1329 PWs)					bands (ev):		
-13.3526	-12.3421	-5.6512	-1.4411	2.5786	8.4955	11.7203	11.8701
k = 0.4802 0.3230 0.0000 ( 1327 PWs)					bands (ev):		
-13.3481	-12.3375	-5.6745	-1.4346	2.5770	8.5272	11.7268	11.8768
k = 0.4782 0.3265 0.0000 ( 1327 PWs)					bands (ev):		
-13.3430	-12.3325	-5.7001	-1.4274	2.5753	8.5620	11.7339	11.8843
k = 0.4762 0.3299 0.0000 ( 1329 PWs)					bands (ev):		
-13.3376	-12.3271	-5.7281	-1.4196	2.5733	8.5999	11.7416	11.8925
k = 0.4742 0.3334 0.0000 ( 1329 PWs)					bands (ev):		
-13.3316	-12.3211	-5.7583	-1.4110	2.5711	8.6409	11.7501	11.9014
k = 0.4722 0.3368 0.0000 ( 1329 PWs)					bands (ev):		
-13.3251	-12.3147	-5.7907	-1.4018	2.5687	8.6850	11.7592	11.9110
k = 0.4702 0.3402 0.0000 ( 1335 PWs)					bands (ev):		
-13.3182	-12.3079	-5.8252	-1.3919	2.5660	8.7320	11.7689	11.9213
k = 0.4683 0.3437 0.0000 ( 1335 PWs)					bands (ev):		
-13.3108	-12.3005	-5.8618	-1.3814	2.5632	8.7820	11.7794	11.9323
k = 0.4663 0.3471 0.0000 ( 1335 PWs)					bands (ev):		
-13.3029	-12.2927	-5.9004	-1.3701	2.5600	8.8349	11.7905	11.9440
k = 0.4643 0.3505 0.0000 ( 1335 PWs)					bands (ev):		
-13.2946	-12.2845	-5.9411	-1.3582	2.5567	8.8906	11.8022	11.9565
k = 0.4623 0.3540 0.0000 ( 1335 PWs)					bands (ev):		
-13.2857	-12.2758	-5.9836	-1.3456	2.5530	8.9490	11.8147	11.9696

k = 0.4603 0.3574 0.0000 ( 1331 PWs) bands (ev):  
-13.2764 -12.2666 -6.0280 -1.3323 2.5491 9.0102 11.8278 11.9834

k = 0.4583 0.3608 0.0000 ( 1333 PWs) bands (ev):  
-13.2666 -12.2570 -6.0744 -1.3183 2.5449 9.0739 11.8415 11.9980

k = 0.4563 0.3643 0.0000 ( 1341 PWs) bands (ev):  
-13.2564 -12.2469 -6.1224 -1.3037 2.5404 9.1402 11.8559 12.0132

k = 0.4544 0.3677 0.0000 ( 1341 PWs) bands (ev):  
-13.2456 -12.2364 -6.1721 -1.2884 2.5355 9.2090 11.8709 12.0291

k = 0.4524 0.3712 0.0000 ( 1341 PWs) bands (ev):  
-13.2344 -12.2254 -6.2235 -1.2724 2.5303 9.2802 11.8866 12.0457

k = 0.4504 0.3746 0.0000 ( 1341 PWs) bands (ev):  
-13.2227 -12.2140 -6.2764 -1.2557 2.5248 9.3538 11.9030 12.0631

k = 0.4484 0.3780 0.0000 ( 1341 PWs) bands (ev):  
-13.2105 -12.2022 -6.3309 -1.2383 2.5189 9.4297 11.9200 12.0811

k = 0.4464 0.3815 0.0000 ( 1341 PWs) bands (ev):  
-13.1979 -12.1900 -6.3868 -1.2203 2.5125 9.5078 11.9376 12.0998

k = 0.4444 0.3849 0.0000 ( 1341 PWs) bands (ev):  
-13.1847 -12.1773 -6.4442 -1.2016 2.5058 9.5880 11.9559 12.1192

k = 0.4425 0.3883 0.0000 ( 1341 PWs) bands (ev):  
-13.1711 -12.1642 -6.5028 -1.1822 2.4987 9.6703 11.9748 12.1392

k = 0.4405 0.3918 0.0000 ( 1341 PWs) bands (ev):  
-13.1571 -12.1507 -6.5628 -1.1621 2.4911 9.7546 11.9943 12.1600

k = 0.4385 0.3952 0.0000 ( 1341 PWs) bands (ev):  
-13.1425 -12.1368 -6.6240 -1.1414 2.4830 9.8408 12.0144 12.1815

k = 0.4365 0.3986 0.0000 ( 1341 PWs) bands (ev):  
-13.1275 -12.1224 -6.6863 -1.1200 2.4745 9.9288 12.0352 12.2036

k = 0.4345 0.4021 0.0000 ( 1341 PWs) bands (ev):  
-13.1120 -12.1077 -6.7498 -1.0979 2.4654 10.0186 12.0566 12.2264

k = 0.4325 0.4055 0.0000 ( 1341 PWs) bands (ev):  
-13.0960 -12.0926 -6.8142 -1.0751 2.4558 10.1101 12.0786 12.2499

k = 0.4306 0.4090 0.0000 ( 1347 PWs) bands (ev):

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-13.0795	-12.0772	-6.8798	-1.0517	2.4457	10.2032	12.1012	12.2741
k = 0.4286 0.4124 0.0000 ( 1339 PWs) bands (ev):							
-13.0626	-12.0613	-6.9461	-1.0276	2.4350	10.2979	12.1244	12.2990
k = 0.4266 0.4158 0.0000 ( 1339 PWs) bands (ev):							
-13.0452	-12.0451	-7.0134	-1.0028	2.4237	10.3940	12.1482	12.3245
k = 0.4246 0.4193 0.0000 ( 1335 PWs) bands (ev):							
-13.0273	-12.0286	-7.0815	-0.9773	2.4118	10.4915	12.1726	12.3507
k = 0.4226 0.4227 0.0000 ( 1335 PWs) bands (ev):							
-13.0089	-12.0117	-7.1503	-0.9512	2.3993	10.5903	12.1975	12.3776
k = 0.4206 0.4261 0.0000 ( 1335 PWs) bands (ev):							
-12.9901	-11.9944	-7.2199	-0.9245	2.3861	10.6903	12.2231	12.4051
k = 0.4186 0.4296 0.0000 ( 1335 PWs) bands (ev):							
-12.9708	-11.9769	-7.2900	-0.8970	2.3722	10.7913	12.2492	12.4333
k = 0.4167 0.4330 0.0000 ( 1335 PWs) bands (ev):							
-12.9510	-11.9591	-7.3608	-0.8689	2.3577	10.8935	12.2758	12.4622
k = 0.4147 0.4364 0.0000 ( 1335 PWs) bands (ev):							
-12.9307	-11.9410	-7.4321	-0.8401	2.3424	10.9965	12.3031	12.4918
k = 0.4127 0.4399 0.0000 ( 1337 PWs) bands (ev):							
-12.9100	-11.9226	-7.5039	-0.8106	2.3263	11.1004	12.3308	12.5220
k = 0.4107 0.4433 0.0000 ( 1337 PWs) bands (ev):							
-12.8888	-11.9039	-7.5760	-0.7805	2.3095	11.2050	12.3591	12.5530
k = 0.4087 0.4468 0.0000 ( 1337 PWs) bands (ev):							
-12.8671	-11.8851	-7.6486	-0.7497	2.2919	11.3103	12.3879	12.5846
k = 0.4067 0.4502 0.0000 ( 1341 PWs) bands (ev):							
-12.8449	-11.8660	-7.7214	-0.7183	2.2735	11.4161	12.4172	12.6082
k = 0.4048 0.4536 0.0000 ( 1349 PWs) bands (ev):							
-12.8223	-11.8468	-7.7946	-0.6862	2.2542	11.5222	12.4470	12.5609
k = 0.4028 0.4571 0.0000 ( 1349 PWs) bands (ev):							
-12.7992	-11.8274	-7.8678	-0.6534	2.2341	11.6286	12.4773	12.5141
k = 0.4008 0.4605 0.0000 ( 1349 PWs) bands (ev):							
-12.7756	-11.8078	-7.9412	-0.6200	2.2131	11.7351	12.4678	12.5081



k = 0.3988 0.4639 0.0000 ( 1345 PWs) bands (ev):  
-12.7516 -11.7882 -8.0146 -0.5859 2.1912 11.8416 12.4221 12.5393

k = 0.3968 0.4674 0.0000 ( 1345 PWs) bands (ev):  
-12.7271 -11.7685 -8.0879 -0.5512 2.1684 11.9478 12.3771 12.5709

k = 0.3948 0.4708 0.0000 ( 1345 PWs) bands (ev):  
-12.7021 -11.7488 -8.1612 -0.5158 2.1447 12.0536 12.3328 12.6030

k = 0.3929 0.4742 0.0000 ( 1341 PWs) bands (ev):  
-12.6766 -11.7292 -8.2344 -0.4797 2.1200 12.1586 12.2893 12.6355

k = 0.3909 0.4777 0.0000 ( 1347 PWs) bands (ev):  
-12.6506 -11.7096 -8.3073 -0.4430 2.0944 12.2468 12.2626 12.6684

k = 0.3889 0.4811 0.0000 ( 1347 PWs) bands (ev):  
-12.6242 -11.6901 -8.3799 -0.4056 2.0677 12.2052 12.3652 12.7017

k = 0.3869 0.4846 0.0000 ( 1347 PWs) bands (ev):  
-12.5973 -11.6708 -8.4521 -0.3676 2.0401 12.1646 12.4659 12.7353

k = 0.3849 0.4880 0.0000 ( 1347 PWs) bands (ev):  
-12.5700 -11.6518 -8.5238 -0.3289 2.0115 12.1251 12.5641 12.7692

k = 0.3829 0.4914 0.0000 ( 1347 PWs) bands (ev):  
-12.5422 -11.6331 -8.5949 -0.2896 1.9818 12.0868 12.6592 12.8035

k = 0.3810 0.4949 0.0000 ( 1347 PWs) bands (ev):  
-12.5139 -11.6148 -8.6652 -0.2496 1.9511 12.0497 12.7501 12.8380

k = 0.3790 0.4983 0.0000 ( 1335 PWs) bands (ev):  
-12.4851 -11.5970 -8.7348 -0.2089 1.9194 12.0139 12.8359 12.8728

k = 0.3770 0.5017 0.0000 ( 1335 PWs) bands (ev):  
-12.4558 -11.5798 -8.8035 -0.1676 1.8865 11.9794 12.9078 12.9156

k = 0.3750 0.5052 0.0000 ( 1335 PWs) bands (ev):  
-12.4261 -11.5633 -8.8710 -0.1257 1.8527 11.9462 12.9430 12.9885

k = 0.3730 0.5086 0.0000 ( 1335 PWs) bands (ev):  
-12.3959 -11.5477 -8.9374 -0.0832 1.8178 11.9145 12.9783 13.0546

k = 0.3710 0.5121 0.0000 ( 1335 PWs) bands (ev):  
-12.3653 -11.5330 -9.0023 -0.0399 1.7818 11.8841 13.0138 13.1145

k = 0.3690 0.5155 0.0000 ( 1335 PWs) bands (ev):

-12.3342 -11.5195 -9.0658 0.0039 1.7447 11.8553 13.0494 13.1693  
k = 0.3671 0.5189 0.0000 ( 1335 PWs) bands (ev):

-12.3026 -11.5073 -9.1274 0.0484 1.7066 11.8279 13.0850 13.2200  
k = 0.3651 0.5224 0.0000 ( 1343 PWs) bands (ev):

-12.2706 -11.4966 -9.1872 0.0935 1.6673 11.8021 13.1206 13.2675  
k = 0.3631 0.5258 0.0000 ( 1343 PWs) bands (ev):

-12.2380 -11.4876 -9.2448 0.1392 1.6271 11.7778 13.1561 13.3125  
k = 0.3611 0.5292 0.0000 ( 1347 PWs) bands (ev):

-12.2051 -11.4805 -9.3000 0.1856 1.5857 11.7551 13.1916 13.3554  
k = 0.3591 0.5327 0.0000 ( 1343 PWs) bands (ev):

-12.1716 -11.4755 -9.3526 0.2327 1.5433 11.7339 13.2269 13.3965  
k = 0.3571 0.5361 0.0000 ( 1343 PWs) bands (ev):

-12.1377 -11.4729 -9.4023 0.2803 1.4999 11.7144 13.2620 13.4360  
k = 0.3552 0.5395 0.0000 ( 1343 PWs) bands (ev):

-12.1033 -11.4729 -9.4489 0.3286 1.4554 11.6965 13.2969 13.4738  
k = 0.3532 0.5430 0.0000 ( 1343 PWs) bands (ev):

-12.0684 -11.4757 -9.4921 0.3776 1.4099 11.6801 13.3314 13.5098  
k = 0.3512 0.5464 0.0000 ( 1343 PWs) bands (ev):

-12.0331 -11.4816 -9.5317 0.4271 1.3633 11.6654 13.3656 13.5439  
k = 0.3492 0.5499 0.0000 ( 1343 PWs) bands (ev):

-11.9973 -11.4907 -9.5675 0.4773 1.3158 11.6523 13.3993 13.5756  
k = 0.3472 0.5533 0.0000 ( 1343 PWs) bands (ev):

-11.9611 -11.5034 -9.5992 0.5281 1.2672 11.6407 13.4325 13.6045  
k = 0.3452 0.5567 0.0000 ( 1355 PWs) bands (ev):

-11.9244 -11.5196 -9.6268 0.5795 1.2176 11.6308 13.4652 13.6299  
k = 0.3433 0.5602 0.0000 ( 1355 PWs) bands (ev):

-11.8872 -11.5395 -9.6500 0.6315 1.1672 11.6225 13.4971 13.6509  
k = 0.3413 0.5636 0.0000 ( 1359 PWs) bands (ev):

-11.8496 -11.5632 -9.6689 0.6842 1.1157 11.6157 13.5283 13.6665  
k = 0.3393 0.5670 0.0000 ( 1363 PWs) bands (ev):

-11.8115 -11.5906 -9.6835 0.7374 1.0634 11.6104 13.5587 13.6752

k = 0.3373 0.5705 0.0000 ( 1365 PWs) bands (ev):  
-11.7729 -11.6217 -9.6938 0.7913 1.0101 11.6067 13.5882 13.6753

k = 0.3353 0.5739 0.0000 ( 1365 PWs) bands (ev):  
-11.7339 -11.6563 -9.6998 0.8458 0.9560 11.6045 13.6167 13.6654

k = 0.3333 0.5773 0.0000 ( 1365 PWs) bands (ev):  
-11.6944 -11.6943 -9.7018 0.9009 0.9010 11.6038 13.6442 13.6443

k = 0.3314 0.5739 0.0000 ( 1365 PWs) bands (ev):  
-11.7355 -11.6546 -9.6999 0.8454 0.9564 11.6045 13.6117 13.6705

k = 0.3294 0.5705 0.0000 ( 1365 PWs) bands (ev):  
-11.7795 -11.6144 -9.6944 0.7891 1.0124 11.6066 13.5682 13.6954

k = 0.3274 0.5671 0.0000 ( 1357 PWs) bands (ev):  
-11.8264 -11.5738 -9.6853 0.7320 1.0690 11.6101 13.5146 13.7191

k = 0.3254 0.5637 0.0000 ( 1355 PWs) bands (ev):  
-11.8757 -11.5328 -9.6731 0.6742 1.1262 11.6148 13.4524 13.7415

k = 0.3235 0.5603 0.0000 ( 1347 PWs) bands (ev):  
-11.9274 -11.4912 -9.6579 0.6156 1.1840 11.6209 13.3828 13.7625

k = 0.3215 0.5568 0.0000 ( 1347 PWs) bands (ev):  
-11.9813 -11.4492 -9.6399 0.5564 1.2423 11.6281 13.3070 13.7820

k = 0.3195 0.5534 0.0000 ( 1351 PWs) bands (ev):  
-12.0370 -11.4068 -9.6193 0.4964 1.3013 11.6366 13.2262 13.8000

k = 0.3176 0.5500 0.0000 ( 1351 PWs) bands (ev):  
-12.0944 -11.3640 -9.5964 0.4358 1.3608 11.6461 13.1412 13.8164

k = 0.3156 0.5466 0.0000 ( 1355 PWs) bands (ev):  
-12.1533 -11.3206 -9.5712 0.3746 1.4209 11.6567 13.0528 13.8313

k = 0.3136 0.5432 0.0000 ( 1355 PWs) bands (ev):  
-12.2136 -11.2769 -9.5440 0.3128 1.4815 11.6682 12.9615 13.8445

k = 0.3116 0.5398 0.0000 ( 1351 PWs) bands (ev):  
-12.2751 -11.2327 -9.5149 0.2504 1.5428 11.6807 12.8680 13.8561

k = 0.3097 0.5363 0.0000 ( 1351 PWs) bands (ev):  
-12.3375 -11.1880 -9.4840 0.1875 1.6046 11.6941 12.7726 13.8661

k = 0.3077 0.5329 0.0000 ( 1351 PWs) bands (ev):

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-12.4009	-11.1429	-9.4515	0.1240	1.6670	11.7082	12.6757	13.8744
k = 0.3057 0.5295 0.0000 ( 1351 PWs) bands (ev):							
-12.4651	-11.0974	-9.4176	0.0601	1.7299	11.7230	12.5775	13.8811
k = 0.3037 0.5261 0.0000 ( 1351 PWs) bands (ev):							
-12.5300	-11.0514	-9.3822	-0.0044	1.7934	11.7383	12.4784	13.8862
k = 0.3018 0.5227 0.0000 ( 1351 PWs) bands (ev):							
-12.5954	-11.0050	-9.3455	-0.0692	1.8575	11.7542	12.3784	13.8897
k = 0.2998 0.5193 0.0000 ( 1351 PWs) bands (ev):							
-12.6614	-10.9581	-9.3076	-0.1345	1.9221	11.7704	12.2779	13.8916
k = 0.2978 0.5159 0.0000 ( 1351 PWs) bands (ev):							
-12.7278	-10.9108	-9.2685	-0.2002	1.9873	11.7870	12.1769	13.8921
k = 0.2959 0.5124 0.0000 ( 1355 PWs) bands (ev):							
-12.7945	-10.8630	-9.2284	-0.2662	2.0530	11.8037	12.0756	13.8910
k = 0.2939 0.5090 0.0000 ( 1355 PWs) bands (ev):							
-12.8614	-10.8148	-9.1873	-0.3326	2.1193	11.8204	11.9741	13.8885
k = 0.2919 0.5056 0.0000 ( 1351 PWs) bands (ev):							
-12.9287	-10.7662	-9.1451	-0.3993	2.1861	11.8370	11.8725	13.8847
k = 0.2899 0.5022 0.0000 ( 1351 PWs) bands (ev):							
-12.9960	-10.7171	-9.1021	-0.4662	2.2535	11.7709	11.8534	13.8796
k = 0.2880 0.4988 0.0000 ( 1351 PWs) bands (ev):							
-13.0635	-10.6676	-9.0583	-0.5335	2.3214	11.6693	11.8694	13.8731
k = 0.2860 0.4954 0.0000 ( 1351 PWs) bands (ev):							
-13.1311	-10.6177	-9.0136	-0.6009	2.3898	11.5679	11.8849	13.8655
k = 0.2840 0.4919 0.0000 ( 1351 PWs) bands (ev):							
-13.1987	-10.5674	-8.9681	-0.6686	2.4588	11.4666	11.8996	13.8567
k = 0.2820 0.4885 0.0000 ( 1351 PWs) bands (ev):							
-13.2663	-10.5166	-8.9219	-0.7365	2.5283	11.3656	11.9135	13.8469
k = 0.2801 0.4851 0.0000 ( 1351 PWs) bands (ev):							
-13.3339	-10.4653	-8.8750	-0.8045	2.5983	11.2648	11.9263	13.8360
k = 0.2781 0.4817 0.0000 ( 1355 PWs) bands (ev):							
-13.4014	-10.4137	-8.8274	-0.8728	2.6688	11.1644	11.9378	13.8241

k = 0.2761 0.4783 0.0000 ( 1355 PWs) bands (ev):  
-13.4688 -10.3616 -8.7792 -0.9411 2.7398 11.0643 11.9479 13.8060

k = 0.2742 0.4749 0.0000 ( 1355 PWs) bands (ev):  
-13.5361 -10.3091 -8.7304 -1.0095 2.8114 10.9646 11.9563 13.7614

k = 0.2722 0.4714 0.0000 ( 1355 PWs) bands (ev):  
-13.6032 -10.2562 -8.6809 -1.0780 2.8834 10.8653 11.9629 13.7155

k = 0.2702 0.4680 0.0000 ( 1353 PWs) bands (ev):  
-13.6702 -10.2028 -8.6308 -1.1466 2.9559 10.7665 11.9674 13.6683

k = 0.2682 0.4646 0.0000 ( 1353 PWs) bands (ev):  
-13.7370 -10.1491 -8.5802 -1.2152 3.0290 10.6681 11.9698 13.6199

k = 0.2663 0.4612 0.0000 ( 1353 PWs) bands (ev):  
-13.8036 -10.0949 -8.5291 -1.2838 3.1025 10.5702 11.9697 13.5704

k = 0.2643 0.4578 0.0000 ( 1357 PWs) bands (ev):  
-13.8700 -10.0403 -8.4775 -1.3525 3.1765 10.4728 11.9671 13.5200

k = 0.2623 0.4544 0.0000 ( 1357 PWs) bands (ev):  
-13.9361 -9.9853 -8.4253 -1.4211 3.2510 10.3760 11.9618 13.4687

k = 0.2604 0.4509 0.0000 ( 1357 PWs) bands (ev):  
-14.0020 -9.9298 -8.3727 -1.4897 3.3260 10.2796 11.9537 13.4166

k = 0.2584 0.4475 0.0000 ( 1357 PWs) bands (ev):  
-14.0676 -9.8740 -8.3196 -1.5582 3.4014 10.1839 11.9427 13.3638

k = 0.2564 0.4441 0.0000 ( 1357 PWs) bands (ev):  
-14.1329 -9.8177 -8.2661 -1.6267 3.4773 10.0887 11.9287 13.3104

k = 0.2544 0.4407 0.0000 ( 1361 PWs) bands (ev):  
-14.1979 -9.7611 -8.2121 -1.6951 3.5537 9.9940 11.9117 13.2563

k = 0.2525 0.4373 0.0000 ( 1349 PWs) bands (ev):  
-14.2626 -9.7039 -8.1576 -1.7633 3.6305 9.9000 11.8917 13.2018

k = 0.2505 0.4339 0.0000 ( 1349 PWs) bands (ev):  
-14.3270 -9.6465 -8.1028 -1.8315 3.7078 9.8066 11.8686 13.1469

k = 0.2485 0.4304 0.0000 ( 1349 PWs) bands (ev):  
-14.3911 -9.5886 -8.0476 -1.8995 3.7855 9.7138 11.8426 13.0915

k = 0.2465 0.4270 0.0000 ( 1349 PWs) bands (ev):

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-14.4548	-9.5303	-7.9920	-1.9674	3.8636	9.6216	11.8137	13.0359
k = 0.2446 0.4236 0.0000 ( 1345 PWs)					bands (ev):		
-14.5182	-9.4716	-7.9360	-2.0351	3.9422	9.5300	11.7819	12.9799
k = 0.2426 0.4202 0.0000 ( 1345 PWs)					bands (ev):		
-14.5813	-9.4126	-7.8797	-2.1026	4.0212	9.4390	11.7475	12.9238
k = 0.2406 0.4168 0.0000 ( 1345 PWs)					bands (ev):		
-14.6440	-9.3531	-7.8230	-2.1699	4.1006	9.3487	11.7105	12.8675
k = 0.2387 0.4134 0.0000 ( 1341 PWs)					bands (ev):		
-14.7063	-9.2933	-7.7659	-2.2371	4.1804	9.2591	11.6710	12.8110
k = 0.2367 0.4099 0.0000 ( 1341 PWs)					bands (ev):		
-14.7682	-9.2330	-7.7086	-2.3040	4.2606	9.1701	11.6293	12.7544
k = 0.2347 0.4065 0.0000 ( 1341 PWs)					bands (ev):		
-14.8297	-9.1724	-7.6509	-2.3706	4.3412	9.0818	11.5855	12.6978
k = 0.2327 0.4031 0.0000 ( 1341 PWs)					bands (ev):		
-14.8909	-9.1114	-7.5929	-2.4370	4.4223	8.9941	11.5397	12.6412
k = 0.2308 0.3997 0.0000 ( 1341 PWs)					bands (ev):		
-14.9517	-9.0500	-7.5346	-2.5032	4.5036	8.9071	11.4920	12.5846
k = 0.2288 0.3963 0.0000 ( 1337 PWs)					bands (ev):		
-15.0120	-8.9883	-7.4761	-2.5691	4.5854	8.8208	11.4428	12.5280
k = 0.2268 0.3929 0.0000 ( 1333 PWs)					bands (ev):		
-15.0720	-8.9261	-7.4172	-2.6347	4.6675	8.7351	11.3920	12.4715
k = 0.2248 0.3895 0.0000 ( 1333 PWs)					bands (ev):		
-15.1315	-8.8636	-7.3581	-2.7000	4.7500	8.6502	11.3398	12.4151
k = 0.2229 0.3860 0.0000 ( 1333 PWs)					bands (ev):		
-15.1906	-8.8008	-7.2987	-2.7650	4.8328	8.5659	11.2864	12.3589
k = 0.2209 0.3826 0.0000 ( 1327 PWs)					bands (ev):		
-15.2493	-8.7375	-7.2391	-2.8297	4.9160	8.4823	11.2319	12.3028
k = 0.2189 0.3792 0.0000 ( 1323 PWs)					bands (ev):		
-15.3076	-8.6739	-7.1792	-2.8941	4.9996	8.3994	11.1765	12.2468
k = 0.2170 0.3758 0.0000 ( 1323 PWs)					bands (ev):		
-15.3654	-8.6100	-7.1192	-2.9581	5.0834	8.3172	11.1202	12.1911

k = 0.2150 0.3724 0.0000 ( 1323 PWs) bands (ev):  
-15.4229 -8.5457 -7.0589 -3.0218 5.1676 8.2357 11.0631 12.1356

k = 0.2130 0.3690 0.0000 ( 1323 PWs) bands (ev):  
-15.4798 -8.4811 -6.9984 -3.0851 5.2520 8.1549 11.0054 12.0804

k = 0.2110 0.3655 0.0000 ( 1329 PWs) bands (ev):  
-15.5363 -8.4161 -6.9378 -3.1481 5.3368 8.0748 10.9471 12.0254

k = 0.2091 0.3621 0.0000 ( 1329 PWs) bands (ev):  
-15.5924 -8.3508 -6.8769 -3.2107 5.4218 7.9954 10.8883 11.9707

k = 0.2071 0.3587 0.0000 ( 1329 PWs) bands (ev):  
-15.6480 -8.2851 -6.8159 -3.2729 5.5071 7.9167 10.8292 11.9163

k = 0.2051 0.3553 0.0000 ( 1329 PWs) bands (ev):  
-15.7032 -8.2192 -6.7547 -3.3347 5.5927 7.8388 10.7698 11.8622

k = 0.2032 0.3519 0.0000 ( 1329 PWs) bands (ev):  
-15.7579 -8.1528 -6.6934 -3.3961 5.6786 7.7615 10.7101 11.8084

k = 0.2012 0.3485 0.0000 ( 1329 PWs) bands (ev):  
-15.8122 -8.0862 -6.6319 -3.4572 5.7647 7.6850 10.6503 11.7550

k = 0.1992 0.3450 0.0000 ( 1329 PWs) bands (ev):  
-15.8659 -8.0193 -6.5703 -3.5178 5.8510 7.6092 10.5903 11.7020

k = 0.1972 0.3416 0.0000 ( 1331 PWs) bands (ev):  
-15.9193 -7.9520 -6.5085 -3.5779 5.9376 7.5341 10.5303 11.6493

k = 0.1953 0.3382 0.0000 ( 1331 PWs) bands (ev):  
-15.9721 -7.8844 -6.4467 -3.6377 6.0244 7.4597 10.4702 11.5971

k = 0.1933 0.3348 0.0000 ( 1331 PWs) bands (ev):  
-16.0245 -7.8166 -6.3848 -3.6970 6.1114 7.3860 10.4102 11.5452

k = 0.1913 0.3314 0.0000 ( 1331 PWs) bands (ev):  
-16.0764 -7.7484 -6.3228 -3.7558 6.1986 7.3131 10.3503 11.4938

k = 0.1893 0.3280 0.0000 ( 1337 PWs) bands (ev):  
-16.1278 -7.6800 -6.2607 -3.8143 6.2859 7.2409 10.2906 11.4427

k = 0.1874 0.3245 0.0000 ( 1337 PWs) bands (ev):  
-16.1787 -7.6112 -6.1985 -3.8722 6.3735 7.1694 10.2309 11.3921

k = 0.1854 0.3211 0.0000 ( 1337 PWs) bands (ev):

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-16.2292	-7.5422	-6.1363	-3.9297	6.4612	7.0986	10.1715	11.3420
k = 0.1834 0.3177 0.0000 ( 1337 PWs) bands (ev):							
-16.2792	-7.4729	-6.0741	-3.9867	6.5490	7.0286	10.1123	11.2923
k = 0.1815 0.3143 0.0000 ( 1337 PWs) bands (ev):							
-16.3286	-7.4033	-6.0118	-4.0433	6.6369	6.9593	10.0534	11.2431
k = 0.1795 0.3109 0.0000 ( 1329 PWs) bands (ev):							
-16.3776	-7.3335	-5.9495	-4.0993	6.7250	6.8907	9.9947	11.1944
k = 0.1775 0.3075 0.0000 ( 1329 PWs) bands (ev):							
-16.4261	-7.2634	-5.8872	-4.1549	6.8132	6.8229	9.9364	11.1462
k = 0.1755 0.3040 0.0000 ( 1333 PWs) bands (ev):							
-16.4741	-7.1931	-5.8249	-4.2100	6.7558	6.9014	9.8784	11.0985
k = 0.1736 0.3006 0.0000 ( 1331 PWs) bands (ev):							
-16.5216	-7.1225	-5.7626	-4.2646	6.6894	6.9898	9.8208	11.0513
k = 0.1716 0.2972 0.0000 ( 1335 PWs) bands (ev):							
-16.5687	-7.0517	-5.7003	-4.3186	6.6238	7.0782	9.7635	11.0045
k = 0.1696 0.2938 0.0000 ( 1335 PWs) bands (ev):							
-16.6152	-6.9807	-5.6382	-4.3722	6.5589	7.1666	9.7066	10.9584
k = 0.1677 0.2904 0.0000 ( 1335 PWs) bands (ev):							
-16.6612	-6.9095	-5.5760	-4.4253	6.4948	7.2550	9.6502	10.9127
k = 0.1657 0.2870 0.0000 ( 1335 PWs) bands (ev):							
-16.7067	-6.8381	-5.5140	-4.4778	6.4313	7.3435	9.5942	10.8676
k = 0.1637 0.2835 0.0000 ( 1335 PWs) bands (ev):							
-16.7517	-6.7664	-5.4520	-4.5298	6.3687	7.4319	9.5386	10.8231
k = 0.1617 0.2801 0.0000 ( 1335 PWs) bands (ev):							
-16.7962	-6.6946	-5.3901	-4.5813	6.3067	7.5204	9.4836	10.7790
k = 0.1598 0.2767 0.0000 ( 1333 PWs) bands (ev):							
-16.8402	-6.6226	-5.3283	-4.6322	6.2455	7.6087	9.4290	10.7356
k = 0.1578 0.2733 0.0000 ( 1333 PWs) bands (ev):							
-16.8837	-6.5505	-5.2667	-4.6827	6.1850	7.6971	9.3749	10.6927
k = 0.1558 0.2699 0.0000 ( 1333 PWs) bands (ev):							
-16.9266	-6.4781	-5.2052	-4.7325	6.1253	7.7853	9.3213	10.6504



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k = 0.1538 0.2665 0.0000 ( 1333 PWs)	bands (ev):
-16.9691 -6.4057 -5.1438 -4.7819 6.0663	7.8735 9.2682 10.6086
k = 0.1519 0.2631 0.0000 ( 1327 PWs)	bands (ev):
-17.0110 -6.3331 -5.0826 -4.8306 6.0081	7.9615 9.2156 10.5675
k = 0.1499 0.2596 0.0000 ( 1327 PWs)	bands (ev):
-17.0525 -6.2603 -5.0216 -4.8789 5.9506	8.0494 9.1636 10.5269
k = 0.1479 0.2562 0.0000 ( 1335 PWs)	bands (ev):
-17.0934 -6.1875 -4.9608 -4.9266 5.8939	8.1372 9.1121 10.4869
k = 0.1460 0.2528 0.0000 ( 1327 PWs)	bands (ev):
-17.1338 -6.1145 -4.9737 -4.9001 5.8379	8.2248 9.0612 10.4476
k = 0.1440 0.2494 0.0000 ( 1327 PWs)	bands (ev):
-17.1737 -6.0415 -5.0202 -4.8397 5.7826	8.3122 9.0109 10.4088
k = 0.1420 0.2460 0.0000 ( 1327 PWs)	bands (ev):
-17.2130 -5.9683 -5.0662 -4.7796 5.7281	8.3993 8.9611 10.3706
k = 0.1400 0.2426 0.0000 ( 1327 PWs)	bands (ev):
-17.2519 -5.8951 -5.1116 -4.7198 5.6743	8.4863 8.9119 10.3331
k = 0.1381 0.2391 0.0000 ( 1331 PWs)	bands (ev):
-17.2902 -5.8219 -5.1565 -4.6602 5.6213	8.5729 8.8633 10.2961
k = 0.1361 0.2357 0.0000 ( 1327 PWs)	bands (ev):
-17.3280 -5.7486 -5.2007 -4.6008 5.5690	8.6593 8.8153 10.2597
k = 0.1341 0.2323 0.0000 ( 1327 PWs)	bands (ev):
-17.3652 -5.6753 -5.2444 -4.5418 5.5175	8.7454 8.7679 10.2240
k = 0.1321 0.2289 0.0000 ( 1327 PWs)	bands (ev):
-17.4020 -5.6020 -5.2875 -4.4831 5.4667	8.7211 8.8312 10.1890
k = 0.1302 0.2255 0.0000 ( 1327 PWs)	bands (ev):
-17.4382 -5.5287 -5.3300 -4.4248 5.4166	8.6749 8.9166 10.1545
k = 0.1282 0.2221 0.0000 ( 1327 PWs)	bands (ev):
-17.4739 -5.4554 -5.3719 -4.3668 5.3674	8.6294 9.0016 10.1207
k = 0.1262 0.2186 0.0000 ( 1323 PWs)	bands (ev):
-17.5091 -5.4133 -5.3821 -4.3092 5.3188	8.5844 9.0863 10.0875
k = 0.1243 0.2152 0.0000 ( 1323 PWs)	bands (ev):

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-17.5437	-5.4540	-5.3089	-4.2519	5.2710	8.5401	9.1705	10.0550
k = 0.1223 0.2118 0.0000 ( 1327 PWs)					bands (ev):		
-17.5778	-5.4942	-5.2358	-4.1951	5.2240	8.4965	9.2542	10.0231
k = 0.1203 0.2084 0.0000 ( 1327 PWs)					bands (ev):		
-17.6114	-5.5338	-5.1628	-4.1387	5.1777	8.4534	9.3375	9.9918
k = 0.1183 0.2050 0.0000 ( 1327 PWs)					bands (ev):		
-17.6444	-5.5727	-5.0900	-4.0827	5.1321	8.4110	9.4203	9.9612
k = 0.1164 0.2016 0.0000 ( 1327 PWs)					bands (ev):		
-17.6769	-5.6111	-5.0172	-4.0272	5.0874	8.3693	9.5026	9.9313
k = 0.1144 0.1981 0.0000 ( 1327 PWs)					bands (ev):		
-17.7089	-5.6488	-4.9446	-3.9722	5.0433	8.3282	9.5843	9.9020
k = 0.1124 0.1947 0.0000 ( 1331 PWs)					bands (ev):		
-17.7404	-5.6859	-4.8722	-3.9176	5.0000	8.2877	9.6654	9.8733
k = 0.1105 0.1913 0.0000 ( 1331 PWs)					bands (ev):		
-17.7713	-5.7225	-4.8000	-3.8636	4.9575	8.2480	9.7459	9.8453
k = 0.1085 0.1879 0.0000 ( 1331 PWs)					bands (ev):		
-17.8016	-5.7584	-4.7280	-3.8101	4.9157	8.2088	9.8180	9.8257
k = 0.1065 0.1845 0.0000 ( 1327 PWs)					bands (ev):		
-17.8315	-5.7937	-4.6563	-3.7571	4.8746	8.1704	9.7913	9.9050
k = 0.1045 0.1811 0.0000 ( 1323 PWs)					bands (ev):		
-17.8608	-5.8283	-4.5848	-3.7046	4.8344	8.1326	9.7652	9.9835
k = 0.1026 0.1776 0.0000 ( 1323 PWs)					bands (ev):		
-17.8896	-5.8624	-4.5136	-3.6527	4.7948	8.0955	9.7398	10.0612
k = 0.1006 0.1742 0.0000 ( 1323 PWs)					bands (ev):		
-17.9178	-5.8958	-4.4428	-3.6015	4.7560	8.0590	9.7151	10.1383
k = 0.0986 0.1708 0.0000 ( 1323 PWs)					bands (ev):		
-17.9455	-5.9287	-4.3723	-3.5509	4.7180	8.0232	9.6910	10.2145
k = 0.0966 0.1674 0.0000 ( 1319 PWs)					bands (ev):		
-17.9726	-5.9609	-4.3022	-3.5008	4.6807	7.9881	9.6676	10.2899
k = 0.0947 0.1640 0.0000 ( 1319 PWs)					bands (ev):		
-17.9992	-5.9924	-4.2325	-3.4515	4.6442	7.9537	9.6449	10.3645

k = 0.0927 0.1606 0.0000 ( 1325 PWs) bands (ev):  
-18.0253 -6.0234 -4.1632 -3.4028 4.6084 7.9200 9.6227 10.3315

k = 0.0907 0.1571 0.0000 ( 1325 PWs) bands (ev):  
-18.0508 -6.0537 -4.0944 -3.3548 4.5734 7.8869 9.6012 10.2972

k = 0.0888 0.1537 0.0000 ( 1319 PWs) bands (ev):  
-18.0758 -6.0834 -4.0262 -3.3075 4.5391 7.8546 9.5804 10.2636

k = 0.0868 0.1503 0.0000 ( 1319 PWs) bands (ev):  
-18.1003 -6.1124 -3.9584 -3.2609 4.5056 7.8229 9.5603 10.2306

k = 0.0848 0.1469 0.0000 ( 1315 PWs) bands (ev):  
-18.1242 -6.1408 -3.8912 -3.2151 4.4728 7.7919 9.5408 10.1983

k = 0.0828 0.1435 0.0000 ( 1315 PWs) bands (ev):  
-18.1475 -6.1686 -3.8246 -3.1700 4.4408 7.7616 9.5219 10.1666

k = 0.0809 0.1401 0.0000 ( 1315 PWs) bands (ev):  
-18.1703 -6.1958 -3.7587 -3.1257 4.4096 7.7320 9.5037 10.1356

k = 0.0789 0.1366 0.0000 ( 1315 PWs) bands (ev):  
-18.1926 -6.2223 -3.6934 -3.0822 4.3791 7.7031 9.4861 10.1052

k = 0.0769 0.1332 0.0000 ( 1315 PWs) bands (ev):  
-18.2143 -6.2481 -3.6289 -3.0395 4.3493 7.6749 9.4692 10.0754

k = 0.0749 0.1298 0.0000 ( 1315 PWs) bands (ev):  
-18.2355 -6.2734 -3.5652 -2.9976 4.3203 7.6474 9.4529 10.0463

k = 0.0730 0.1264 0.0000 ( 1315 PWs) bands (ev):  
-18.2562 -6.2980 -3.5022 -2.9566 4.2921 7.6206 9.4372 10.0179

k = 0.0710 0.1230 0.0000 ( 1315 PWs) bands (ev):  
-18.2762 -6.3219 -3.4401 -2.9165 4.2646 7.5944 9.4222 9.9900

k = 0.0690 0.1196 0.0000 ( 1315 PWs) bands (ev):  
-18.2958 -6.3452 -3.3789 -2.8772 4.2378 7.5690 9.4077 9.9628

k = 0.0671 0.1162 0.0000 ( 1307 PWs) bands (ev):  
-18.3148 -6.3679 -3.3185 -2.8387 4.2118 7.5443 9.3940 9.9363

k = 0.0651 0.1127 0.0000 ( 1307 PWs) bands (ev):  
-18.3332 -6.3899 -3.2592 -2.8013 4.1866 7.5203 9.3808 9.9104

k = 0.0631 0.1093 0.0000 ( 1311 PWs) bands (ev):

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-18.3511	-6.4112	-3.2009	-2.7647	4.1621	7.4970	9.3682	9.8851
k = 0.0611 0.1059 0.0000 ( 1311 PWs)					bands (ev):		
-18.3685	-6.4320	-3.1437	-2.7291	4.1384	7.4744	9.3563	9.8605
k = 0.0592 0.1025 0.0000 ( 1311 PWs)					bands (ev):		
-18.3853	-6.4520	-3.0876	-2.6945	4.1154	7.4526	9.3449	9.8365
k = 0.0572 0.0991 0.0000 ( 1301 PWs)					bands (ev):		
-18.4016	-6.4714	-3.0325	-2.6608	4.0932	7.4314	9.3341	9.8131
k = 0.0552 0.0957 0.0000 ( 1301 PWs)					bands (ev):		
-18.4173	-6.4902	-2.9788	-2.6281	4.0718	7.4109	9.3239	9.7904
k = 0.0533 0.0922 0.0000 ( 1301 PWs)					bands (ev):		
-18.4324	-6.5083	-2.9263	-2.5965	4.0511	7.3912	9.3143	9.7683
k = 0.0513 0.0888 0.0000 ( 1301 PWs)					bands (ev):		
-18.4471	-6.5258	-2.8751	-2.5658	4.0311	7.3721	9.3053	9.7469
k = 0.0493 0.0854 0.0000 ( 1301 PWs)					bands (ev):		
-18.4611	-6.5426	-2.8253	-2.5362	4.0119	7.3538	9.2968	9.7261
k = 0.0473 0.0820 0.0000 ( 1305 PWs)					bands (ev):		
-18.4746	-6.5588	-2.7769	-2.5076	3.9934	7.3362	9.2889	9.7060
k = 0.0454 0.0786 0.0000 ( 1305 PWs)					bands (ev):		
-18.4876	-6.5743	-2.7300	-2.4801	3.9758	7.3193	9.2815	9.6866
k = 0.0434 0.0752 0.0000 ( 1301 PWs)					bands (ev):		
-18.5000	-6.5891	-2.6846	-2.4537	3.9588	7.3031	9.2746	9.6678
k = 0.0414 0.0717 0.0000 ( 1297 PWs)					bands (ev):		
-18.5119	-6.6033	-2.6407	-2.4283	3.9426	7.2876	9.2683	9.6496
k = 0.0394 0.0683 0.0000 ( 1293 PWs)					bands (ev):		
-18.5232	-6.6169	-2.5984	-2.4040	3.9272	7.2729	9.2625	9.6322
k = 0.0375 0.0649 0.0000 ( 1293 PWs)					bands (ev):		
-18.5340	-6.6297	-2.5579	-2.3809	3.9125	7.2588	9.2572	9.6154
k = 0.0355 0.0615 0.0000 ( 1293 PWs)					bands (ev):		
-18.5442	-6.6420	-2.5191	-2.3589	3.8986	7.2455	9.2523	9.5942
k = 0.0335 0.0581 0.0000 ( 1291 PWs)					bands (ev):		
-18.5538	-6.6535	-2.4820	-2.3380	3.8854	7.2329	9.2480	9.5562

k = 0.0316 0.0547 0.0000 ( 1295 PWs)	bands (ev):
-18.5630 -6.6644 -2.4468 -2.3182 3.8730	7.2210 9.2440 9.5199
k = 0.0296 0.0512 0.0000 ( 1295 PWs)	bands (ev):
-18.5715 -6.6747 -2.4134 -2.2996 3.8613	7.2098 9.2405 9.4854
k = 0.0276 0.0478 0.0000 ( 1295 PWs)	bands (ev):
-18.5795 -6.6843 -2.3820 -2.2821 3.8504	7.1994 9.2374 9.4528
k = 0.0256 0.0444 0.0000 ( 1295 PWs)	bands (ev):
-18.5870 -6.6932 -2.3525 -2.2659 3.8402	7.1897 9.2347 9.4221
k = 0.0237 0.0410 0.0000 ( 1295 PWs)	bands (ev):
-18.5939 -6.7015 -2.3250 -2.2507 3.8308	7.1806 9.2324 9.3934
k = 0.0217 0.0376 0.0000 ( 1293 PWs)	bands (ev):
-18.6002 -6.7091 -2.2996 -2.2368 3.8222	7.1724 9.2304 9.3668
k = 0.0197 0.0342 0.0000 ( 1293 PWs)	bands (ev):
-18.6060 -6.7160 -2.2762 -2.2241 3.8143	7.1648 9.2287 9.3423
k = 0.0178 0.0307 0.0000 ( 1293 PWs)	bands (ev):
-18.6113 -6.7223 -2.2549 -2.2125 3.8071	7.1579 9.2273 9.3200
k = 0.0158 0.0273 0.0000 ( 1297 PWs)	bands (ev):
-18.6160 -6.7280 -2.2358 -2.2022 3.8007	7.1518 9.2262 9.2999
k = 0.0138 0.0239 0.0000 ( 1297 PWs)	bands (ev):
-18.6201 -6.7329 -2.2189 -2.1930 3.7951	7.1464 9.2253 9.2821
k = 0.0118 0.0205 0.0000 ( 1301 PWs)	bands (ev):
-18.6237 -6.7372 -2.2042 -2.1851 3.7902	7.1417 9.2246 9.2665
k = 0.0099 0.0171 0.0000 ( 1301 PWs)	bands (ev):
-18.6268 -6.7409 -2.1917 -2.1784 3.7860	7.1377 9.2240 9.2533
k = 0.0079 0.0137 0.0000 ( 1301 PWs)	bands (ev):
-18.6292 -6.7439 -2.1814 -2.1729 3.7826	7.1345 9.2236 9.2424
k = 0.0059 0.0102 0.0000 ( 1301 PWs)	bands (ev):
-18.6312 -6.7462 -2.1734 -2.1686 3.7800	7.1320 9.2234 9.2340
k = 0.0039 0.0068 0.0000 ( 1301 PWs)	bands (ev):
-18.6326 -6.7478 -2.1677 -2.1655 3.7781	7.1302 9.2232 9.2279
k = 0.0020 0.0034 0.0000 ( 1301 PWs)	bands (ev):

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-18.6334 -6.7488 -2.1642 -2.1637 3.7770 7.1291 9.2231 9.2243
      k = 0.0000 0.0000 0.0000 ( 1301 PWs) bands (ev):
-18.6337 -6.7492 -2.1631 -2.1631 3.7766 7.1287 9.2231 9.2231
----- SPIN DOWN -----

      k = 0.0000 0.0000 0.0000 ( 1301 PWs) bands (ev):
-18.6259 -6.7295 -2.1598 -2.1598 3.7794 7.1344 9.2257 9.2257
      k = 0.0034 0.0020 0.0000 ( 1301 PWs) bands (ev):
-18.6256 -6.7292 -2.1610 -2.1604 3.7798 7.1348 9.2258 9.2269
      k = 0.0068 0.0040 0.0000 ( 1301 PWs) bands (ev):
-18.6247 -6.7282 -2.1644 -2.1623 3.7810 7.1358 9.2259 9.2306
      k = 0.0103 0.0059 0.0000 ( 1301 PWs) bands (ev):
-18.6234 -6.7265 -2.1702 -2.1654 3.7828 7.1377 9.2260 9.2367
      k = 0.0137 0.0079 0.0000 ( 1301 PWs) bands (ev):
-18.6214 -6.7242 -2.1782 -2.1697 3.7855 7.1402 9.2263 9.2452
      k = 0.0171 0.0099 0.0000 ( 1301 PWs) bands (ev):
-18.6189 -6.7212 -2.1886 -2.1752 3.7889 7.1435 9.2267 9.2562
      k = 0.0205 0.0119 0.0000 ( 1301 PWs) bands (ev):
-18.6159 -6.7175 -2.2012 -2.1819 3.7931 7.1474 9.2271 9.2696
      k = 0.0240 0.0138 0.0000 ( 1297 PWs) bands (ev):
-18.6122 -6.7132 -2.2160 -2.1898 3.7980 7.1522 9.2277 9.2854
      k = 0.0274 0.0158 0.0000 ( 1297 PWs) bands (ev):
-18.6081 -6.7082 -2.2331 -2.1989 3.8036 7.1576 9.2284 9.3035
      k = 0.0308 0.0178 0.0000 ( 1293 PWs) bands (ev):
-18.6034 -6.7026 -2.2524 -2.2092 3.8101 7.1638 9.2292 9.3241
      k = 0.0342 0.0198 0.0000 ( 1293 PWs) bands (ev):
-18.5981 -6.6962 -2.2739 -2.2206 3.8173 7.1706 9.2302 9.3470
      k = 0.0377 0.0217 0.0000 ( 1293 PWs) bands (ev):
-18.5923 -6.6893 -2.2976 -2.2332 3.8252 7.1783 9.2313 9.3723
      k = 0.0411 0.0237 0.0000 ( 1293 PWs) bands (ev):
-18.5859 -6.6816 -2.3235 -2.2469 3.8339 7.1866 9.2326 9.3999
      k = 0.0445 0.0257 0.0000 ( 1297 PWs) bands (ev):

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-18.5789	-6.6733	-2.3515	-2.2617	3.8434	7.1956	9.2340	9.4298
k = 0.0479 0.0277 0.0000 ( 1297 PWs)					bands (ev):		
-18.5714	-6.6643	-2.3815	-2.2775	3.8536	7.2054	9.2356	9.4619
k = 0.0514 0.0297 0.0000 ( 1295 PWs)					bands (ev):		
-18.5634	-6.6547	-2.4137	-2.2945	3.8645	7.2159	9.2373	9.4964
k = 0.0548 0.0316 0.0000 ( 1295 PWs)					bands (ev):		
-18.5548	-6.6444	-2.4479	-2.3124	3.8763	7.2272	9.2391	9.5331
k = 0.0582 0.0336 0.0000 ( 1295 PWs)					bands (ev):		
-18.5456	-6.6334	-2.4841	-2.3314	3.8888	7.2391	9.2410	9.5719
k = 0.0616 0.0356 0.0000 ( 1295 PWs)					bands (ev):		
-18.5359	-6.6218	-2.5222	-2.3514	3.9020	7.2518	9.2431	9.6020
k = 0.0651 0.0376 0.0000 ( 1299 PWs)					bands (ev):		
-18.5257	-6.6095	-2.5624	-2.3723	3.9160	7.2652	9.2451	9.6178
k = 0.0685 0.0395 0.0000 ( 1299 PWs)					bands (ev):		
-18.5149	-6.5965	-2.6044	-2.3942	3.9307	7.2793	9.2473	9.6342
k = 0.0719 0.0415 0.0000 ( 1299 PWs)					bands (ev):		
-18.5035	-6.5829	-2.6482	-2.4170	3.9463	7.2941	9.2494	9.6512
k = 0.0753 0.0435 0.0000 ( 1297 PWs)					bands (ev):		
-18.4916	-6.5687	-2.6939	-2.4406	3.9625	7.3097	9.2516	9.6688
k = 0.0788 0.0455 0.0000 ( 1301 PWs)					bands (ev):		
-18.4791	-6.5537	-2.7415	-2.4652	3.9796	7.3259	9.2538	9.6870
k = 0.0822 0.0475 0.0000 ( 1301 PWs)					bands (ev):		
-18.4661	-6.5381	-2.7906	-2.4905	3.9973	7.3429	9.2559	9.7059
k = 0.0856 0.0494 0.0000 ( 1301 PWs)					bands (ev):		
-18.4525	-6.5219	-2.8415	-2.5166	4.0159	7.3606	9.2580	9.7252
k = 0.0890 0.0514 0.0000 ( 1305 PWs)					bands (ev):		
-18.4383	-6.5050	-2.8941	-2.5435	4.0352	7.3790	9.2599	9.7452
k = 0.0925 0.0534 0.0000 ( 1305 PWs)					bands (ev):		
-18.4237	-6.4874	-2.9483	-2.5712	4.0552	7.3981	9.2618	9.7658
k = 0.0959 0.0554 0.0000 ( 1305 PWs)					bands (ev):		
-18.4084	-6.4692	-3.0040	-2.5995	4.0760	7.4180	9.2635	9.7869

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k = 0.0993 0.0573 0.0000 ( 1299 PWs) bands (ev):
-18.3926 -6.4503 -3.0612 -2.6284 4.0976 7.4385 9.2650 9.8087

k = 0.1027 0.0593 0.0000 ( 1301 PWs) bands (ev):
-18.3763 -6.4308 -3.1200 -2.6581 4.1199 7.4598 9.2663 9.8310

k = 0.1062 0.0613 0.0000 ( 1305 PWs) bands (ev):
-18.3594 -6.4107 -3.1802 -2.6883 4.1430 7.4818 9.2674 9.8538

k = 0.1096 0.0633 0.0000 ( 1309 PWs) bands (ev):
-18.3420 -6.3898 -3.2419 -2.7192 4.1668 7.5045 9.2682 9.8773

k = 0.1130 0.0652 0.0000 ( 1309 PWs) bands (ev):
-18.3240 -6.3684 -3.3049 -2.7506 4.1914 7.5278 9.2687 9.9014

k = 0.1164 0.0672 0.0000 ( 1309 PWs) bands (ev):
-18.3054 -6.3462 -3.3692 -2.7825 4.2168 7.5519 9.2689 9.9261

k = 0.1199 0.0692 0.0000 ( 1309 PWs) bands (ev):
-18.2863 -6.3235 -3.4348 -2.8149 4.2429 7.5767 9.2688 9.9514

k = 0.1233 0.0712 0.0000 ( 1309 PWs) bands (ev):
-18.2667 -6.3000 -3.5016 -2.8478 4.2698 7.6022 9.2684 9.9773

k = 0.1267 0.0732 0.0000 ( 1313 PWs) bands (ev):
-18.2465 -6.2760 -3.5697 -2.8812 4.2974 7.6284 9.2676 10.0038

k = 0.1301 0.0751 0.0000 ( 1313 PWs) bands (ev):
-18.2258 -6.2512 -3.6389 -2.9149 4.3257 7.6553 9.2665 10.0310

k = 0.1336 0.0771 0.0000 ( 1321 PWs) bands (ev):
-18.2045 -6.2259 -3.7093 -2.9491 4.3549 7.6829 9.2649 10.0588

k = 0.1370 0.0791 0.0000 ( 1321 PWs) bands (ev):
-18.1827 -6.1999 -3.7807 -2.9836 4.3848 7.7111 9.2629 10.0872

k = 0.1404 0.0811 0.0000 ( 1321 PWs) bands (ev):
-18.1603 -6.1732 -3.8532 -3.0184 4.4154 7.7401 9.2606 10.1163

k = 0.1438 0.0830 0.0000 ( 1319 PWs) bands (ev):
-18.1374 -6.1460 -3.9266 -3.0536 4.4468 7.7697 9.2578 10.1460

k = 0.1473 0.0850 0.0000 ( 1319 PWs) bands (ev):
-18.1139 -6.1180 -4.0011 -3.0890 4.4790 7.8000 9.2546 10.1764

k = 0.1507 0.0870 0.0000 ( 1319 PWs) bands (ev):
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-18.0899 -6.0895 -4.0765 -3.1246 4.5119 7.8310 9.2510 10.2075
      k = 0.1541 0.0890 0.0000 ( 1319 PWs) bands (ev):
-18.0653 -6.0603 -4.1528 -3.1605 4.5455 7.8626 9.2470 10.2392
      k = 0.1575 0.0910 0.0000 ( 1319 PWs) bands (ev):
-18.0402 -6.0305 -4.2300 -3.1966 4.5800 7.8949 9.2425 10.2717
      k = 0.1610 0.0929 0.0000 ( 1319 PWs) bands (ev):
-18.0145 -6.0000 -4.3080 -3.2329 4.6151 7.9278 9.2376 10.3047
      k = 0.1644 0.0949 0.0000 ( 1323 PWs) bands (ev):
-17.9883 -5.9689 -4.3869 -3.2693 4.6511 7.9614 9.2323 10.3385
      k = 0.1678 0.0969 0.0000 ( 1323 PWs) bands (ev):
-17.9616 -5.9372 -4.4665 -3.3059 4.6878 7.9955 9.2265 10.2976
      k = 0.1712 0.0989 0.0000 ( 1323 PWs) bands (ev):
-17.9343 -5.9049 -4.5468 -3.3426 4.7252 8.0303 9.2204 10.2206
      k = 0.1747 0.1008 0.0000 ( 1323 PWs) bands (ev):
-17.9065 -5.8719 -4.6278 -3.3793 4.7634 8.0656 9.2138 10.1428
      k = 0.1781 0.1028 0.0000 ( 1323 PWs) bands (ev):
-17.8781 -5.8383 -4.7096 -3.4162 4.8023 8.1015 9.2069 10.0642
      k = 0.1815 0.1048 0.0000 ( 1323 PWs) bands (ev):
-17.8492 -5.8041 -4.7919 -3.4531 4.8420 8.1379 9.1996 9.9849
      k = 0.1849 0.1068 0.0000 ( 1319 PWs) bands (ev):
-17.8198 -5.7693 -4.8749 -3.4900 4.8825 8.1748 9.1919 9.9050
      k = 0.1884 0.1087 0.0000 ( 1321 PWs) bands (ev):
-17.7898 -5.7338 -4.9585 -3.5271 4.9237 8.2121 9.1838 9.8245
      k = 0.1918 0.1107 0.0000 ( 1321 PWs) bands (ev):
-17.7592 -5.6977 -5.0426 -3.5640 4.9657 8.2498 9.1754 9.7436
      k = 0.1952 0.1127 0.0000 ( 1317 PWs) bands (ev):
-17.7282 -5.6611 -5.1273 -3.6009 5.0084 8.2877 9.1667 9.6623
      k = 0.1986 0.1147 0.0000 ( 1317 PWs) bands (ev):
-17.6966 -5.6238 -5.2124 -3.6378 5.0518 8.3257 9.1576 9.5808
      k = 0.2021 0.1167 0.0000 ( 1317 PWs) bands (ev):
-17.6644 -5.5859 -5.2981 -3.6746 5.0960 8.3635 9.1482 9.4994
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k = 0.2055 0.1186 0.0000 ( 1319 PWs) bands (ev):
-17.6317 -5.5474 -5.3842 -3.7114 5.1410 8.4010 9.1385 9.4184

k = 0.2089 0.1206 0.0000 ( 1319 PWs) bands (ev):
-17.5985 -5.5084 -5.4708 -3.7481 5.1867 8.4377 9.1285 9.3382

k = 0.2123 0.1226 0.0000 ( 1317 PWs) bands (ev):
-17.5648 -5.5577 -5.4687 -3.7846 5.2332 8.4727 9.1183 9.2597

k = 0.2158 0.1246 0.0000 ( 1321 PWs) bands (ev):
-17.5305 -5.6450 -5.4284 -3.8211 5.2804 8.5049 9.1078 9.1840

k = 0.2192 0.1265 0.0000 ( 1321 PWs) bands (ev):
-17.4957 -5.7327 -5.3876 -3.8573 5.3284 8.5323 9.0970 9.1132

k = 0.2226 0.1285 0.0000 ( 1321 PWs) bands (ev):
-17.4604 -5.8208 -5.3461 -3.8935 5.3771 8.5515 9.0508 9.0861

k = 0.2260 0.1305 0.0000 ( 1321 PWs) bands (ev):
-17.4245 -5.9091 -5.3041 -3.9295 5.4266 8.5571 9.0020 9.0749

k = 0.2295 0.1325 0.0000 ( 1321 PWs) bands (ev):
-17.3881 -5.9977 -5.2615 -3.9653 5.4768 8.5435 8.9726 9.0635

k = 0.2329 0.1345 0.0000 ( 1321 PWs) bands (ev):
-17.3511 -6.0866 -5.2183 -4.0009 5.5278 8.5080 8.9653 9.0519

k = 0.2363 0.1364 0.0000 ( 1321 PWs) bands (ev):
-17.3137 -6.1758 -5.1746 -4.0363 5.5795 8.4537 8.9769 9.0402

k = 0.2397 0.1384 0.0000 ( 1325 PWs) bands (ev):
-17.2757 -6.2653 -5.1302 -4.0715 5.6320 8.3863 9.0019 9.0283

k = 0.2432 0.1404 0.0000 ( 1325 PWs) bands (ev):
-17.2372 -6.3549 -5.0853 -4.1064 5.6852 8.3104 9.0163 9.0356

k = 0.2466 0.1424 0.0000 ( 1325 PWs) bands (ev):
-17.1981 -6.4447 -5.0399 -4.1411 5.7391 8.2291 9.0041 9.0749

k = 0.2500 0.1443 0.0000 ( 1325 PWs) bands (ev):
-17.1586 -6.5347 -4.9939 -4.1756 5.7938 8.1443 8.9919 9.1181

k = 0.2534 0.1463 0.0000 ( 1325 PWs) bands (ev):
-17.1185 -6.6249 -4.9473 -4.2098 5.8493 8.0571 8.9795 9.1640

k = 0.2568 0.1483 0.0000 ( 1325 PWs) bands (ev):
```

-17.0779	-6.7152	-4.9002	-4.2437	5.9055	7.9680	8.9671	9.2121
k = 0.2603 0.1503 0.0000 ( 1325 PWs)				bands (ev):			
-17.0367	-6.8056	-4.8526	-4.2773	5.9624	7.8776	8.9546	9.2618
k = 0.2637 0.1522 0.0000 ( 1323 PWs)				bands (ev):			
-16.9951	-6.8961	-4.8044	-4.3106	6.0201	7.7862	8.9420	9.3130
k = 0.2671 0.1542 0.0000 ( 1315 PWs)				bands (ev):			
-16.9529	-6.9867	-4.7557	-4.3436	6.0785	7.6939	8.9294	9.3654
k = 0.2705 0.1562 0.0000 ( 1315 PWs)				bands (ev):			
-16.9102	-7.0774	-4.7065	-4.3763	6.1376	7.6009	8.9168	9.4189
k = 0.2740 0.1582 0.0000 ( 1315 PWs)				bands (ev):			
-16.8670	-7.1682	-4.6568	-4.4087	6.1975	7.5074	8.9041	9.4734
k = 0.2774 0.1602 0.0000 ( 1319 PWs)				bands (ev):			
-16.8232	-7.2590	-4.6065	-4.4408	6.2582	7.4134	8.8914	9.5288
k = 0.2808 0.1621 0.0000 ( 1319 PWs)				bands (ev):			
-16.7790	-7.3499	-4.5558	-4.4725	6.3195	7.3190	8.8788	9.5851
k = 0.2842 0.1641 0.0000 ( 1319 PWs)				bands (ev):			
-16.7343	-7.4407	-4.5045	-4.5039	6.3816	7.2243	8.8661	9.6423
k = 0.2877 0.1661 0.0000 ( 1319 PWs)				bands (ev):			
-16.6890	-7.5316	-4.5349	-4.4528	6.4445	7.1293	8.8535	9.7002
k = 0.2911 0.1681 0.0000 ( 1319 PWs)				bands (ev):			
-16.6432	-7.6225	-4.5655	-4.4006	6.5081	7.0341	8.8409	9.7589
k = 0.2945 0.1700 0.0000 ( 1319 PWs)				bands (ev):			
-16.5970	-7.7133	-4.5958	-4.3479	6.5724	6.9387	8.8284	9.8184
k = 0.2979 0.1720 0.0000 ( 1319 PWs)				bands (ev):			
-16.5502	-7.8041	-4.6257	-4.2948	6.6374	6.8432	8.8159	9.8786
k = 0.3014 0.1740 0.0000 ( 1322 PWs)				bands (ev):			
-16.5029	-7.8948	-4.6552	-4.2412	6.7032	6.7475	8.8035	9.9395
k = 0.3048 0.1760 0.0000 ( 1322 PWs)				bands (ev):			
-16.4551	-7.9855	-4.6843	-4.1872	6.6518	6.7696	8.7912	10.0011
k = 0.3082 0.1780 0.0000 ( 1322 PWs)				bands (ev):			
-16.4068	-8.0761	-4.7130	-4.1327	6.5561	6.8368	8.7790	10.0634

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k = 0.3116 0.1799 0.0000 ( 1322 PWs) bands (ev):
-16.3580 -8.1666 -4.7413 -4.0779 6.4604 6.9047 8.7669 10.1263

k = 0.3151 0.1819 0.0000 ( 1322 PWs) bands (ev):
-16.3088 -8.2570 -4.7692 -4.0226 6.3647 6.9734 8.7550 10.1900

k = 0.3185 0.1839 0.0000 ( 1326 PWs) bands (ev):
-16.2590 -8.3473 -4.7966 -3.9669 6.2691 7.0427 8.7431 10.2543

k = 0.3219 0.1859 0.0000 ( 1326 PWs) bands (ev):
-16.2087 -8.4375 -4.8237 -3.9109 6.1735 7.1127 8.7314 10.3192

k = 0.3253 0.1878 0.0000 ( 1322 PWs) bands (ev):
-16.1580 -8.5275 -4.8502 -3.8544 6.0781 7.1835 8.7199 10.3848

k = 0.3288 0.1898 0.0000 ( 1330 PWs) bands (ev):
-16.1067 -8.6175 -4.8764 -3.7976 5.9829 7.2549 8.7085 10.4510

k = 0.3322 0.1918 0.0000 ( 1330 PWs) bands (ev):
-16.0550 -8.7072 -4.9021 -3.7405 5.8878 7.3270 8.6973 10.5179

k = 0.3356 0.1938 0.0000 ( 1330 PWs) bands (ev):
-16.0028 -8.7968 -4.9274 -3.6830 5.7930 7.3997 8.6864 10.5853

k = 0.3390 0.1957 0.0000 ( 1326 PWs) bands (ev):
-15.9501 -8.8862 -4.9522 -3.6252 5.6984 7.4731 8.6757 10.6534

k = 0.3425 0.1977 0.0000 ( 1330 PWs) bands (ev):
-15.8969 -8.9754 -4.9766 -3.5672 5.6041 7.5471 8.6652 10.7221

k = 0.3459 0.1997 0.0000 ( 1326 PWs) bands (ev):
-15.8433 -9.0644 -5.0005 -3.5088 5.5101 7.6217 8.6551 10.7913

k = 0.3493 0.2017 0.0000 ( 1326 PWs) bands (ev):
-15.7892 -9.1532 -5.0239 -3.4503 5.4165 7.6968 8.6453 10.8612

k = 0.3527 0.2037 0.0000 ( 1326 PWs) bands (ev):
-15.7346 -9.2418 -5.0469 -3.3915 5.3233 7.7724 8.6359 10.9316

k = 0.3562 0.2056 0.0000 ( 1326 PWs) bands (ev):
-15.6796 -9.3301 -5.0694 -3.3324 5.2305 7.8485 8.6271 11.0026

k = 0.3596 0.2076 0.0000 ( 1326 PWs) bands (ev):
-15.6241 -9.4182 -5.0914 -3.2733 5.1381 7.9248 8.6188 11.0742

k = 0.3630 0.2096 0.0000 ( 1326 PWs) bands (ev):
```

-15.5682	-9.5060	-5.1129	-3.2139	5.0463	8.0012	8.6114	11.1463
k = 0.3664 0.2116 0.0000 ( 1326 PWs)					bands (ev):		
-15.5118	-9.5936	-5.1340	-3.1545	4.9550	8.0773	8.6051	11.2189
k = 0.3699 0.2135 0.0000 ( 1326 PWs)					bands (ev):		
-15.4550	-9.6809	-5.1545	-3.0949	4.8643	8.1527	8.6006	11.2921
k = 0.3733 0.2155 0.0000 ( 1326 PWs)					bands (ev):		
-15.3977	-9.7679	-5.1746	-3.0353	4.7742	8.2263	8.5987	11.3658
k = 0.3767 0.2175 0.0000 ( 1324 PWs)					bands (ev):		
-15.3400	-9.8546	-5.1941	-2.9757	4.6848	8.2963	8.6014	11.4400
k = 0.3801 0.2195 0.0000 ( 1328 PWs)					bands (ev):		
-15.2819	-9.9410	-5.2132	-2.9160	4.5960	8.3590	8.6123	11.5147
k = 0.3836 0.2214 0.0000 ( 1328 PWs)					bands (ev):		
-15.2234	-10.0271	-5.2317	-2.8565	4.5081	8.4087	8.6371	11.5899
k = 0.3870 0.2234 0.0000 ( 1328 PWs)					bands (ev):		
-15.1645	-10.1128	-5.2498	-2.7970	4.4210	8.4408	8.6805	11.6656
k = 0.3904 0.2254 0.0000 ( 1328 PWs)					bands (ev):		
-15.1051	-10.1982	-5.2673	-2.7377	4.3348	8.4573	8.7404	11.7417
k = 0.3938 0.2274 0.0000 ( 1332 PWs)					bands (ev):		
-15.0454	-10.2832	-5.2844	-2.6785	4.2494	8.4638	8.8112	11.8183
k = 0.3973 0.2294 0.0000 ( 1328 PWs)					bands (ev):		
-14.9853	-10.3678	-5.3008	-2.6196	4.1651	8.4650	8.8883	11.8953
k = 0.4007 0.2313 0.0000 ( 1328 PWs)					bands (ev):		
-14.9249	-10.4520	-5.3168	-2.5610	4.0819	8.4632	8.9693	11.9728
k = 0.4041 0.2333 0.0000 ( 1328 PWs)					bands (ev):		
-14.8640	-10.5358	-5.3323	-2.5028	3.9998	8.4599	9.0528	12.0506
k = 0.4075 0.2353 0.0000 ( 1328 PWs)					bands (ev):		
-14.8029	-10.6192	-5.3473	-2.4450	3.9188	8.4557	9.1382	12.1288
k = 0.4110 0.2373 0.0000 ( 1324 PWs)					bands (ev):		
-14.7414	-10.7021	-5.3617	-2.3876	3.8392	8.4509	9.2250	12.2074
k = 0.4144 0.2392 0.0000 ( 1324 PWs)					bands (ev):		
-14.6796	-10.7846	-5.3756	-2.3309	3.7609	8.4459	9.3130	12.2863

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k = 0.4178 0.2412 0.0000 ( 1324 PWs) bands (ev):
-14.6176 -10.8665 -5.3889 -2.2748 3.6841 8.4407 9.4021 12.3655

k = 0.4212 0.2432 0.0000 ( 1324 PWs) bands (ev):
-14.5553 -10.9479 -5.4018 -2.2195 3.6088 8.4356 9.4922 12.4449

k = 0.4247 0.2452 0.0000 ( 1324 PWs) bands (ev):
-14.4927 -11.0287 -5.4141 -2.1651 3.5352 8.4304 9.5831 12.5247

k = 0.4281 0.2472 0.0000 ( 1322 PWs) bands (ev):
-14.4300 -11.1089 -5.4259 -2.1115 3.4633 8.4254 9.6750 12.6046

k = 0.4315 0.2491 0.0000 ( 1322 PWs) bands (ev):
-14.3671 -11.1885 -5.4371 -2.0590 3.3933 8.4205 9.7676 12.6847

k = 0.4349 0.2511 0.0000 ( 1326 PWs) bands (ev):
-14.3041 -11.2674 -5.4478 -2.0077 3.3252 8.4158 9.8610 12.7649

k = 0.4384 0.2531 0.0000 ( 1326 PWs) bands (ev):
-14.2411 -11.3456 -5.4579 -1.9577 3.2593 8.4112 9.9552 12.8451

k = 0.4418 0.2551 0.0000 ( 1326 PWs) bands (ev):
-14.1781 -11.4229 -5.4676 -1.9090 3.1957 8.4068 10.0501 12.9253

k = 0.4452 0.2570 0.0000 ( 1326 PWs) bands (ev):
-14.1152 -11.4993 -5.4766 -1.8620 3.1344 8.4027 10.1457 13.0055

k = 0.4486 0.2590 0.0000 ( 1326 PWs) bands (ev):
-14.0525 -11.5747 -5.4852 -1.8166 3.0757 8.3987 10.2420 13.0854

k = 0.4521 0.2610 0.0000 ( 1334 PWs) bands (ev):
-13.9901 -11.6490 -5.4932 -1.7731 3.0196 8.3950 10.3391 13.1651

k = 0.4555 0.2630 0.0000 ( 1338 PWs) bands (ev):
-13.9281 -11.7221 -5.5007 -1.7316 2.9664 8.3915 10.4368 13.1984

k = 0.4589 0.2649 0.0000 ( 1330 PWs) bands (ev):
-13.8668 -11.7936 -5.5075 -1.6922 2.9163 8.3882 10.5352 13.0863

k = 0.4623 0.2669 0.0000 ( 1330 PWs) bands (ev):
-13.8063 -11.8636 -5.5139 -1.6552 2.8693 8.3852 10.6342 12.9746

k = 0.4658 0.2689 0.0000 ( 1330 PWs) bands (ev):
-13.7470 -11.9315 -5.5197 -1.6207 2.8256 8.3825 10.7339 12.8633

k = 0.4692 0.2709 0.0000 ( 1332 PWs) bands (ev):
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-13.6892 -11.9972 -5.5249 -1.5888 2.7855 8.3800 10.8342 12.7525
      k = 0.4726 0.2729 0.0000 ( 1336 PWs) bands (ev):
-13.6333 -12.0601 -5.5296 -1.5598 2.7491 8.3777 10.9350 12.6421
      k = 0.4760 0.2748 0.0000 ( 1336 PWs) bands (ev):
-13.5800 -12.1195 -5.5338 -1.5337 2.7165 8.3757 11.0364 12.5322
      k = 0.4795 0.2768 0.0000 ( 1336 PWs) bands (ev):
-13.5300 -12.1749 -5.5374 -1.5108 2.6879 8.3740 11.1383 12.4230
      k = 0.4829 0.2788 0.0000 ( 1332 PWs) bands (ev):
-13.4842 -12.2252 -5.5404 -1.4911 2.6634 8.3726 11.2406 12.3145
      k = 0.4863 0.2808 0.0000 ( 1332 PWs) bands (ev):
-13.4439 -12.2693 -5.5429 -1.4748 2.6432 8.3714 11.3432 12.2068
      k = 0.4897 0.2827 0.0000 ( 1332 PWs) bands (ev):
-13.4102 -12.3058 -5.5448 -1.4620 2.6274 8.3704 11.4455 12.1005
      k = 0.4932 0.2847 0.0000 ( 1332 PWs) bands (ev):
-13.3848 -12.3333 -5.5462 -1.4529 2.6160 8.3698 11.5465 11.9967
      k = 0.4966 0.2867 0.0000 ( 1332 PWs) bands (ev):
-13.3688 -12.3505 -5.5470 -1.4473 2.6092 8.3694 11.6416 11.8999
      k = 0.5000 0.2887 0.0000 ( 1332 PWs) bands (ev):
-13.3634 -12.3563 -5.5473 -1.4455 2.6069 8.3692 11.6972 11.8437
      k = 0.4980 0.2921 0.0000 ( 1332 PWs) bands (ev):
-13.3632 -12.3561 -5.5485 -1.4451 2.6068 8.3709 11.6976 11.8440
      k = 0.4960 0.2955 0.0000 ( 1332 PWs) bands (ev):
-13.3624 -12.3554 -5.5523 -1.4441 2.6066 8.3760 11.6986 11.8451
      k = 0.4940 0.2990 0.0000 ( 1332 PWs) bands (ev):
-13.3612 -12.3542 -5.5586 -1.4424 2.6062 8.3845 11.7003 11.8469
      k = 0.4921 0.3024 0.0000 ( 1332 PWs) bands (ev):
-13.3596 -12.3525 -5.5674 -1.4400 2.6057 8.3963 11.7027 11.8494
      k = 0.4901 0.3059 0.0000 ( 1336 PWs) bands (ev):
-13.3574 -12.3503 -5.5787 -1.4369 2.6049 8.4115 11.7057 11.8526
      k = 0.4881 0.3093 0.0000 ( 1336 PWs) bands (ev):
-13.3548 -12.3477 -5.5924 -1.4332 2.6041 8.4301 11.7094 11.8565

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k = 0.4861 0.3127 0.0000 ( 1328 PWs) bands (ev):
-13.3517 -12.3446 -5.6085 -1.4287 2.6030 8.4520 11.7138 11.8611

k = 0.4841 0.3162 0.0000 ( 1328 PWs) bands (ev):
-13.3481 -12.3410 -5.6271 -1.4236 2.6018 8.4771 11.7189 11.8665

k = 0.4821 0.3196 0.0000 ( 1329 PWs) bands (ev):
-13.3441 -12.3370 -5.6481 -1.4178 2.6004 8.5055 11.7247 11.8725

k = 0.4802 0.3230 0.0000 ( 1327 PWs) bands (ev):
-13.3395 -12.3324 -5.6714 -1.4113 2.5989 8.5371 11.7311 11.8793

k = 0.4782 0.3265 0.0000 ( 1327 PWs) bands (ev):
-13.3345 -12.3274 -5.6970 -1.4042 2.5971 8.5719 11.7382 11.8868

k = 0.4762 0.3299 0.0000 ( 1329 PWs) bands (ev):
-13.3290 -12.3220 -5.7250 -1.3963 2.5951 8.6098 11.7460 11.8950

k = 0.4742 0.3334 0.0000 ( 1329 PWs) bands (ev):
-13.3231 -12.3160 -5.7551 -1.3878 2.5930 8.6508 11.7544 11.9039

k = 0.4722 0.3368 0.0000 ( 1329 PWs) bands (ev):
-13.3166 -12.3096 -5.7875 -1.3786 2.5906 8.6949 11.7635 11.9135

k = 0.4702 0.3402 0.0000 ( 1335 PWs) bands (ev):
-13.3097 -12.3028 -5.8220 -1.3687 2.5880 8.7419 11.7733 11.9238

k = 0.4683 0.3437 0.0000 ( 1335 PWs) bands (ev):
-13.3023 -12.2954 -5.8586 -1.3581 2.5851 8.7919 11.7837 11.9348

k = 0.4663 0.3471 0.0000 ( 1335 PWs) bands (ev):
-13.2944 -12.2876 -5.8972 -1.3469 2.5820 8.8447 11.7948 11.9465

k = 0.4643 0.3505 0.0000 ( 1335 PWs) bands (ev):
-13.2861 -12.2794 -5.9378 -1.3349 2.5787 8.9004 11.8066 11.9589

k = 0.4623 0.3540 0.0000 ( 1335 PWs) bands (ev):
-13.2772 -12.2706 -5.9803 -1.3223 2.5751 8.9588 11.8190 11.9721

k = 0.4603 0.3574 0.0000 ( 1331 PWs) bands (ev):
-13.2679 -12.2614 -6.0248 -1.3090 2.5712 9.0199 11.8321 11.9859

k = 0.4583 0.3608 0.0000 ( 1333 PWs) bands (ev):
-13.2581 -12.2518 -6.0710 -1.2950 2.5670 9.0836 11.8459 12.0004

k = 0.4563 0.3643 0.0000 ( 1341 PWs) bands (ev):
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-13.2479 -12.2417 -6.1191 -1.2804 2.5625 9.1499 11.8603 12.0157
      k = 0.4544 0.3677 0.0000 ( 1341 PWs) bands (ev):
-13.2371 -12.2312 -6.1688 -1.2651 2.5577 9.2187 11.8753 12.0316
      k = 0.4524 0.3712 0.0000 ( 1341 PWs) bands (ev):
-13.2259 -12.2203 -6.2201 -1.2491 2.5526 9.2899 11.8911 12.0482
      k = 0.4504 0.3746 0.0000 ( 1341 PWs) bands (ev):
-13.2142 -12.2089 -6.2730 -1.2324 2.5471 9.3635 11.9074 12.0655
      k = 0.4484 0.3780 0.0000 ( 1341 PWs) bands (ev):
-13.2020 -12.1970 -6.3275 -1.2150 2.5412 9.4393 11.9244 12.0836
      k = 0.4464 0.3815 0.0000 ( 1341 PWs) bands (ev):
-13.1894 -12.1848 -6.3834 -1.1970 2.5349 9.5174 11.9420 12.1023
      k = 0.4444 0.3849 0.0000 ( 1341 PWs) bands (ev):
-13.1763 -12.1721 -6.4407 -1.1782 2.5282 9.5975 11.9603 12.1217
      k = 0.4425 0.3883 0.0000 ( 1341 PWs) bands (ev):
-13.1627 -12.1590 -6.4994 -1.1589 2.5211 9.6798 11.9792 12.1417
      k = 0.4405 0.3918 0.0000 ( 1341 PWs) bands (ev):
-13.1486 -12.1455 -6.5593 -1.1388 2.5136 9.7641 11.9988 12.1625
      k = 0.4385 0.3952 0.0000 ( 1341 PWs) bands (ev):
-13.1341 -12.1315 -6.6204 -1.1180 2.5056 9.8502 12.0189 12.1840
      k = 0.4365 0.3986 0.0000 ( 1341 PWs) bands (ev):
-13.1190 -12.1172 -6.6828 -1.0966 2.4971 9.9383 12.0397 12.2061
      k = 0.4345 0.4021 0.0000 ( 1341 PWs) bands (ev):
-13.1035 -12.1025 -6.7462 -1.0745 2.4881 10.0280 12.0611 12.2289
      k = 0.4325 0.4055 0.0000 ( 1341 PWs) bands (ev):
-13.0876 -12.0874 -6.8107 -1.0518 2.4785 10.1195 12.0831 12.2524
      k = 0.4306 0.4090 0.0000 ( 1347 PWs) bands (ev):
-13.0711 -12.0719 -6.8762 -1.0283 2.4684 10.2126 12.1057 12.2766
      k = 0.4286 0.4124 0.0000 ( 1339 PWs) bands (ev):
-13.0542 -12.0560 -6.9425 -1.0042 2.4578 10.3072 12.1289 12.3014
      k = 0.4266 0.4158 0.0000 ( 1339 PWs) bands (ev):
-13.0368 -12.0398 -7.0098 -0.9794 2.4466 10.4033 12.1528 12.3270
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k = 0.4246 0.4193 0.0000 ( 1335 PWs) bands (ev):  
-13.0189 -12.0232 -7.0778 -0.9539 2.4347 10.5008 12.1772 12.3532

k = 0.4226 0.4227 0.0000 ( 1335 PWs) bands (ev):  
-13.0005 -12.0063 -7.1466 -0.9278 2.4223 10.5995 12.2021 12.3800

k = 0.4206 0.4261 0.0000 ( 1335 PWs) bands (ev):  
-12.9817 -11.9891 -7.2162 -0.9010 2.4091 10.6995 12.2277 12.4076

k = 0.4186 0.4296 0.0000 ( 1335 PWs) bands (ev):  
-12.9624 -11.9715 -7.2863 -0.8736 2.3953 10.8006 12.2538 12.4358

k = 0.4167 0.4330 0.0000 ( 1335 PWs) bands (ev):  
-12.9426 -11.9537 -7.3571 -0.8454 2.3808 10.9027 12.2805 12.4647

k = 0.4147 0.4364 0.0000 ( 1335 PWs) bands (ev):  
-12.9224 -11.9356 -7.4284 -0.8166 2.3656 11.0057 12.3077 12.4942

k = 0.4127 0.4399 0.0000 ( 1337 PWs) bands (ev):  
-12.9016 -11.9171 -7.5001 -0.7872 2.3496 11.1096 12.3355 12.5245

k = 0.4107 0.4433 0.0000 ( 1337 PWs) bands (ev):  
-12.8804 -11.8985 -7.5723 -0.7571 2.3328 11.2142 12.3638 12.5554

k = 0.4087 0.4468 0.0000 ( 1337 PWs) bands (ev):  
-12.8588 -11.8796 -7.6448 -0.7263 2.3153 11.3195 12.3926 12.5870

k = 0.4067 0.4502 0.0000 ( 1341 PWs) bands (ev):  
-12.8366 -11.8605 -7.7177 -0.6948 2.2969 11.4252 12.4220 12.6154

k = 0.4048 0.4536 0.0000 ( 1349 PWs) bands (ev):  
-12.8140 -11.8412 -7.7908 -0.6627 2.2777 11.5314 12.4518 12.5681

k = 0.4028 0.4571 0.0000 ( 1349 PWs) bands (ev):  
-12.7909 -11.8218 -7.8641 -0.6299 2.2576 11.6378 12.4821 12.5212

k = 0.4008 0.4605 0.0000 ( 1349 PWs) bands (ev):  
-12.7673 -11.8023 -7.9374 -0.5965 2.2367 11.7443 12.4748 12.5129

k = 0.3988 0.4639 0.0000 ( 1345 PWs) bands (ev):  
-12.7433 -11.7826 -8.0108 -0.5624 2.2148 11.8508 12.4290 12.5442

k = 0.3968 0.4674 0.0000 ( 1345 PWs) bands (ev):  
-12.7188 -11.7629 -8.0842 -0.5276 2.1921 11.9570 12.3839 12.5758

k = 0.3948 0.4708 0.0000 ( 1345 PWs) bands (ev):

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-12.6938 -11.7432 -8.1575 -0.4922 2.1684 12.0627 12.3395 12.6080
      k = 0.3929 0.4742 0.0000 ( 1341 PWs)  bands (ev):
-12.6683 -11.7234 -8.2306 -0.4561 2.1438 12.1678 12.2959 12.6405
      k = 0.3909 0.4777 0.0000 ( 1347 PWs)  bands (ev):
-12.6424 -11.7038 -8.3036 -0.4194 2.1182 12.2533 12.2718 12.6734
      k = 0.3889 0.4811 0.0000 ( 1347 PWs)  bands (ev):
-12.6160 -11.6843 -8.3762 -0.3820 2.0916 12.2116 12.3744 12.7067
      k = 0.3869 0.4846 0.0000 ( 1347 PWs)  bands (ev):
-12.5891 -11.6649 -8.4484 -0.3439 2.0640 12.1710 12.4751 12.7404
      k = 0.3849 0.4880 0.0000 ( 1347 PWs)  bands (ev):
-12.5618 -11.6459 -8.5201 -0.3052 2.0354 12.1314 12.5733 12.7744
      k = 0.3829 0.4914 0.0000 ( 1347 PWs)  bands (ev):
-12.5340 -11.6271 -8.5912 -0.2659 2.0057 12.0930 12.6684 12.8087
      k = 0.3810 0.4949 0.0000 ( 1347 PWs)  bands (ev):
-12.5057 -11.6088 -8.6616 -0.2259 1.9751 12.0559 12.7592 12.8432
      k = 0.3790 0.4983 0.0000 ( 1335 PWs)  bands (ev):
-12.4769 -11.5909 -8.7312 -0.1852 1.9434 12.0200 12.8449 12.8781
      k = 0.3770 0.5017 0.0000 ( 1335 PWs)  bands (ev):
-12.4477 -11.5736 -8.7999 -0.1439 1.9106 11.9854 12.9131 12.9243
      k = 0.3750 0.5052 0.0000 ( 1335 PWs)  bands (ev):
-12.4180 -11.5571 -8.8675 -0.1020 1.8768 11.9521 12.9483 12.9968
      k = 0.3730 0.5086 0.0000 ( 1335 PWs)  bands (ev):
-12.3878 -11.5414 -8.9339 -0.0594 1.8419 11.9203 12.9837 13.0625
      k = 0.3710 0.5121 0.0000 ( 1335 PWs)  bands (ev):
-12.3572 -11.5267 -8.9990 -0.0162 1.8059 11.8899 13.0193 13.1219
      k = 0.3690 0.5155 0.0000 ( 1335 PWs)  bands (ev):
-12.3261 -11.5131 -9.0624 0.0277 1.7689 11.8610 13.0549 13.1763
      k = 0.3671 0.5189 0.0000 ( 1335 PWs)  bands (ev):
-12.2945 -11.5008 -9.1242 0.0722 1.7307 11.8336 13.0905 13.2267
      k = 0.3651 0.5224 0.0000 ( 1343 PWs)  bands (ev):
-12.2625 -11.4900 -9.1840 0.1173 1.6915 11.8077 13.1262 13.2739
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k = 0.3631 0.5258 0.0000 ( 1343 PWs) bands (ev):
-12.2300 -11.4809 -9.2417 0.1630 1.6513 11.7834 13.1618 13.3187

k = 0.3611 0.5292 0.0000 ( 1347 PWs) bands (ev):
-12.1970 -11.4737 -9.2970 0.2095 1.6099 11.7606 13.1973 13.3615

k = 0.3591 0.5327 0.0000 ( 1343 PWs) bands (ev):
-12.1636 -11.4686 -9.3496 0.2565 1.5676 11.7394 13.2327 13.4026

k = 0.3571 0.5361 0.0000 ( 1343 PWs) bands (ev):
-12.1297 -11.4659 -9.3994 0.3042 1.5241 11.7198 13.2679 13.4420

k = 0.3552 0.5395 0.0000 ( 1343 PWs) bands (ev):
-12.0953 -11.4658 -9.4461 0.3525 1.4796 11.7018 13.3029 13.4798

k = 0.3532 0.5430 0.0000 ( 1343 PWs) bands (ev):
-12.0605 -11.4685 -9.4894 0.4015 1.4341 11.6855 13.3375 13.5159

k = 0.3512 0.5464 0.0000 ( 1343 PWs) bands (ev):
-12.0251 -11.4743 -9.5290 0.4510 1.3876 11.6707 13.3718 13.5500

k = 0.3492 0.5499 0.0000 ( 1343 PWs) bands (ev):
-11.9894 -11.4834 -9.5648 0.5012 1.3400 11.6576 13.4056 13.5818

k = 0.3472 0.5533 0.0000 ( 1343 PWs) bands (ev):
-11.9531 -11.4959 -9.5966 0.5520 1.2915 11.6460 13.4389 13.6109

k = 0.3452 0.5567 0.0000 ( 1355 PWs) bands (ev):
-11.9165 -11.5121 -9.6243 0.6035 1.2419 11.6360 13.4716 13.6364

k = 0.3433 0.5602 0.0000 ( 1355 PWs) bands (ev):
-11.8793 -11.5319 -9.6476 0.6555 1.1914 11.6277 13.5037 13.6577

k = 0.3413 0.5636 0.0000 ( 1359 PWs) bands (ev):
-11.8417 -11.5555 -9.6665 0.7082 1.1399 11.6209 13.5350 13.6734

k = 0.3393 0.5670 0.0000 ( 1363 PWs) bands (ev):
-11.8036 -11.5829 -9.6811 0.7615 1.0876 11.6156 13.5655 13.6822

k = 0.3373 0.5705 0.0000 ( 1365 PWs) bands (ev):
-11.7651 -11.6139 -9.6914 0.8154 1.0343 11.6119 13.5951 13.6825

k = 0.3353 0.5739 0.0000 ( 1365 PWs) bands (ev):
-11.7261 -11.6485 -9.6975 0.8699 0.9801 11.6097 13.6238 13.6726

k = 0.3333 0.5773 0.0000 ( 1365 PWs) bands (ev):
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-11.6866 -11.6865 -9.6995 0.9250 0.9252 11.6090 13.6514 13.6515
    k = 0.3314 0.5739 0.0000 ( 1365 PWs) bands (ev):
-11.7277 -11.6468 -9.6976 0.8695 0.9806 11.6097 13.6187 13.6778
    k = 0.3294 0.5705 0.0000 ( 1365 PWs) bands (ev):
-11.7717 -11.6067 -9.6920 0.8132 1.0366 11.6118 13.5749 13.7029
    k = 0.3274 0.5671 0.0000 ( 1357 PWs) bands (ev):
-11.8185 -11.5661 -9.6830 0.7561 1.0932 11.6153 13.5211 13.7267
    k = 0.3254 0.5637 0.0000 ( 1355 PWs) bands (ev):
-11.8679 -11.5250 -9.6707 0.6982 1.1504 11.6201 13.4585 13.7492
    k = 0.3235 0.5603 0.0000 ( 1347 PWs) bands (ev):
-11.9196 -11.4835 -9.6555 0.6396 1.2082 11.6261 13.3886 13.7703
    k = 0.3215 0.5568 0.0000 ( 1347 PWs) bands (ev):
-11.9735 -11.4415 -9.6374 0.5803 1.2666 11.6334 13.3126 13.7900
    k = 0.3195 0.5534 0.0000 ( 1351 PWs) bands (ev):
-12.0292 -11.3991 -9.6168 0.5203 1.3256 11.6418 13.2315 13.8081
    k = 0.3176 0.5500 0.0000 ( 1351 PWs) bands (ev):
-12.0866 -11.3563 -9.5939 0.4597 1.3851 11.6514 13.1463 13.8247
    k = 0.3156 0.5466 0.0000 ( 1355 PWs) bands (ev):
-12.1456 -11.3130 -9.5686 0.3984 1.4452 11.6620 13.0577 13.8397
    k = 0.3136 0.5432 0.0000 ( 1355 PWs) bands (ev):
-12.2059 -11.2693 -9.5414 0.3366 1.5059 11.6736 12.9664 13.8531
    k = 0.3116 0.5398 0.0000 ( 1351 PWs) bands (ev):
-12.2674 -11.2251 -9.5123 0.2742 1.5672 11.6861 12.8727 13.8648
    k = 0.3097 0.5363 0.0000 ( 1351 PWs) bands (ev):
-12.3299 -11.1804 -9.4814 0.2112 1.6290 11.6995 12.7772 13.8749
    k = 0.3077 0.5329 0.0000 ( 1351 PWs) bands (ev):
-12.3933 -11.1354 -9.4489 0.1477 1.6914 11.7136 12.6801 13.8834
    k = 0.3057 0.5295 0.0000 ( 1351 PWs) bands (ev):
-12.4575 -11.0898 -9.4149 0.0837 1.7544 11.7284 12.5818 13.8902
    k = 0.3037 0.5261 0.0000 ( 1351 PWs) bands (ev):
-12.5224 -11.0439 -9.3794 0.0192 1.8180 11.7438 12.4826 13.8954
```

```
k = 0.3018 0.5227 0.0000 ( 1351 PWs) bands (ev):
-12.5878 -10.9975 -9.3427 -0.0457 1.8821 11.7597 12.3826 13.8990

k = 0.2998 0.5193 0.0000 ( 1351 PWs) bands (ev):
-12.6538 -10.9506 -9.3048 -0.1110 1.9467 11.7760 12.2820 13.9011

k = 0.2978 0.5159 0.0000 ( 1351 PWs) bands (ev):
-12.7202 -10.9033 -9.2657 -0.1767 2.0119 11.7926 12.1809 13.9017

k = 0.2959 0.5124 0.0000 ( 1355 PWs) bands (ev):
-12.7869 -10.8556 -9.2256 -0.2428 2.0777 11.8093 12.0796 13.9007

k = 0.2939 0.5090 0.0000 ( 1355 PWs) bands (ev):
-12.8539 -10.8074 -9.1844 -0.3092 2.1440 11.8261 11.9780 13.8984

k = 0.2919 0.5056 0.0000 ( 1351 PWs) bands (ev):
-12.9211 -10.7588 -9.1422 -0.3760 2.2108 11.8428 11.8764 13.8946

k = 0.2899 0.5022 0.0000 ( 1351 PWs) bands (ev):
-12.9885 -10.7098 -9.0992 -0.4430 2.2782 11.7747 11.8592 13.8896

k = 0.2880 0.4988 0.0000 ( 1351 PWs) bands (ev):
-13.0560 -10.6603 -9.0553 -0.5103 2.3462 11.6731 11.8753 13.8832

k = 0.2860 0.4954 0.0000 ( 1351 PWs) bands (ev):
-13.1236 -10.6104 -9.0106 -0.5778 2.4146 11.5716 11.8908 13.8757

k = 0.2840 0.4919 0.0000 ( 1351 PWs) bands (ev):
-13.1912 -10.5600 -8.9652 -0.6455 2.4836 11.4703 11.9056 13.8670

k = 0.2820 0.4885 0.0000 ( 1351 PWs) bands (ev):
-13.2588 -10.5093 -8.9189 -0.7134 2.5531 11.3692 11.9195 13.8573

k = 0.2801 0.4851 0.0000 ( 1351 PWs) bands (ev):
-13.3264 -10.4581 -8.8720 -0.7815 2.6232 11.2684 11.9323 13.8464

k = 0.2781 0.4817 0.0000 ( 1355 PWs) bands (ev):
-13.3939 -10.4064 -8.8244 -0.8498 2.6937 11.1680 11.9439 13.8347

k = 0.2761 0.4783 0.0000 ( 1355 PWs) bands (ev):
-13.4613 -10.3544 -8.7762 -0.9182 2.7648 11.0679 11.9540 13.8112

k = 0.2742 0.4749 0.0000 ( 1355 PWs) bands (ev):
-13.5286 -10.3019 -8.7273 -0.9867 2.8364 10.9681 11.9625 13.7667

k = 0.2722 0.4714 0.0000 ( 1355 PWs) bands (ev):
```

```
-13.5957 -10.2490 -8.6778 -1.0552 2.9085 10.8688 11.9691 13.7208
      k = 0.2702 0.4680 0.0000 ( 1353 PWs) bands (ev):
-13.6627 -10.1957 -8.6278 -1.1238 2.9810 10.7700 11.9737 13.6736
      k = 0.2682 0.4646 0.0000 ( 1353 PWs) bands (ev):
-13.7295 -10.1419 -8.5772 -1.1925 3.0541 10.6716 11.9761 13.6252
      k = 0.2663 0.4612 0.0000 ( 1353 PWs) bands (ev):
-13.7961 -10.0878 -8.5260 -1.2612 3.1277 10.5736 11.9761 13.5757
      k = 0.2643 0.4578 0.0000 ( 1357 PWs) bands (ev):
-13.8625 -10.0332 -8.4744 -1.3299 3.2017 10.4762 11.9735 13.5253
      k = 0.2623 0.4544 0.0000 ( 1357 PWs) bands (ev):
-13.9286 -9.9782 -8.4222 -1.3985 3.2762 10.3794 11.9683 13.4740
      k = 0.2604 0.4509 0.0000 ( 1357 PWs) bands (ev):
-13.9945 -9.9228 -8.3696 -1.4672 3.3513 10.2830 11.9602 13.4219
      k = 0.2584 0.4475 0.0000 ( 1357 PWs) bands (ev):
-14.0601 -9.8670 -8.3165 -1.5358 3.4267 10.1872 11.9492 13.3691
      k = 0.2564 0.4441 0.0000 ( 1357 PWs) bands (ev):
-14.1254 -9.8107 -8.2629 -1.6043 3.5027 10.0920 11.9353 13.3156
      k = 0.2544 0.4407 0.0000 ( 1361 PWs) bands (ev):
-14.1904 -9.7541 -8.2089 -1.6727 3.5791 9.9974 11.9183 13.2616
      k = 0.2525 0.4373 0.0000 ( 1349 PWs) bands (ev):
-14.2552 -9.6970 -8.1545 -1.7410 3.6560 9.9033 11.8983 13.2071
      k = 0.2505 0.4339 0.0000 ( 1349 PWs) bands (ev):
-14.3196 -9.6395 -8.0997 -1.8092 3.7333 9.8099 11.8752 13.1521
      k = 0.2485 0.4304 0.0000 ( 1349 PWs) bands (ev):
-14.3836 -9.5817 -8.0444 -1.8773 3.8110 9.7170 11.8492 13.0968
      k = 0.2465 0.4270 0.0000 ( 1349 PWs) bands (ev):
-14.4474 -9.5235 -7.9888 -1.9452 3.8892 9.6248 11.8203 13.0411
      k = 0.2446 0.4236 0.0000 ( 1345 PWs) bands (ev):
-14.5108 -9.4648 -7.9328 -2.0130 3.9679 9.5332 11.7885 12.9852
      k = 0.2426 0.4202 0.0000 ( 1345 PWs) bands (ev):
-14.5738 -9.4057 -7.8765 -2.0805 4.0469 9.4423 11.7541 12.9290
```

```
k = 0.2406 0.4168 0.0000 ( 1345 PWs) bands (ev):
-14.6365 -9.3463 -7.8198 -2.1479 4.1263 9.3520 11.7171 12.8727

k = 0.2387 0.4134 0.0000 ( 1341 PWs) bands (ev):
-14.6988 -9.2865 -7.7627 -2.2151 4.2062 9.2623 11.6776 12.8162

k = 0.2367 0.4099 0.0000 ( 1341 PWs) bands (ev):
-14.7607 -9.2263 -7.7054 -2.2820 4.2865 9.1733 11.6359 12.7596

k = 0.2347 0.4065 0.0000 ( 1341 PWs) bands (ev):
-14.8223 -9.1657 -7.6477 -2.3487 4.3671 9.0850 11.5921 12.7030

k = 0.2327 0.4031 0.0000 ( 1341 PWs) bands (ev):
-14.8834 -9.1047 -7.5897 -2.4152 4.4482 8.9973 11.5463 12.6463

k = 0.2308 0.3997 0.0000 ( 1341 PWs) bands (ev):
-14.9442 -9.0434 -7.5314 -2.4814 4.5296 8.9103 11.4986 12.5897

k = 0.2288 0.3963 0.0000 ( 1337 PWs) bands (ev):
-15.0045 -8.9816 -7.4728 -2.5473 4.6114 8.8239 11.4493 12.5331

k = 0.2268 0.3929 0.0000 ( 1333 PWs) bands (ev):
-15.0645 -8.9195 -7.4140 -2.6130 4.6936 8.7383 11.3985 12.4766

k = 0.2248 0.3895 0.0000 ( 1333 PWs) bands (ev):
-15.1240 -8.8571 -7.3549 -2.6783 4.7761 8.6533 11.3463 12.4202

k = 0.2229 0.3860 0.0000 ( 1333 PWs) bands (ev):
-15.1831 -8.7942 -7.2955 -2.7434 4.8590 8.5690 11.2929 12.3639

k = 0.2209 0.3826 0.0000 ( 1327 PWs) bands (ev):
-15.2418 -8.7310 -7.2358 -2.8081 4.9423 8.4854 11.2384 12.3078

k = 0.2189 0.3792 0.0000 ( 1323 PWs) bands (ev):
-15.3001 -8.6674 -7.1760 -2.8725 5.0258 8.4025 11.1829 12.2519

k = 0.2170 0.3758 0.0000 ( 1323 PWs) bands (ev):
-15.3579 -8.6035 -7.1159 -2.9366 5.1097 8.3203 11.1266 12.1962

k = 0.2150 0.3724 0.0000 ( 1323 PWs) bands (ev):
-15.4153 -8.5393 -7.0557 -3.0003 5.1939 8.2388 11.0695 12.1407

k = 0.2130 0.3690 0.0000 ( 1323 PWs) bands (ev):
-15.4723 -8.4747 -6.9952 -3.0637 5.2785 8.1580 11.0118 12.0854

k = 0.2110 0.3655 0.0000 ( 1329 PWs) bands (ev):
```



-15.5288	-8.4097	-6.9345	-3.1267	5.3633	8.0779	10.9535	12.0304
k = 0.2091 0.3621 0.0000 ( 1329 PWs)					bands (ev):		
-15.5849	-8.3444	-6.8737	-3.1893	5.4484	7.9985	10.8947	11.9756
k = 0.2071 0.3587 0.0000 ( 1329 PWs)					bands (ev):		
-15.6405	-8.2788	-6.8127	-3.2516	5.5338	7.9198	10.8356	11.9212
k = 0.2051 0.3553 0.0000 ( 1329 PWs)					bands (ev):		
-15.6957	-8.2128	-6.7515	-3.3134	5.6194	7.8418	10.7761	11.8671
k = 0.2032 0.3519 0.0000 ( 1329 PWs)					bands (ev):		
-15.7504	-8.1466	-6.6901	-3.3749	5.7053	7.7646	10.7164	11.8134
k = 0.2012 0.3485 0.0000 ( 1329 PWs)					bands (ev):		
-15.8046	-8.0800	-6.6287	-3.4359	5.7915	7.6880	10.6566	11.7600
k = 0.1992 0.3450 0.0000 ( 1329 PWs)					bands (ev):		
-15.8584	-8.0130	-6.5671	-3.4966	5.8779	7.6122	10.5966	11.7069
k = 0.1972 0.3416 0.0000 ( 1331 PWs)					bands (ev):		
-15.9117	-7.9458	-6.5053	-3.5568	5.9646	7.5371	10.5365	11.6542
k = 0.1953 0.3382 0.0000 ( 1331 PWs)					bands (ev):		
-15.9646	-7.8783	-6.4435	-3.6166	6.0514	7.4627	10.4765	11.6019
k = 0.1933 0.3348 0.0000 ( 1331 PWs)					bands (ev):		
-16.0169	-7.8104	-6.3816	-3.6759	6.1385	7.3891	10.4165	11.5501
k = 0.1913 0.3314 0.0000 ( 1331 PWs)					bands (ev):		
-16.0688	-7.7423	-6.3195	-3.7348	6.2257	7.3161	10.3566	11.4986
k = 0.1893 0.3280 0.0000 ( 1337 PWs)					bands (ev):		
-16.1202	-7.6739	-6.2575	-3.7932	6.3131	7.2439	10.2968	11.4475
k = 0.1874 0.3245 0.0000 ( 1337 PWs)					bands (ev):		
-16.1712	-7.6052	-6.1953	-3.8512	6.4007	7.1724	10.2371	11.3969
k = 0.1854 0.3211 0.0000 ( 1337 PWs)					bands (ev):		
-16.2216	-7.5362	-6.1331	-3.9087	6.4885	7.1017	10.1777	11.3468
k = 0.1834 0.3177 0.0000 ( 1337 PWs)					bands (ev):		
-16.2716	-7.4669	-6.0708	-3.9658	6.5764	7.0316	10.1185	11.2971
k = 0.1815 0.3143 0.0000 ( 1337 PWs)					bands (ev):		
-16.3211	-7.3974	-6.0086	-4.0224	6.6644	6.9623	10.0595	11.2479

```
k = 0.1795 0.3109 0.0000 ( 1329 PWs) bands (ev):
-16.3700 -7.3275 -5.9462 -4.0785 6.7526 6.8937 10.0009 11.1992

k = 0.1775 0.3075 0.0000 ( 1329 PWs) bands (ev):
-16.4185 -7.2575 -5.8839 -4.1341 6.8259 6.8408 9.9425 11.1510

k = 0.1755 0.3040 0.0000 ( 1333 PWs) bands (ev):
-16.4665 -7.1872 -5.8217 -4.1892 6.7588 6.9291 9.8845 11.1032

k = 0.1736 0.3006 0.0000 ( 1331 PWs) bands (ev):
-16.5140 -7.1167 -5.7594 -4.2438 6.6924 7.0175 9.8269 11.0560

k = 0.1716 0.2972 0.0000 ( 1335 PWs) bands (ev):
-16.5611 -7.0459 -5.6971 -4.2979 6.6268 7.1060 9.7696 11.0092

k = 0.1696 0.2938 0.0000 ( 1335 PWs) bands (ev):
-16.6076 -6.9750 -5.6349 -4.3515 6.5619 7.1945 9.7127 10.9630

k = 0.1677 0.2904 0.0000 ( 1335 PWs) bands (ev):
-16.6536 -6.9038 -5.5728 -4.4046 6.4977 7.2830 9.6563 10.9174

k = 0.1657 0.2870 0.0000 ( 1335 PWs) bands (ev):
-16.6991 -6.8324 -5.5107 -4.4571 6.4343 7.3715 9.6003 10.8722

k = 0.1637 0.2835 0.0000 ( 1335 PWs) bands (ev):
-16.7441 -6.7608 -5.4488 -4.5092 6.3716 7.4601 9.5447 10.8277

k = 0.1617 0.2801 0.0000 ( 1335 PWs) bands (ev):
-16.7886 -6.6890 -5.3869 -4.5607 6.3097 7.5486 9.4896 10.7836

k = 0.1598 0.2767 0.0000 ( 1333 PWs) bands (ev):
-16.8325 -6.6170 -5.3251 -4.6117 6.2485 7.6370 9.4350 10.7402

k = 0.1578 0.2733 0.0000 ( 1333 PWs) bands (ev):
-16.8760 -6.5449 -5.2635 -4.6621 6.1880 7.7254 9.3809 10.6973

k = 0.1558 0.2699 0.0000 ( 1333 PWs) bands (ev):
-16.9190 -6.4726 -5.2020 -4.7120 6.1283 7.8138 9.3273 10.6549

k = 0.1538 0.2665 0.0000 ( 1333 PWs) bands (ev):
-16.9614 -6.4002 -5.1406 -4.7614 6.0693 7.9020 9.2742 10.6132

k = 0.1519 0.2631 0.0000 ( 1327 PWs) bands (ev):
-17.0034 -6.3276 -5.0794 -4.8102 6.0111 7.9901 9.2216 10.5720

k = 0.1499 0.2596 0.0000 ( 1327 PWs) bands (ev):
```

-17.0448	-6.2549	-5.0184	-4.8584	5.9536	8.0781	9.1696	10.5314
k = 0.1479 0.2562 0.0000 ( 1335 PWs)					bands (ev):		
-17.0857	-6.1821	-4.9576	-4.9061	5.8968	8.1659	9.1181	10.4914
k = 0.1460 0.2528 0.0000 ( 1327 PWs)					bands (ev):		
-17.1261	-6.1091	-4.9533	-4.8969	5.8408	8.2536	9.0672	10.4520
k = 0.1440 0.2494 0.0000 ( 1327 PWs)					bands (ev):		
-17.1660	-6.0361	-4.9998	-4.8366	5.7855	8.3411	9.0168	10.4132
k = 0.1420 0.2460 0.0000 ( 1327 PWs)					bands (ev):		
-17.2053	-5.9630	-5.0458	-4.7764	5.7310	8.4284	8.9670	10.3750
k = 0.1400 0.2426 0.0000 ( 1327 PWs)					bands (ev):		
-17.2442	-5.8899	-5.0913	-4.7166	5.6772	8.5154	8.9178	10.3374
k = 0.1381 0.2391 0.0000 ( 1331 PWs)					bands (ev):		
-17.2825	-5.8167	-5.1361	-4.6570	5.6242	8.6021	8.8692	10.3004
k = 0.1361 0.2357 0.0000 ( 1327 PWs)					bands (ev):		
-17.3203	-5.7434	-5.1804	-4.5976	5.5719	8.6886	8.8212	10.2641
k = 0.1341 0.2323 0.0000 ( 1327 PWs)					bands (ev):		
-17.3576	-5.6701	-5.2241	-4.5386	5.5204	8.7738	8.7748	10.2284
k = 0.1321 0.2289 0.0000 ( 1327 PWs)					bands (ev):		
-17.3943	-5.5969	-5.2672	-4.4800	5.4696	8.7270	8.8607	10.1933
k = 0.1302 0.2255 0.0000 ( 1327 PWs)					bands (ev):		
-17.4305	-5.5236	-5.3098	-4.4216	5.4196	8.6808	8.9462	10.1588
k = 0.1282 0.2221 0.0000 ( 1327 PWs)					bands (ev):		
-17.4662	-5.4504	-5.3517	-4.3636	5.3703	8.6353	9.0313	10.1250
k = 0.1262 0.2186 0.0000 ( 1323 PWs)					bands (ev):		
-17.5014	-5.3931	-5.3771	-4.3060	5.3217	8.5903	9.1160	10.0918
k = 0.1243 0.2152 0.0000 ( 1323 PWs)					bands (ev):		
-17.5360	-5.4339	-5.3039	-4.2488	5.2739	8.5460	9.2003	10.0592
k = 0.1223 0.2118 0.0000 ( 1327 PWs)					bands (ev):		
-17.5701	-5.4741	-5.2309	-4.1919	5.2269	8.5023	9.2842	10.0273
k = 0.1203 0.2084 0.0000 ( 1327 PWs)					bands (ev):		
-17.6037	-5.5136	-5.1579	-4.1355	5.1806	8.4593	9.3676	9.9960

```
k = 0.1183 0.2050 0.0000 ( 1327 PWs) bands (ev):
-17.6367 -5.5526 -5.0851 -4.0796 5.1350 8.4169 9.4504 9.9654

k = 0.1164 0.2016 0.0000 ( 1327 PWs) bands (ev):
-17.6692 -5.5910 -5.0124 -4.0240 5.0902 8.3751 9.5328 9.9354

k = 0.1144 0.1981 0.0000 ( 1327 PWs) bands (ev):
-17.7012 -5.6287 -4.9398 -3.9690 5.0462 8.3340 9.6146 9.9061

k = 0.1124 0.1947 0.0000 ( 1331 PWs) bands (ev):
-17.7326 -5.6659 -4.8675 -3.9144 5.0029 8.2936 9.6958 9.8774

k = 0.1105 0.1913 0.0000 ( 1331 PWs) bands (ev):
-17.7636 -5.7024 -4.7953 -3.8604 4.9604 8.2538 9.7764 9.8494

k = 0.1085 0.1879 0.0000 ( 1331 PWs) bands (ev):
-17.7939 -5.7383 -4.7233 -3.8069 4.9186 8.2147 9.8220 9.8563

k = 0.1065 0.1845 0.0000 ( 1327 PWs) bands (ev):
-17.8238 -5.7736 -4.6516 -3.7539 4.8775 8.1762 9.7953 9.9357

k = 0.1045 0.1811 0.0000 ( 1323 PWs) bands (ev):
-17.8531 -5.8083 -4.5802 -3.7014 4.8372 8.1384 9.7692 10.0143

k = 0.1026 0.1776 0.0000 ( 1323 PWs) bands (ev):
-17.8818 -5.8424 -4.5090 -3.6496 4.7977 8.1013 9.7438 10.0921

k = 0.1006 0.1742 0.0000 ( 1323 PWs) bands (ev):
-17.9100 -5.8759 -4.4382 -3.5983 4.7589 8.0648 9.7190 10.1693

k = 0.0986 0.1708 0.0000 ( 1323 PWs) bands (ev):
-17.9377 -5.9087 -4.3678 -3.5477 4.7209 8.0290 9.6949 10.2456

k = 0.0966 0.1674 0.0000 ( 1319 PWs) bands (ev):
-17.9649 -5.9409 -4.2977 -3.4976 4.6836 7.9939 9.6715 10.3211

k = 0.0947 0.1640 0.0000 ( 1319 PWs) bands (ev):
-17.9915 -5.9725 -4.2280 -3.4483 4.6471 7.9595 9.6487 10.3696

k = 0.0927 0.1606 0.0000 ( 1325 PWs) bands (ev):
-18.0176 -6.0035 -4.1588 -3.3996 4.6113 7.9258 9.6265 10.3347

k = 0.0907 0.1571 0.0000 ( 1325 PWs) bands (ev):
-18.0431 -6.0338 -4.0901 -3.3516 4.5763 7.8927 9.6050 10.3004

k = 0.0888 0.1537 0.0000 ( 1319 PWs) bands (ev):
```

-18.0681	-6.0635	-4.0218	-3.3043	4.5420	7.8603	9.5842	10.2668
k = 0.0868 0.1503 0.0000 ( 1319 PWs)					bands (ev):		
-18.0925	-6.0925	-3.9541	-3.2577	4.5085	7.8287	9.5640	10.2339
k = 0.0848 0.1469 0.0000 ( 1315 PWs)					bands (ev):		
-18.1164	-6.1210	-3.8869	-3.2119	4.4757	7.7977	9.5445	10.2015
k = 0.0828 0.1435 0.0000 ( 1315 PWs)					bands (ev):		
-18.1398	-6.1488	-3.8204	-3.1668	4.4437	7.7674	9.5256	10.1699
k = 0.0809 0.1401 0.0000 ( 1315 PWs)					bands (ev):		
-18.1626	-6.1759	-3.7545	-3.1225	4.4124	7.7378	9.5073	10.1388
k = 0.0789 0.1366 0.0000 ( 1315 PWs)					bands (ev):		
-18.1848	-6.2024	-3.6893	-3.0790	4.3819	7.7088	9.4897	10.1084
k = 0.0769 0.1332 0.0000 ( 1315 PWs)					bands (ev):		
-18.2066	-6.2283	-3.6248	-3.0363	4.3522	7.6806	9.4728	10.0787
k = 0.0749 0.1298 0.0000 ( 1315 PWs)					bands (ev):		
-18.2277	-6.2536	-3.5611	-2.9944	4.3232	7.6531	9.4564	10.0496
k = 0.0730 0.1264 0.0000 ( 1315 PWs)					bands (ev):		
-18.2484	-6.2782	-3.4982	-2.9534	4.2949	7.6263	9.4407	10.0211
k = 0.0710 0.1230 0.0000 ( 1315 PWs)					bands (ev):		
-18.2685	-6.3021	-3.4361	-2.9133	4.2674	7.6002	9.4257	9.9933
k = 0.0690 0.1196 0.0000 ( 1315 PWs)					bands (ev):		
-18.2880	-6.3254	-3.3749	-2.8740	4.2407	7.5748	9.4112	9.9661
k = 0.0671 0.1162 0.0000 ( 1307 PWs)					bands (ev):		
-18.3070	-6.3481	-3.3146	-2.8355	4.2147	7.5501	9.3974	9.9396
k = 0.0651 0.1127 0.0000 ( 1307 PWs)					bands (ev):		
-18.3254	-6.3701	-3.2553	-2.7981	4.1895	7.5261	9.3842	9.9136
k = 0.0631 0.1093 0.0000 ( 1311 PWs)					bands (ev):		
-18.3434	-6.3915	-3.1970	-2.7615	4.1650	7.5028	9.3716	9.8884
k = 0.0611 0.1059 0.0000 ( 1311 PWs)					bands (ev):		
-18.3607	-6.4122	-3.1398	-2.7259	4.1412	7.4802	9.3596	9.8637
k = 0.0592 0.1025 0.0000 ( 1311 PWs)					bands (ev):		
-18.3775	-6.4323	-3.0838	-2.6913	4.1183	7.4583	9.3482	9.8398

```
k = 0.0572 0.0991 0.0000 ( 1301 PWs) bands (ev):
-18.3938 -6.4517 -3.0287 -2.6576 4.0961 7.4371 9.3375 9.8164

k = 0.0552 0.0957 0.0000 ( 1301 PWs) bands (ev):
-18.4095 -6.4705 -2.9750 -2.6249 4.0746 7.4166 9.3272 9.7937

k = 0.0533 0.0922 0.0000 ( 1301 PWs) bands (ev):
-18.4246 -6.4886 -2.9225 -2.5932 4.0539 7.3969 9.3176 9.7716

k = 0.0513 0.0888 0.0000 ( 1301 PWs) bands (ev):
-18.4393 -6.5061 -2.8714 -2.5626 4.0339 7.3778 9.3085 9.7502

k = 0.0493 0.0854 0.0000 ( 1301 PWs) bands (ev):
-18.4533 -6.5229 -2.8216 -2.5330 4.0147 7.3595 9.3000 9.7295

k = 0.0473 0.0820 0.0000 ( 1305 PWs) bands (ev):
-18.4668 -6.5391 -2.7733 -2.5044 3.9963 7.3419 9.2920 9.7094

k = 0.0454 0.0786 0.0000 ( 1305 PWs) bands (ev):
-18.4798 -6.5546 -2.7264 -2.4769 3.9786 7.3250 9.2846 9.6899

k = 0.0434 0.0752 0.0000 ( 1301 PWs) bands (ev):
-18.4922 -6.5694 -2.6810 -2.4505 3.9616 7.3088 9.2777 9.6711

k = 0.0414 0.0717 0.0000 ( 1297 PWs) bands (ev):
-18.5041 -6.5836 -2.6372 -2.4251 3.9454 7.2933 9.2714 9.6530

k = 0.0394 0.0683 0.0000 ( 1293 PWs) bands (ev):
-18.5154 -6.5972 -2.5949 -2.4008 3.9300 7.2786 9.2656 9.6355

k = 0.0375 0.0649 0.0000 ( 1293 PWs) bands (ev):
-18.5262 -6.6101 -2.5544 -2.3777 3.9153 7.2645 9.2602 9.6188

k = 0.0355 0.0615 0.0000 ( 1293 PWs) bands (ev):
-18.5364 -6.6223 -2.5156 -2.3556 3.9014 7.2512 9.2554 9.5969

k = 0.0335 0.0581 0.0000 ( 1291 PWs) bands (ev):
-18.5460 -6.6339 -2.4785 -2.3347 3.8882 7.2386 9.2510 9.5589

k = 0.0316 0.0547 0.0000 ( 1295 PWs) bands (ev):
-18.5551 -6.6448 -2.4434 -2.3150 3.8758 7.2267 9.2469 9.5226

k = 0.0296 0.0512 0.0000 ( 1295 PWs) bands (ev):
-18.5637 -6.6550 -2.4100 -2.2964 3.8641 7.2155 9.2434 9.4881

k = 0.0276 0.0478 0.0000 ( 1295 PWs) bands (ev):
```

```

-18.5717  -6.6646  -2.3786  -2.2789   3.8532   7.2051   9.2403   9.4555
      k = 0.0256 0.0444 0.0000 ( 1295 PWs)  bands (ev):
-18.5792  -6.6736  -2.3491  -2.2626   3.8430   7.1954   9.2376   9.4248
      k = 0.0237 0.0410 0.0000 ( 1295 PWs)  bands (ev):
-18.5861  -6.6818  -2.3217  -2.2475   3.8336   7.1863   9.2352   9.3961
      k = 0.0217 0.0376 0.0000 ( 1293 PWs)  bands (ev):
-18.5924  -6.6895  -2.2962  -2.2335   3.8250   7.1780   9.2332   9.3695
      k = 0.0197 0.0342 0.0000 ( 1293 PWs)  bands (ev):
-18.5982  -6.6964  -2.2729  -2.2208   3.8171   7.1705   9.2315   9.3450
      k = 0.0178 0.0307 0.0000 ( 1293 PWs)  bands (ev):
-18.6035  -6.7027  -2.2516  -2.2093   3.8099   7.1636   9.2301   9.3227
      k = 0.0158 0.0273 0.0000 ( 1297 PWs)  bands (ev):
-18.6082  -6.7083  -2.2325  -2.1989   3.8035   7.1575   9.2289   9.3026
      k = 0.0138 0.0239 0.0000 ( 1297 PWs)  bands (ev):
-18.6123  -6.7133  -2.2156  -2.1898   3.7979   7.1521   9.2280   9.2847
      k = 0.0118 0.0205 0.0000 ( 1301 PWs)  bands (ev):
-18.6159  -6.7176  -2.2009  -2.1818   3.7930   7.1474   9.2273   9.2692
      k = 0.0099 0.0171 0.0000 ( 1301 PWs)  bands (ev):
-18.6189  -6.7213  -2.1884  -2.1751   3.7888   7.1434   9.2267   9.2560
      k = 0.0079 0.0137 0.0000 ( 1301 PWs)  bands (ev):
-18.6214  -6.7242  -2.1781  -2.1696   3.7855   7.1402   9.2263   9.2451
      k = 0.0059 0.0102 0.0000 ( 1301 PWs)  bands (ev):
-18.6234  -6.7266  -2.1701  -2.1653   3.7828   7.1376   9.2260   9.2366
      k = 0.0039 0.0068 0.0000 ( 1301 PWs)  bands (ev):
-18.6247  -6.7282  -2.1644  -2.1623   3.7809   7.1358   9.2259   9.2306
      k = 0.0020 0.0034 0.0000 ( 1301 PWs)  bands (ev):
-18.6256  -6.7292  -2.1610  -2.1604   3.7798   7.1348   9.2258   9.2269
      k = 0.0000 0.0000 0.0000 ( 1301 PWs)  bands (ev):
-18.6259  -6.7295  -2.1598  -2.1598   3.7794   7.1344   9.2257   9.2257

```

Writing output data file ./tmp-hetero/A.save/

init\_run : 1.26s CPU 1.31s WALL ( 1 calls)

electrons : 255.35s CPU 227.92s WALL ( 1 calls)

Called by init\_run:

wfcinit : 0.00s CPU 0.00s WALL ( 1 calls)  
wfcinit:atom : 0.46s CPU 0.42s WALL ( 800 calls)  
wfcinit:wfc : 19.12s CPU 16.03s WALL ( 800 calls)  
potinit : 0.62s CPU 0.64s WALL ( 1 calls)  
hinit0 : 0.36s CPU 0.36s WALL ( 1 calls)

Called by electrons:

c\_bands : 255.34s CPU 227.90s WALL ( 1 calls)  
v\_of\_rho : 0.57s CPU 0.60s WALL ( 1 calls)  
v\_h : 0.01s CPU 0.01s WALL ( 1 calls)  
v\_xc : 0.57s CPU 0.59s WALL ( 1 calls)  
newd : 0.04s CPU 0.06s WALL ( 1 calls)

Called by c\_bands:

init\_us\_2 : 0.56s CPU 0.54s WALL ( 800 calls)  
cegterg : 226.36s CPU 184.68s WALL ( 1063 calls)

Called by sum\_band:

Called by \*egterg:

h\_psi : 209.90s CPU 173.40s WALL ( 16855 calls)  
s\_psi : 3.00s CPU 2.30s WALL ( 16855 calls)  
g\_psi : 1.17s CPU 0.85s WALL ( 14992 calls)  
cdiaghg : 10.02s CPU 8.27s WALL ( 15792 calls)  
cegterg:over : 8.54s CPU 6.59s WALL ( 14992 calls)  
cegterg:upda : 6.40s CPU 4.85s WALL ( 14992 calls)  
cegterg:last : 4.07s CPU 2.75s WALL ( 3491 calls)

Called by h\_psi:

h\_psi:calbec : 3.73s CPU 2.93s WALL ( 16855 calls)  
vloc\_psi : 202.44s CPU 167.63s WALL ( 16855 calls)  
add\_vuspsi : 3.19s CPU 2.46s WALL ( 16855 calls)

General routines

calbec : 3.64s CPU 2.87s WALL ( 16855 calls)  
fft : 0.13s CPU 0.13s WALL ( 22 calls)  
ffts : 0.02s CPU 0.02s WALL ( 2 calls)  
fftw : 186.69s CPU 155.76s WALL ( 168114 calls)  
interpolate : 0.03s CPU 0.03s WALL ( 2 calls)  
davcio : 6.37s CPU 24.35s WALL ( 1600 calls)

Parallel routines

PWSCF : 4m17.43s CPU 3m51.58s WALL

This run was terminated on: 19:35:24 250ct2023

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JOB DONE.

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