```
     Program PWSCF v.5.1 starts

     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);
          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     8 processors
     R & G space division:  proc/nbgrp/npool/nimage =       8
     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
               file C.pbe-rrkjus.UPF: wavefunction(s)  2S 2P renormalized

     Subspace diagonalization in iterative solution of the eigenvalue problem:
     scalapack distributed-memory algorithm (size of sub-group:  2*  2 procs)


     Parallelization info
     --------------------
     sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
     Min        1118     446    119               256124    64802    9013
     Max        1119     447    120               256141    64831    9030
     Sum        8947    3571    955              2049049   518527   72155

     Generating pointlists ...
     new r_m :   0.0595 (alat units)  1.0721 (a.u.) for type    1
     new r_m :   0.0595 (alat units)  1.0719 (a.u.) for type    2
     new r_m :   0.0595 (alat units)  1.0719 (a.u.) for type    3


     bravais-lattice index     =            4
     lattice parameter (alat)  =      18.0060  a.u.
     unit-cell volume          =   15167.1375 (a.u.)^3
     number of atoms/cell      =           64
     number of atomic types    =            3
     number of electrons       =       256.00
     number of Kohn-Sham states=          154
     kinetic-energy cutoff     =      40.0000  Ry
     charge density cutoff     =     400.0000  Ry
     convergence threshold     =      1.0E-06
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation      = PBE ( 1  4  3  4 0)

     celldm(1)=  18.006000  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 )
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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


PseudoPot. # 2 for  B read from file:
./pseudo/B.pbe-n-rrkjus_psl.0.1.UPF
MD5 check sum: 82e190d381d3269bb317afd43cf1db29
Pseudo is Ultrasoft + core correction, Zval =  3.0
Generated using "atomic" code by A. Dal Corso  (Quantum ESPRESSO distribution)
Using radial grid of 1059 points,  4 beta functions with:
           l(1) =   0
           l(2) =   0
           l(3) =   1
           l(4) =   1
Q(r) pseudized with 0 coefficients


PseudoPot. # 3 for  N read from file:
./pseudo/N.pbe-n-rrkjus_psl.0.1.UPF
MD5 check sum: c8986a496cba5b831c7822586319e126
Pseudo is Ultrasoft + core correction, Zval =  5.0
Generated using "atomic" code by A. Dal Corso  (Quantum ESPRESSO distribution)
Using radial grid of 1085 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)
   B              3.00    10.81000      B( 1.00)
   N              5.00    14.01000      N( 1.00)

Starting magnetic structure
atomic species   magnetization
   C            0.500
   B           -0.500
   N            0.000

No symmetry found

                                s                       frac. trans.
```

```
      isym =  1     identity

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

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


     point group C_1 (1)
     there are  1 classes
     the character table:

       E
A      1.00

     the symmetry operations in each class:
     E        1

   Cartesian axes

     site n.     atom                  positions (alat units)
         1           C   tau(   1) = (  -0.3722375   0.7921450   1.5717749  )
         2           C   tau(   2) = (  -0.2473937   0.7200621   1.5623312  )
         3           C   tau(   3) = (  -0.2474672   0.5755947   1.5610503  )
         4           C   tau(   4) = (  -0.1224101   0.5034082   1.5545272  )
         5           C   tau(   5) = (  -0.1223487   0.3591504   1.5625054  )
         6           C   tau(   6) = (   0.0027039   0.2869919   1.5671389  )
         7           C   tau(   7) = (   0.1277631   0.3591980   1.5678735  )
         8           C   tau(   8) = (   0.2525680   0.2870921   1.5788444  )
         9           C   tau(   9) = (   0.1278264   0.5033915   1.5583770  )
        10           C   tau(  10) = (   0.0027713   0.5755675   1.5496450  )
        11           C   tau(  11) = (   0.0026935   0.7201541   1.5517755  )
        12           C   tau(  12) = (  -0.1223495   0.7923689   1.5590566  )
        13           C   tau(  13) = (   0.1277242   0.7922795   1.5584410  )
        14           C   tau(  14) = (   0.2527545   0.7200131   1.5636008  )
        15           C   tau(  15) = (   0.2527616   0.5755804   1.5658001  )
        16           C   tau(  16) = (   0.3775246   0.5035911   1.5781177  )
        17           C   tau(  17) = (   0.3776089   0.3592186   1.5826729  )
        18           C   tau(  18) = (   0.5027638   0.2869259   1.5823156  )
        19           C   tau(  19) = (   0.3776228   0.7921513   1.5714527  )
        20           C   tau(  20) = (   0.5026924   0.7200085   1.5742543  )
        21           C   tau(  21) = (   0.5027082   0.5756984   1.5772995  )
        22           C   tau(  22) = (   0.6278335   0.5035639   1.5733955  )
        23           C   tau(  23) = (   0.6277597   0.3591836   1.5767004  )
        24           C   tau(  24) = (   0.7527147   0.2870630   1.5705184  )
        25           C   tau(  25) = (   0.7526826   0.1426472   1.5707590  )
        26           C   tau(  26) = (   0.8776967   0.0704876   1.5715409  )
        27           C   tau(  27) = (   0.6276465   0.0704622   1.5677100  )
        28           C   tau(  28) = (   0.5027096   0.1426048   1.5746582  )
        29           C   tau(  29) = (   0.3777101   0.0703786   1.5713144  )
        30           C   tau(  30) = (   0.2527081   0.1426074   1.5773510  )
        31           C   tau(  31) = (   0.1277052   0.0704799   1.5750035  )
        32           C   tau(  32) = (   0.0026733   0.1427159   1.5735559  )
        33           B   tau(  33) = (  -0.3722930   0.7921719   1.0499985  )
        34           N   tau(  34) = (  -0.2472939   0.7200032   1.0499987  )
        35           B   tau(  35) = (  -0.2473184   0.5756731   1.0499987  )
        36           N   tau(  36) = (  -0.1223232   0.5035014   1.0499977  )
        37           B   tau(  37) = (  -0.1223036   0.3591545   1.0499986  )
        38           N   tau(  38) = (   0.0027018   0.2870027   1.0499986  )
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      39           B   tau(  39) = (   0.1276928   0.3591775   1.0499986  )
      40           N   tau(  40) = (   0.2526728   0.2870002   1.0499988  )
      41           N   tau(  41) = (   0.1277082   0.5034989   1.0499979  )
      42           B   tau(  42) = (   0.0027070   0.5756602   1.0499991  )
      43           N   tau(  43) = (   0.0026889   0.7200266   1.0499976  )
      44           B   tau(  44) = (  -0.1223171   0.7921996   1.0499987  )
      45           B   tau(  45) = (   0.1277154   0.7921930   1.0499986  )
      46           N   tau(  46) = (   0.2526964   0.7200017   1.0499982  )
      47           B   tau(  47) = (   0.2526871   0.5756705   1.0499986  )
      48           N   tau(  48) = (   0.3776797   0.5035212   1.0499988  )
      49           B   tau(  49) = (   0.3776924   0.3591732   1.0499978  )
      50           N   tau(  50) = (   0.5027047   0.2869886   1.0499988  )
      51           B   tau(  51) = (   0.3776931   0.7921707   1.0499980  )
      52           N   tau(  52) = (   0.5027012   0.7200196   1.0499986  )
      53           B   tau(  53) = (   0.5026998   0.5756503   1.0499979  )
      54           N   tau(  54) = (   0.6277079   0.5035044   1.0499985  )
      55           B   tau(  55) = (   0.6277035   0.3591749   1.0499979  )
      56           N   tau(  56) = (   0.7527054   0.2869984   1.0499984  )
      57           B   tau(  57) = (   0.7526904   0.1426600   1.0499982  )
      58           N   tau(  58) = (   0.8777103   0.0704830   1.0499986  )
      59           N   tau(  59) = (   0.6276960   0.0704893   1.0499983  )
      60           B   tau(  60) = (   0.5026952   0.1426459   1.0499981  )
      61           N   tau(  61) = (   0.3777058   0.0704853   1.0499984  )
      62           B   tau(  62) = (   0.2527205   0.1426623   1.0499979  )
      63           N   tau(  63) = (   0.1276933   0.0704829   1.0499987  )
      64           B   tau(  64) = (   0.0027020   0.1426665   1.0499981  )

   Crystallographic axes

     site n.     atom                  positions (cryst. coord.)
          1           C   tau(   1) = (  0.0851076  0.9146903  0.5239250  )
          2           C   tau(   2) = (  0.1683343  0.8314561  0.5207771  )
          3           C   tau(   3) = (  0.0848525  0.6646395  0.5203501  )
          4           C   tau(   4) = (  0.1682328  0.5812857  0.5181757  )
          5           C   tau(   5) = (  0.0850069  0.4147111  0.5208351  )
          6           C   tau(   6) = (  0.1683988  0.3313897  0.5223796  )
          7           C   tau(   7) = (  0.3351462  0.4147662  0.5226245  )
          8           C   tau(   8) = (  0.4183207  0.3315054  0.5262815  )
          9           C   tau(   9) = (  0.4184596  0.5812664  0.5194590  )
         10           C   tau(  10) = (  0.3350754  0.6646081  0.5165483  )
         11           C   tau(  11) = (  0.4184747  0.8315623  0.5172585  )
         12           C   tau(  12) = (  0.3351248  0.9149488  0.5196855  )
         13           C   tau(  13) = (  0.5851470  0.9148455  0.5194803  )
         14           C   tau(  14) = (  0.6684543  0.8313995  0.5212003  )
         15           C   tau(  15) = (  0.5850731  0.6646230  0.5219334  )
         16           C   tau(  16) = (  0.6682730  0.5814969  0.5260392  )
         17           C   tau(  17) = (  0.5850039  0.4147900  0.5275576  )
         18           C   tau(  18) = (  0.6684206  0.3313135  0.5274385  )
         19           C   tau(  19) = (  0.8349716  0.9146975  0.5238176  )
         20           C   tau(  20) = (  0.9183895  0.8313942  0.5247514  )
         21           C   tau(  21) = (  0.8350878  0.6647592  0.5257665  )
         22           C   tau(  22) = (  0.9185663  0.5814655  0.5244652  )
         23           C   tau(  23) = (  0.8351344  0.4147495  0.5255668  )
         24           C   tau(  24) = (  0.9184506  0.3314718  0.5235061  )
         25           C   tau(  25) = (  0.8350400  0.1647148  0.5235863  )
         26           C   tau(  26) = (  0.9183927  0.0813920  0.5238470  )
         27           C   tau(  27) = (  0.6683279  0.0813627  0.5225700  )
         28           C   tau(  28) = (  0.5850426  0.1646659  0.5248861  )
         29           C   tau(  29) = (  0.4183432  0.0812662  0.5237715  )
         30           C   tau(  30) = (  0.3350425  0.1646688  0.5257837  )
         31           C   tau(  31) = (  0.1683968  0.0813831  0.5250012  )
         32           C   tau(  32) = (  0.0850703  0.1647941  0.5245186  )
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     33           B   tau(  33) = (  0.0850676  0.9147213  0.3499995  )
     34           N   tau(  34) = (  0.1684001  0.8313880  0.3499996  )
     35           B   tau(  35) = (  0.0850466  0.6647301  0.3499996  )
     36           N   tau(  36) = (  0.1683735  0.5813934  0.3499992  )
     37           B   tau(  37) = (  0.0850543  0.4147159  0.3499995  )
     38           N   tau(  38) = (  0.1684028  0.3314021  0.3499995  )
     39           B   tau(  39) = (  0.3350640  0.4147425  0.3499995  )
     40           N   tau(  40) = (  0.4183724  0.3313993  0.3499996  )
     41           N   tau(  41) = (  0.4184034  0.5813905  0.3499993  )
     42           B   tau(  42) = (  0.3350646  0.6647152  0.3499997  )
     43           N   tau(  43) = (  0.4183964  0.8314151  0.3499992  )
     44           B   tau(  44) = (  0.3350596  0.9147533  0.3499996  )
     45           B   tau(  45) = (  0.5850883  0.9147457  0.3499995  )
     46           N   tau(  46) = (  0.6683896  0.8313864  0.3499994  )
     47           B   tau(  47) = (  0.5850506  0.6647271  0.3499995  )
     48           N   tau(  48) = (  0.6683878  0.5814163  0.3499996  )
     49           B   tau(  49) = (  0.5850611  0.4147375  0.3499993  )
     50           N   tau(  50) = (  0.6683977  0.3313859  0.3499996  )
     51           B   tau(  51) = (  0.8350530  0.9147199  0.3499993  )
     52           N   tau(  52) = (  0.9184048  0.8314070  0.3499995  )
     53           B   tau(  53) = (  0.8350516  0.6647037  0.3499993  )
     54           N   tau(  54) = (  0.9184063  0.5813968  0.3499995  )
     55           B   tau(  55) = (  0.8350732  0.4147395  0.3499993  )
     56           N   tau(  56) = (  0.9184040  0.3313972  0.3499995  )
     57           B   tau(  57) = (  0.8350552  0.1647295  0.3499994  )
     58           N   tau(  58) = (  0.9184036  0.0813868  0.3499995  )
     59           N   tau(  59) = (  0.6683931  0.0813941  0.3499994  )
     60           B   tau(  60) = (  0.5850518  0.1647133  0.3499994  )
     61           N   tau(  61) = (  0.4184006  0.0813894  0.3499995  )
     62           B   tau(  62) = (  0.3350866  0.1647322  0.3499993  )
     63           N   tau(  63) = (  0.1683866  0.0813866  0.3499996  )
     64           B   tau(  64) = (  0.0850706  0.1647371  0.3499994  )

  number of k points=    40  Marzari-Vanderbilt smearing, width (Ry)=  0.0010
                    cart. coord. in units 2pi/alat
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0277778
     k(    2) = (   0.0000000   0.1924501   0.0000000), wk =   0.0555556
     k(    3) = (   0.0000000   0.3849002   0.0000000), wk =   0.0555556
     k(    4) = (   0.0000000  -0.5773503   0.0000000), wk =   0.0277778
     k(    5) = (   0.1666667   0.2886751   0.0000000), wk =   0.0555556
     k(    6) = (   0.1666667   0.4811252   0.0000000), wk =   0.0555556
     k(    7) = (   0.3333333   0.5773503   0.0000000), wk =   0.0555556
     k(    8) = (  -0.1666667   0.0962250   0.0000000), wk =   0.0555556
     k(    9) = (   0.1666667   0.0962250   0.0000000), wk =   0.0555556
     k(   10) = (  -0.3333333   0.1924501   0.0000000), wk =   0.0555556
     k(   11) = (   0.3333333   0.1924501   0.0000000), wk =   0.0555556
     k(   12) = (   0.5000000  -0.2886751   0.0000000), wk =   0.0277778
     k(   13) = (  -0.5000000  -0.2886751   0.0000000), wk =   0.0277778
     k(   14) = (  -0.1666667   0.2886751   0.0000000), wk =   0.0555556
     k(   15) = (   0.3333333   0.0000000   0.0000000), wk =   0.0555556
     k(   16) = (  -0.1666667   0.4811252   0.0000000), wk =   0.0555556
     k(   17) = (  -0.3333333   0.3849002   0.0000000), wk =   0.0555556
     k(   18) = (   0.5000000   0.0962250   0.0000000), wk =   0.0555556
     k(   19) = (  -0.3333333  -0.3849002   0.0000000), wk =   0.0555556
     k(   20) = (   0.5000000  -0.0962250   0.0000000), wk =   0.0555556
     k(   21) = (   0.0000000   0.0000000   0.0000000), wk =   0.0277778
     k(   22) = (   0.0000000   0.1924501   0.0000000), wk =   0.0555556
     k(   23) = (   0.0000000   0.3849002   0.0000000), wk =   0.0555556
     k(   24) = (   0.0000000  -0.5773503   0.0000000), wk =   0.0277778
     k(   25) = (   0.1666667   0.2886751   0.0000000), wk =   0.0555556
     k(   26) = (   0.1666667   0.4811252   0.0000000), wk =   0.0555556
     k(   27) = (   0.3333333   0.5773503   0.0000000), wk =   0.0555556
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     k(   28) = (  -0.1666667   0.0962250   0.0000000), wk =   0.0555556
     k(   29) = (   0.1666667   0.0962250   0.0000000), wk =   0.0555556
     k(   30) = (  -0.3333333   0.1924501   0.0000000), wk =   0.0555556
     k(   31) = (   0.3333333   0.1924501   0.0000000), wk =   0.0555556
     k(   32) = (   0.5000000  -0.2886751   0.0000000), wk =   0.0277778
     k(   33) = (  -0.5000000  -0.2886751   0.0000000), wk =   0.0277778
     k(   34) = (  -0.1666667   0.2886751   0.0000000), wk =   0.0555556
     k(   35) = (   0.3333333   0.0000000   0.0000000), wk =   0.0555556
     k(   36) = (  -0.1666667   0.4811252   0.0000000), wk =   0.0555556
     k(   37) = (  -0.3333333   0.3849002   0.0000000), wk =   0.0555556
     k(   38) = (   0.5000000   0.0962250   0.0000000), wk =   0.0555556
     k(   39) = (  -0.3333333  -0.3849002   0.0000000), wk =   0.0555556
     k(   40) = (   0.5000000  -0.0962250   0.0000000), wk =   0.0555556

                    cryst. coord.
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0277778
     k(    2) = (   0.0000000   0.1666667   0.0000000), wk =   0.0555556
     k(    3) = (   0.0000000   0.3333333   0.0000000), wk =   0.0555556
     k(    4) = (   0.0000000  -0.5000000   0.0000000), wk =   0.0277778
     k(    5) = (   0.1666667   0.1666667   0.0000000), wk =   0.0555556
     k(    6) = (   0.1666667   0.3333333   0.0000000), wk =   0.0555556
     k(    7) = (   0.3333333   0.3333333   0.0000000), wk =   0.0555556
     k(    8) = (  -0.1666667   0.1666667   0.0000000), wk =   0.0555556
     k(    9) = (   0.1666667   0.0000000   0.0000000), wk =   0.0555556
     k(   10) = (  -0.3333333   0.3333333   0.0000000), wk =   0.0555556
     k(   11) = (   0.3333333   0.0000000   0.0000000), wk =   0.0555556
     k(   12) = (   0.5000000  -0.5000000   0.0000000), wk =   0.0277778
     k(   13) = (  -0.5000000   0.0000000   0.0000000), wk =   0.0277778
     k(   14) = (  -0.1666667   0.3333333   0.0000000), wk =   0.0555556
     k(   15) = (   0.3333333  -0.1666667   0.0000000), wk =   0.0555556
     k(   16) = (  -0.1666667   0.5000000   0.0000000), wk =   0.0555556
     k(   17) = (  -0.3333333   0.5000000   0.0000000), wk =   0.0555556
     k(   18) = (   0.5000000  -0.1666667   0.0000000), wk =   0.0555556
     k(   19) = (  -0.3333333  -0.1666667   0.0000000), wk =   0.0555556
     k(   20) = (   0.5000000  -0.3333333   0.0000000), wk =   0.0555556
     k(   21) = (   0.0000000   0.0000000   0.0000000), wk =   0.0277778
     k(   22) = (   0.0000000   0.1666667   0.0000000), wk =   0.0555556
     k(   23) = (   0.0000000   0.3333333   0.0000000), wk =   0.0555556
     k(   24) = (   0.0000000  -0.5000000   0.0000000), wk =   0.0277778
     k(   25) = (   0.1666667   0.1666667   0.0000000), wk =   0.0555556
     k(   26) = (   0.1666667   0.3333333   0.0000000), wk =   0.0555556
     k(   27) = (   0.3333333   0.3333333   0.0000000), wk =   0.0555556
     k(   28) = (  -0.1666667   0.1666667   0.0000000), wk =   0.0555556
     k(   29) = (   0.1666667   0.0000000   0.0000000), wk =   0.0555556
     k(   30) = (  -0.3333333   0.3333333   0.0000000), wk =   0.0555556
     k(   31) = (   0.3333333   0.0000000   0.0000000), wk =   0.0555556
     k(   32) = (   0.5000000  -0.5000000   0.0000000), wk =   0.0277778
     k(   33) = (  -0.5000000   0.0000000   0.0000000), wk =   0.0277778
     k(   34) = (  -0.1666667   0.3333333   0.0000000), wk =   0.0555556
     k(   35) = (   0.3333333  -0.1666667   0.0000000), wk =   0.0555556
     k(   36) = (  -0.1666667   0.5000000   0.0000000), wk =   0.0555556
     k(   37) = (  -0.3333333   0.5000000   0.0000000), wk =   0.0555556
     k(   38) = (   0.5000000  -0.1666667   0.0000000), wk =   0.0555556
     k(   39) = (  -0.3333333  -0.1666667   0.0000000), wk =   0.0555556
     k(   40) = (   0.5000000  -0.3333333   0.0000000), wk =   0.0555556

   Dense  grid:  2049049 G-vectors     FFT dimensions: ( 120, 120, 360)

   Smooth grid:   518527 G-vectors     FFT dimensions: (  75,  75, 225)

   Largest allocated arrays     est. size (Mb)     dimensions
      Kohn-Sham Wavefunctions        19.13 Mb     (    8143,  154)
```

```
   NL pseudopotentials            63.62 Mb     (    8143,  512)
   Each V/rho on FFT grid         19.78 Mb     (  648000,   2)
   Each G-vector array             1.95 Mb     (  256128)
   G-vector shells                 0.06 Mb     (    7983)
Largest temporary arrays     est. size (Mb)     dimensions
   Auxiliary wavefunctions        76.54 Mb     (    8143,  616)
   Each subspace H/S matrix        1.45 Mb     (     308,  308)
   Each <psi_i|beta_j> matrix      1.20 Mb     (     512,  154)
   Arrays for rho mixing          79.10 Mb     (  648000,    8)

Check: negative/imaginary core charge=   -0.000004    0.000000

Initial potential from superposition of free atoms
Check: negative starting charge=(component1):   -0.000364
Check: negative starting charge=(component2):   -0.000374

starting charge  255.99368, renormalised to  256.00000

negative rho (up, down):  3.644E-04 3.744E-04
Starting wfc are  256 randomized atomic wfcs

total cpu time spent up to now is      934.5 secs

per-process dynamical memory:  1023.8 Mb

Self-consistent Calculation

iteration #  1     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  2.8

negative rho (up, down):  7.421E-04 6.544E-04

Magnetic moment per site:
atom:    1    charge:    1.6717    magn:    0.2647    constr:    0.0000
atom:    2    charge:    1.6700    magn:    0.2640    constr:    0.0000
atom:    3    charge:    1.6699    magn:    0.2644    constr:    0.0000
atom:    4    charge:    1.6687    magn:    0.2640    constr:    0.0000
atom:    5    charge:    1.6707    magn:    0.2645    constr:    0.0000
atom:    6    charge:    1.6718    magn:    0.2644    constr:    0.0000
atom:    7    charge:    1.6707    magn:    0.2644    constr:    0.0000
atom:    8    charge:    1.6699    magn:    0.2645    constr:    0.0000
atom:    9    charge:    1.6691    magn:    0.2642    constr:    0.0000
atom:   10    charge:    1.6682    magn:    0.2646    constr:    0.0000
atom:   11    charge:    1.6685    magn:    0.2641    constr:    0.0000
atom:   12    charge:    1.6699    magn:    0.2645    constr:    0.0000
atom:   13    charge:    1.6706    magn:    0.2646    constr:    0.0000
atom:   14    charge:    1.6705    magn:    0.2643    constr:    0.0000
atom:   15    charge:    1.6706    magn:    0.2643    constr:    0.0000
atom:   16    charge:    1.6699    magn:    0.2646    constr:    0.0000
atom:   17    charge:    1.6714    magn:    0.2641    constr:    0.0000
atom:   18    charge:    1.6697    magn:    0.2648    constr:    0.0000
atom:   19    charge:    1.6721    magn:    0.2646    constr:    0.0000
atom:   20    charge:    1.6727    magn:    0.2646    constr:    0.0000
atom:   21    charge:    1.6717    magn:    0.2643    constr:    0.0000
atom:   22    charge:    1.6703    magn:    0.2645    constr:    0.0000
atom:   23    charge:    1.6716    magn:    0.2642    constr:    0.0000
atom:   24    charge:    1.6710    magn:    0.2645    constr:    0.0000
atom:   25    charge:    1.6722    magn:    0.2645    constr:    0.0000
atom:   26    charge:    1.6726    magn:    0.2645    constr:    0.0000
atom:   27    charge:    1.6713    magn:    0.2646    constr:    0.0000
atom:   28    charge:    1.6716    magn:    0.2642    constr:    0.0000
```

```
atom:   29    charge:    1.6697    magn:    0.2643    constr:    0.0000
atom:   30    charge:    1.6714    magn:    0.2644    constr:    0.0000
atom:   31    charge:    1.6729    magn:    0.2645    constr:    0.0000
atom:   32    charge:    1.6726    magn:    0.2648    constr:    0.0000
atom:   33    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   34    charge:    2.9202    magn:    0.0205    constr:    0.0000
atom:   35    charge:    0.7749    magn:   -0.1060    constr:    0.0000
atom:   36    charge:    2.9200    magn:    0.0206    constr:    0.0000
atom:   37    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   38    charge:    2.9202    magn:    0.0205    constr:    0.0000
atom:   39    charge:    0.7749    magn:   -0.1060    constr:    0.0000
atom:   40    charge:    2.9202    magn:    0.0206    constr:    0.0000
atom:   41    charge:    2.9203    magn:    0.0205    constr:    0.0000
atom:   42    charge:    0.7744    magn:   -0.1060    constr:    0.0000
atom:   43    charge:    2.9198    magn:    0.0205    constr:    0.0000
atom:   44    charge:    0.7748    magn:   -0.1060    constr:    0.0000
atom:   45    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   46    charge:    2.9202    magn:    0.0205    constr:    0.0000
atom:   47    charge:    0.7749    magn:   -0.1060    constr:    0.0000
atom:   48    charge:    2.9202    magn:    0.0205    constr:    0.0000
atom:   49    charge:    0.7744    magn:   -0.1060    constr:    0.0000
atom:   50    charge:    2.9200    magn:    0.0206    constr:    0.0000
atom:   51    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   52    charge:    2.9200    magn:    0.0206    constr:    0.0000
atom:   53    charge:    0.7745    magn:   -0.1060    constr:    0.0000
atom:   54    charge:    2.9203    magn:    0.0205    constr:    0.0000
atom:   55    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   56    charge:    2.9202    magn:    0.0205    constr:    0.0000
atom:   57    charge:    0.7746    magn:   -0.1060    constr:    0.0000
atom:   58    charge:    2.9200    magn:    0.0206    constr:    0.0000
atom:   59    charge:    2.9203    magn:    0.0205    constr:    0.0000
atom:   60    charge:    0.7747    magn:   -0.1060    constr:    0.0000
atom:   61    charge:    2.9204    magn:    0.0205    constr:    0.0000
atom:   62    charge:    0.7746    magn:   -0.1060    constr:    0.0000
atom:   63    charge:    2.9201    magn:    0.0205    constr:    0.0000
atom:   64    charge:    0.7747    magn:   -0.1060    constr:    0.0000

total cpu time spent up to now is     3400.9 secs

total energy              =    -786.60522118 Ry
Harris-Foulkes estimate   =    -790.69499750 Ry
estimated scf accuracy    <      13.82448816 Ry

total magnetization       =     3.11 Bohr mag/cell
absolute magnetization    =     6.81 Bohr mag/cell

iteration #  2     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.40E-03,  avg # of iterations =  4.0

negative rho (up, down):  7.631E-04 6.921E-04

Magnetic moment per site:
atom:    1    charge:    1.6597    magn:    0.1370    constr:    0.0000
atom:    2    charge:    1.6584    magn:    0.1366    constr:    0.0000
atom:    3    charge:    1.6586    magn:    0.1368    constr:    0.0000
atom:    4    charge:    1.6576    magn:    0.1366    constr:    0.0000
atom:    5    charge:    1.6591    magn:    0.1368    constr:    0.0000
atom:    6    charge:    1.6598    magn:    0.1368    constr:    0.0000
atom:    7    charge:    1.6592    magn:    0.1368    constr:    0.0000
atom:    8    charge:    1.6585    magn:    0.1369    constr:    0.0000
atom:    9    charge:    1.6582    magn:    0.1367    constr:    0.0000
```

```
atom:   10    charge:    1.6578    magn:    0.1371    constr:    0.0000
atom:   11    charge:    1.6577    magn:    0.1366    constr:    0.0000
atom:   12    charge:    1.6588    magn:    0.1369    constr:    0.0000
atom:   13    charge:    1.6593    magn:    0.1369    constr:    0.0000
atom:   14    charge:    1.6587    magn:    0.1367    constr:    0.0000
atom:   15    charge:    1.6592    magn:    0.1367    constr:    0.0000
atom:   16    charge:    1.6586    magn:    0.1370    constr:    0.0000
atom:   17    charge:    1.6598    magn:    0.1366    constr:    0.0000
atom:   18    charge:    1.6585    magn:    0.1371    constr:    0.0000
atom:   19    charge:    1.6598    magn:    0.1369    constr:    0.0000
atom:   20    charge:    1.6603    magn:    0.1369    constr:    0.0000
atom:   21    charge:    1.6598    magn:    0.1367    constr:    0.0000
atom:   22    charge:    1.6587    magn:    0.1369    constr:    0.0000
atom:   23    charge:    1.6597    magn:    0.1366    constr:    0.0000
atom:   24    charge:    1.6590    magn:    0.1368    constr:    0.0000
atom:   25    charge:    1.6599    magn:    0.1368    constr:    0.0000
atom:   26    charge:    1.6598    magn:    0.1368    constr:    0.0000
atom:   27    charge:    1.6594    magn:    0.1369    constr:    0.0000
atom:   28    charge:    1.6598    magn:    0.1367    constr:    0.0000
atom:   29    charge:    1.6582    magn:    0.1367    constr:    0.0000
atom:   30    charge:    1.6597    magn:    0.1368    constr:    0.0000
atom:   31    charge:    1.6604    magn:    0.1368    constr:    0.0000
atom:   32    charge:    1.6603    magn:    0.1370    constr:    0.0000
atom:   33    charge:    0.8631    magn:   -0.0631    constr:    0.0000
atom:   34    charge:    2.6741    magn:    0.0319    constr:    0.0000
atom:   35    charge:    0.8631    magn:   -0.0632    constr:    0.0000
atom:   36    charge:    2.6741    magn:    0.0319    constr:    0.0000
atom:   37    charge:    0.8630    magn:   -0.0632    constr:    0.0000
atom:   38    charge:    2.6741    magn:    0.0319    constr:    0.0000
atom:   39    charge:    0.8632    magn:   -0.0631    constr:    0.0000
atom:   40    charge:    2.6741    magn:    0.0319    constr:    0.0000
atom:   41    charge:    2.6744    magn:    0.0318    constr:    0.0000
atom:   42    charge:    0.8632    magn:   -0.0632    constr:    0.0000
atom:   43    charge:    2.6739    magn:    0.0318    constr:    0.0000
atom:   44    charge:    0.8632    magn:   -0.0632    constr:    0.0000
atom:   45    charge:    0.8631    magn:   -0.0631    constr:    0.0000
atom:   46    charge:    2.6742    magn:    0.0319    constr:    0.0000
atom:   47    charge:    0.8631    magn:   -0.0632    constr:    0.0000
atom:   48    charge:    2.6742    magn:    0.0318    constr:    0.0000
atom:   49    charge:    0.8630    magn:   -0.0630    constr:    0.0000
atom:   50    charge:    2.6739    magn:    0.0318    constr:    0.0000
atom:   51    charge:    0.8631    magn:   -0.0631    constr:    0.0000
atom:   52    charge:    2.6739    magn:    0.0319    constr:    0.0000
atom:   53    charge:    0.8630    magn:   -0.0631    constr:    0.0000
atom:   54    charge:    2.6744    magn:    0.0318    constr:    0.0000
atom:   55    charge:    0.8630    magn:   -0.0631    constr:    0.0000
atom:   56    charge:    2.6742    magn:    0.0319    constr:    0.0000
atom:   57    charge:    0.8630    magn:   -0.0630    constr:    0.0000
atom:   58    charge:    2.6740    magn:    0.0318    constr:    0.0000
atom:   59    charge:    2.6743    magn:    0.0319    constr:    0.0000
atom:   60    charge:    0.8631    magn:   -0.0631    constr:    0.0000
atom:   61    charge:    2.6745    magn:    0.0318    constr:    0.0000
atom:   62    charge:    0.8629    magn:   -0.0631    constr:    0.0000
atom:   63    charge:    2.6739    magn:    0.0318    constr:    0.0000
atom:   64    charge:    0.8631    magn:   -0.0631    constr:    0.0000

total cpu time spent up to now is     6151.5 secs

total energy              =    -789.65223522 Ry
Harris-Foulkes estimate   =    -791.11587958 Ry
estimated scf accuracy    <       3.42057657 Ry
```

```
     total magnetization       =     0.18 Bohr mag/cell
     absolute magnetization    =     2.75 Bohr mag/cell

     iteration #  3     ecut=    40.00 Ry     beta=0.70
     Davidson diagonalization with overlap
     ethr =  1.34E-03,  avg # of iterations = 11.8

     negative rho (up, down):  8.659E-04 8.237E-04

     Magnetic moment per site:
     atom:    1    charge:    1.6527    magn:    0.0355    constr:    0.0000
     atom:    2    charge:    1.6509    magn:    0.0353    constr:    0.0000
     atom:    3    charge:    1.6507    magn:    0.0355    constr:    0.0000
     atom:    4    charge:    1.6495    magn:    0.0353    constr:    0.0000
     atom:    5    charge:    1.6516    magn:    0.0355    constr:    0.0000
     atom:    6    charge:    1.6527    magn:    0.0354    constr:    0.0000
     atom:    7    charge:    1.6515    magn:    0.0354    constr:    0.0000
     atom:    8    charge:    1.6507    magn:    0.0355    constr:    0.0000
     atom:    9    charge:    1.6500    magn:    0.0354    constr:    0.0000
     atom:   10    charge:    1.6490    magn:    0.0356    constr:    0.0000
     atom:   11    charge:    1.6493    magn:    0.0353    constr:    0.0000
     atom:   12    charge:    1.6506    magn:    0.0355    constr:    0.0000
     atom:   13    charge:    1.6515    magn:    0.0355    constr:    0.0000
     atom:   14    charge:    1.6514    magn:    0.0354    constr:    0.0000
     atom:   15    charge:    1.6514    magn:    0.0354    constr:    0.0000
     atom:   16    charge:    1.6507    magn:    0.0355    constr:    0.0000
     atom:   17    charge:    1.6522    magn:    0.0353    constr:    0.0000
     atom:   18    charge:    1.6506    magn:    0.0356    constr:    0.0000
     atom:   19    charge:    1.6531    magn:    0.0355    constr:    0.0000
     atom:   20    charge:    1.6535    magn:    0.0354    constr:    0.0000
     atom:   21    charge:    1.6525    magn:    0.0354    constr:    0.0000
     atom:   22    charge:    1.6511    magn:    0.0355    constr:    0.0000
     atom:   23    charge:    1.6524    magn:    0.0353    constr:    0.0000
     atom:   24    charge:    1.6519    magn:    0.0355    constr:    0.0000
     atom:   25    charge:    1.6532    magn:    0.0354    constr:    0.0000
     atom:   26    charge:    1.6534    magn:    0.0354    constr:    0.0000
     atom:   27    charge:    1.6521    magn:    0.0355    constr:    0.0000
     atom:   28    charge:    1.6523    magn:    0.0353    constr:    0.0000
     atom:   29    charge:    1.6505    magn:    0.0354    constr:    0.0000
     atom:   30    charge:    1.6523    magn:    0.0354    constr:    0.0000
     atom:   31    charge:    1.6537    magn:    0.0354    constr:    0.0000
     atom:   32    charge:    1.6536    magn:    0.0356    constr:    0.0000
     atom:   33    charge:    0.8606    magn:   -0.0245    constr:    0.0000
     atom:   34    charge:    2.7054    magn:    0.0311    constr:    0.0000
     atom:   35    charge:    0.8607    magn:   -0.0245    constr:    0.0000
     atom:   36    charge:    2.7051    magn:    0.0310    constr:    0.0000
     atom:   37    charge:    0.8606    magn:   -0.0245    constr:    0.0000
     atom:   38    charge:    2.7054    magn:    0.0311    constr:    0.0000
     atom:   39    charge:    0.8606    magn:   -0.0245    constr:    0.0000
     atom:   40    charge:    2.7054    magn:    0.0310    constr:    0.0000
     atom:   41    charge:    2.7052    magn:    0.0310    constr:    0.0000
     atom:   42    charge:    0.8599    magn:   -0.0246    constr:    0.0000
     atom:   43    charge:    2.7050    magn:    0.0310    constr:    0.0000
     atom:   44    charge:    0.8606    magn:   -0.0245    constr:    0.0000
     atom:   45    charge:    0.8604    magn:   -0.0245    constr:    0.0000
     atom:   46    charge:    2.7053    magn:    0.0311    constr:    0.0000
     atom:   47    charge:    0.8607    magn:   -0.0245    constr:    0.0000
     atom:   48    charge:    2.7053    magn:    0.0310    constr:    0.0000
     atom:   49    charge:    0.8602    magn:   -0.0244    constr:    0.0000
     atom:   50    charge:    2.7053    magn:    0.0311    constr:    0.0000
     atom:   51    charge:    0.8606    magn:   -0.0245    constr:    0.0000
     atom:   52    charge:    2.7054    magn:    0.0310    constr:    0.0000
```

```
atom:   53    charge:    0.8603    magn:   -0.0245    constr:    0.0000
atom:   54    charge:    2.7053    magn:    0.0310    constr:    0.0000
atom:   55    charge:    0.8605    magn:   -0.0245    constr:    0.0000
atom:   56    charge:    2.7054    magn:    0.0311    constr:    0.0000
atom:   57    charge:    0.8604    magn:   -0.0245    constr:    0.0000
atom:   58    charge:    2.7053    magn:    0.0309    constr:    0.0000
atom:   59    charge:    2.7054    magn:    0.0310    constr:    0.0000
atom:   60    charge:    0.8606    magn:   -0.0245    constr:    0.0000
atom:   61    charge:    2.7054    magn:    0.0310    constr:    0.0000
atom:   62    charge:    0.8604    magn:   -0.0245    constr:    0.0000
atom:   63    charge:    2.7054    magn:    0.0310    constr:    0.0000
atom:   64    charge:    0.8606    magn:   -0.0245    constr:    0.0000

total cpu time spent up to now is     9307.1 secs

total energy              =    -790.61099848 Ry
Harris-Foulkes estimate   =    -790.53920183 Ry
estimated scf accuracy    <       0.19167449 Ry

total magnetization       =     0.11 Bohr mag/cell
absolute magnetization    =     1.71 Bohr mag/cell

iteration #  4     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  7.49E-05,  avg # of iterations = 11.8

negative rho (up, down):  9.133E-04 8.878E-04

Magnetic moment per site:
atom:    1    charge:    1.6507    magn:    0.0073    constr:    0.0000
atom:    2    charge:    1.6498    magn:    0.0072    constr:    0.0000
atom:    3    charge:    1.6503    magn:    0.0073    constr:    0.0000
atom:    4    charge:    1.6493    magn:    0.0072    constr:    0.0000
atom:    5    charge:    1.6504    magn:    0.0073    constr:    0.0000
atom:    6    charge:    1.6508    magn:    0.0072    constr:    0.0000
atom:    7    charge:    1.6508    magn:    0.0073    constr:    0.0000
atom:    8    charge:    1.6501    magn:    0.0073    constr:    0.0000
atom:    9    charge:    1.6500    magn:    0.0072    constr:    0.0000
atom:   10    charge:    1.6499    magn:    0.0074    constr:    0.0000
atom:   11    charge:    1.6495    magn:    0.0072    constr:    0.0000
atom:   12    charge:    1.6506    magn:    0.0073    constr:    0.0000
atom:   13    charge:    1.6509    magn:    0.0073    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0073    constr:    0.0000
atom:   15    charge:    1.6509    magn:    0.0072    constr:    0.0000
atom:   16    charge:    1.6502    magn:    0.0074    constr:    0.0000
atom:   17    charge:    1.6512    magn:    0.0072    constr:    0.0000
atom:   18    charge:    1.6501    magn:    0.0074    constr:    0.0000
atom:   19    charge:    1.6505    magn:    0.0073    constr:    0.0000
atom:   20    charge:    1.6511    magn:    0.0073    constr:    0.0000
atom:   21    charge:    1.6510    magn:    0.0073    constr:    0.0000
atom:   22    charge:    1.6502    magn:    0.0073    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0072    constr:    0.0000
atom:   24    charge:    1.6501    magn:    0.0073    constr:    0.0000
atom:   25    charge:    1.6507    magn:    0.0073    constr:    0.0000
atom:   26    charge:    1.6502    magn:    0.0073    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0073    constr:    0.0000
atom:   28    charge:    1.6512    magn:    0.0072    constr:    0.0000
atom:   29    charge:    1.6498    magn:    0.0073    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0073    constr:    0.0000
atom:   31    charge:    1.6511    magn:    0.0073    constr:    0.0000
atom:   32    charge:    1.6509    magn:    0.0074    constr:    0.0000
atom:   33    charge:    0.8539    magn:   -0.0092    constr:    0.0000
```

```
atom:   34    charge:    2.7052    magn:    0.0170    constr:    0.0000
atom:   35    charge:    0.8541    magn:   -0.0092    constr:    0.0000
atom:   36    charge:    2.7053    magn:    0.0169    constr:    0.0000
atom:   37    charge:    0.8540    magn:   -0.0092    constr:    0.0000
atom:   38    charge:    2.7052    magn:    0.0169    constr:    0.0000
atom:   39    charge:    0.8542    magn:   -0.0092    constr:    0.0000
atom:   40    charge:    2.7052    magn:    0.0169    constr:    0.0000
atom:   41    charge:    2.7058    magn:    0.0170    constr:    0.0000
atom:   42    charge:    0.8539    magn:   -0.0091    constr:    0.0000
atom:   43    charge:    2.7052    magn:    0.0169    constr:    0.0000
atom:   44    charge:    0.8542    magn:   -0.0092    constr:    0.0000
atom:   45    charge:    0.8540    magn:   -0.0092    constr:    0.0000
atom:   46    charge:    2.7053    magn:    0.0170    constr:    0.0000
atom:   47    charge:    0.8542    magn:   -0.0092    constr:    0.0000
atom:   48    charge:    2.7054    magn:    0.0169    constr:    0.0000
atom:   49    charge:    0.8539    magn:   -0.0091    constr:    0.0000
atom:   50    charge:    2.7050    magn:    0.0169    constr:    0.0000
atom:   51    charge:    0.8540    magn:   -0.0092    constr:    0.0000
atom:   52    charge:    2.7048    magn:    0.0169    constr:    0.0000
atom:   53    charge:    0.8539    magn:   -0.0091    constr:    0.0000
atom:   54    charge:    2.7055    magn:    0.0169    constr:    0.0000
atom:   55    charge:    0.8540    magn:   -0.0092    constr:    0.0000
atom:   56    charge:    2.7052    magn:    0.0169    constr:    0.0000
atom:   57    charge:    0.8539    magn:   -0.0092    constr:    0.0000
atom:   58    charge:    2.7050    magn:    0.0169    constr:    0.0000
atom:   59    charge:    2.7054    magn:    0.0169    constr:    0.0000
atom:   60    charge:    0.8541    magn:   -0.0092    constr:    0.0000
atom:   61    charge:    2.7056    magn:    0.0169    constr:    0.0000
atom:   62    charge:    0.8539    magn:   -0.0092    constr:    0.0000
atom:   63    charge:    2.7048    magn:    0.0169    constr:    0.0000
atom:   64    charge:    0.8539    magn:   -0.0092    constr:    0.0000

total cpu time spent up to now is    12213.8 secs

total energy              =    -790.65553641 Ry
Harris-Foulkes estimate   =    -790.64593449 Ry
estimated scf accuracy    <       0.00627985 Ry

total magnetization       =     0.11 Bohr mag/cell
absolute magnetization    =     0.82 Bohr mag/cell

iteration #  5     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
c_bands:  2 eigenvalues not converged
ethr =  2.45E-06,  avg # of iterations =  6.8

negative rho (up, down):  9.166E-04 9.023E-04

Magnetic moment per site:
atom:    1    charge:    1.6516    magn:    0.0032    constr:    0.0000
atom:    2    charge:    1.6494    magn:    0.0031    constr:    0.0000
atom:    3    charge:    1.6491    magn:    0.0032    constr:    0.0000
atom:    4    charge:    1.6478    magn:    0.0031    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0032    constr:    0.0000
atom:    6    charge:    1.6515    magn:    0.0031    constr:    0.0000
atom:    7    charge:    1.6499    magn:    0.0031    constr:    0.0000
atom:    8    charge:    1.6491    magn:    0.0032    constr:    0.0000
atom:    9    charge:    1.6481    magn:    0.0031    constr:    0.0000
atom:   10    charge:    1.6471    magn:    0.0032    constr:    0.0000
atom:   11    charge:    1.6475    magn:    0.0031    constr:    0.0000
atom:   12    charge:    1.6489    magn:    0.0032    constr:    0.0000
atom:   13    charge:    1.6499    magn:    0.0032    constr:    0.0000
```

```
atom:   14    charge:    1.6500    magn:    0.0031    constr:    0.0000
atom:   15    charge:    1.6497    magn:    0.0031    constr:    0.0000
atom:   16    charge:    1.6491    magn:    0.0032    constr:    0.0000
atom:   17    charge:    1.6507    magn:    0.0031    constr:    0.0000
atom:   18    charge:    1.6490    magn:    0.0033    constr:    0.0000
atom:   19    charge:    1.6523    magn:    0.0032    constr:    0.0000
atom:   20    charge:    1.6526    magn:    0.0031    constr:    0.0000
atom:   21    charge:    1.6513    magn:    0.0031    constr:    0.0000
atom:   22    charge:    1.6497    magn:    0.0032    constr:    0.0000
atom:   23    charge:    1.6511    magn:    0.0031    constr:    0.0000
atom:   24    charge:    1.6507    magn:    0.0032    constr:    0.0000
atom:   25    charge:    1.6523    magn:    0.0031    constr:    0.0000
atom:   26    charge:    1.6528    magn:    0.0031    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0031    constr:    0.0000
atom:   28    charge:    1.6509    magn:    0.0031    constr:    0.0000
atom:   29    charge:    1.6489    magn:    0.0031    constr:    0.0000
atom:   30    charge:    1.6510    magn:    0.0031    constr:    0.0000
atom:   31    charge:    1.6528    magn:    0.0031    constr:    0.0000
atom:   32    charge:    1.6528    magn:    0.0032    constr:    0.0000
atom:   33    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   34    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   35    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   36    charge:    2.7033    magn:    0.0115    constr:    0.0000
atom:   37    charge:    0.8553    magn:   -0.0054    constr:    0.0000
atom:   38    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   39    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   40    charge:    2.7035    magn:    0.0115    constr:    0.0000
atom:   41    charge:    2.7035    magn:    0.0115    constr:    0.0000
atom:   42    charge:    0.8550    magn:   -0.0054    constr:    0.0000
atom:   43    charge:    2.7032    magn:    0.0115    constr:    0.0000
atom:   44    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   45    charge:    0.8553    magn:   -0.0054    constr:    0.0000
atom:   46    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   47    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   48    charge:    2.7035    magn:    0.0115    constr:    0.0000
atom:   49    charge:    0.8550    magn:   -0.0054    constr:    0.0000
atom:   50    charge:    2.7034    magn:    0.0115    constr:    0.0000
atom:   51    charge:    0.8554    magn:   -0.0054    constr:    0.0000
atom:   52    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   53    charge:    0.8552    magn:   -0.0054    constr:    0.0000
atom:   54    charge:    2.7037    magn:    0.0115    constr:    0.0000
atom:   55    charge:    0.8553    magn:   -0.0054    constr:    0.0000
atom:   56    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   57    charge:    0.8552    magn:   -0.0054    constr:    0.0000
atom:   58    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   59    charge:    2.7037    magn:    0.0115    constr:    0.0000
atom:   60    charge:    0.8553    magn:   -0.0054    constr:    0.0000
atom:   61    charge:    2.7037    magn:    0.0115    constr:    0.0000
atom:   62    charge:    0.8552    magn:   -0.0054    constr:    0.0000
atom:   63    charge:    2.7036    magn:    0.0115    constr:    0.0000
atom:   64    charge:    0.8554    magn:   -0.0054    constr:    0.0000

total cpu time spent up to now is    15264.6 secs

total energy              =    -790.65796711 Ry
Harris-Foulkes estimate   =    -790.65848986 Ry
estimated scf accuracy    <       0.00213293 Ry

total magnetization       =     0.11 Bohr mag/cell
absolute magnetization    =     0.42 Bohr mag/cell

iteration #  6     ecut=    40.00 Ry     beta=0.70
```

```
Davidson diagonalization with overlap
ethr =  8.33E-07,  avg # of iterations =  5.0

negative rho (up, down):  9.175E-04 9.092E-04

Magnetic moment per site:
atom:    1    charge:    1.6509    magn:    0.0017    constr:    0.0000
atom:    2    charge:    1.6495    magn:    0.0016    constr:    0.0000
atom:    3    charge:    1.6495    magn:    0.0017    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0017    constr:    0.0000
atom:    5    charge:    1.6501    magn:    0.0017    constr:    0.0000
atom:    6    charge:    1.6510    magn:    0.0017    constr:    0.0000
atom:    7    charge:    1.6503    magn:    0.0017    constr:    0.0000
atom:    8    charge:    1.6494    magn:    0.0017    constr:    0.0000
atom:    9    charge:    1.6490    magn:    0.0017    constr:    0.0000
atom:   10    charge:    1.6483    magn:    0.0018    constr:    0.0000
atom:   11    charge:    1.6484    magn:    0.0017    constr:    0.0000
atom:   12    charge:    1.6496    magn:    0.0017    constr:    0.0000
atom:   13    charge:    1.6502    magn:    0.0017    constr:    0.0000
atom:   14    charge:    1.6499    magn:    0.0017    constr:    0.0000
atom:   15    charge:    1.6502    magn:    0.0017    constr:    0.0000
atom:   16    charge:    1.6495    magn:    0.0018    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0016    constr:    0.0000
atom:   18    charge:    1.6493    magn:    0.0018    constr:    0.0000
atom:   19    charge:    1.6511    magn:    0.0017    constr:    0.0000
atom:   20    charge:    1.6516    magn:    0.0017    constr:    0.0000
atom:   21    charge:    1.6510    magn:    0.0017    constr:    0.0000
atom:   22    charge:    1.6497    magn:    0.0017    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0017    constr:    0.0000
atom:   24    charge:    1.6502    magn:    0.0017    constr:    0.0000
atom:   25    charge:    1.6513    magn:    0.0017    constr:    0.0000
atom:   26    charge:    1.6513    magn:    0.0017    constr:    0.0000
atom:   27    charge:    1.6505    magn:    0.0017    constr:    0.0000
atom:   28    charge:    1.6509    magn:    0.0017    constr:    0.0000
atom:   29    charge:    1.6492    magn:    0.0017    constr:    0.0000
atom:   30    charge:    1.6508    magn:    0.0017    constr:    0.0000
atom:   31    charge:    1.6517    magn:    0.0017    constr:    0.0000
atom:   32    charge:    1.6516    magn:    0.0018    constr:    0.0000
atom:   33    charge:    0.8561    magn:   -0.0035    constr:    0.0000
atom:   34    charge:    2.7029    magn:    0.0080    constr:    0.0000
atom:   35    charge:    0.8562    magn:   -0.0035    constr:    0.0000
atom:   36    charge:    2.7026    magn:    0.0079    constr:    0.0000
atom:   37    charge:    0.8561    magn:   -0.0035    constr:    0.0000
atom:   38    charge:    2.7028    magn:    0.0079    constr:    0.0000
atom:   39    charge:    0.8562    magn:   -0.0035    constr:    0.0000
atom:   40    charge:    2.7028    magn:    0.0079    constr:    0.0000
atom:   41    charge:    2.7027    magn:    0.0078    constr:    0.0000
atom:   42    charge:    0.8558    magn:   -0.0035    constr:    0.0000
atom:   43    charge:    2.7025    magn:    0.0079    constr:    0.0000
atom:   44    charge:    0.8562    magn:   -0.0035    constr:    0.0000
atom:   45    charge:    0.8560    magn:   -0.0035    constr:    0.0000
atom:   46    charge:    2.7028    magn:    0.0079    constr:    0.0000
atom:   47    charge:    0.8562    magn:   -0.0035    constr:    0.0000
atom:   48    charge:    2.7028    magn:    0.0079    constr:    0.0000
atom:   49    charge:    0.8558    magn:   -0.0035    constr:    0.0000
atom:   50    charge:    2.7026    magn:    0.0079    constr:    0.0000
atom:   51    charge:    0.8561    magn:   -0.0034    constr:    0.0000
atom:   52    charge:    2.7027    magn:    0.0080    constr:    0.0000
atom:   53    charge:    0.8559    magn:   -0.0035    constr:    0.0000
atom:   54    charge:    2.7029    magn:    0.0079    constr:    0.0000
atom:   55    charge:    0.8560    magn:   -0.0035    constr:    0.0000
atom:   56    charge:    2.7028    magn:    0.0080    constr:    0.0000
```

```
atom:   57    charge:    0.8560    magn:   -0.0035    constr:    0.0000
atom:   58    charge:    2.7027    magn:    0.0080    constr:    0.0000
atom:   59    charge:    2.7029    magn:    0.0079    constr:    0.0000
atom:   60    charge:    0.8561    magn:   -0.0035    constr:    0.0000
atom:   61    charge:    2.7029    magn:    0.0079    constr:    0.0000
atom:   62    charge:    0.8559    magn:   -0.0035    constr:    0.0000
atom:   63    charge:    2.7027    magn:    0.0080    constr:    0.0000
atom:   64    charge:    0.8561    magn:   -0.0034    constr:    0.0000

total cpu time spent up to now is    17743.2 secs

total energy              =    -790.65861413 Ry
Harris-Foulkes estimate   =    -790.65899102 Ry
estimated scf accuracy    <       0.00138911 Ry

total magnetization       =     0.10 Bohr mag/cell
absolute magnetization    =     0.30 Bohr mag/cell

iteration #  7     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.43E-07,  avg # of iterations =  2.3

negative rho (up, down):  9.174E-04 9.127E-04

Magnetic moment per site:
atom:    1    charge:    1.6511    magn:    0.0011    constr:    0.0000
atom:    2    charge:    1.6494    magn:    0.0010    constr:    0.0000
atom:    3    charge:    1.6496    magn:    0.0011    constr:    0.0000
atom:    4    charge:    1.6484    magn:    0.0010    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0011    constr:    0.0000
atom:    6    charge:    1.6510    magn:    0.0010    constr:    0.0000
atom:    7    charge:    1.6502    magn:    0.0011    constr:    0.0000
atom:    8    charge:    1.6494    magn:    0.0011    constr:    0.0000
atom:    9    charge:    1.6489    magn:    0.0010    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0011    constr:    0.0000
atom:   11    charge:    1.6484    magn:    0.0010    constr:    0.0000
atom:   12    charge:    1.6496    magn:    0.0011    constr:    0.0000
atom:   13    charge:    1.6502    magn:    0.0011    constr:    0.0000
atom:   14    charge:    1.6498    magn:    0.0010    constr:    0.0000
atom:   15    charge:    1.6501    magn:    0.0010    constr:    0.0000
atom:   16    charge:    1.6495    magn:    0.0011    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0010    constr:    0.0000
atom:   18    charge:    1.6494    magn:    0.0011    constr:    0.0000
atom:   19    charge:    1.6513    magn:    0.0011    constr:    0.0000
atom:   20    charge:    1.6517    magn:    0.0010    constr:    0.0000
atom:   21    charge:    1.6510    magn:    0.0010    constr:    0.0000
atom:   22    charge:    1.6498    magn:    0.0010    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0010    constr:    0.0000
atom:   24    charge:    1.6502    magn:    0.0010    constr:    0.0000
atom:   25    charge:    1.6514    magn:    0.0010    constr:    0.0000
atom:   26    charge:    1.6513    magn:    0.0010    constr:    0.0000
atom:   27    charge:    1.6506    magn:    0.0010    constr:    0.0000
atom:   28    charge:    1.6509    magn:    0.0010    constr:    0.0000
atom:   29    charge:    1.6492    magn:    0.0010    constr:    0.0000
atom:   30    charge:    1.6508    magn:    0.0010    constr:    0.0000
atom:   31    charge:    1.6518    magn:    0.0010    constr:    0.0000
atom:   32    charge:    1.6517    magn:    0.0011    constr:    0.0000
atom:   33    charge:    0.8563    magn:   -0.0015    constr:    0.0000
atom:   34    charge:    2.7025    magn:    0.0035    constr:    0.0000
atom:   35    charge:    0.8565    magn:   -0.0015    constr:    0.0000
atom:   36    charge:    2.7025    magn:    0.0034    constr:    0.0000
atom:   37    charge:    0.8564    magn:   -0.0015    constr:    0.0000
```

```
atom:   38    charge:    2.7025    magn:    0.0035    constr:    0.0000
atom:   39    charge:    0.8565    magn:   -0.0015    constr:    0.0000
atom:   40    charge:    2.7025    magn:    0.0035    constr:    0.0000
atom:   41    charge:    2.7028    magn:    0.0033    constr:    0.0000
atom:   42    charge:    0.8561    magn:   -0.0016    constr:    0.0000
atom:   43    charge:    2.7024    magn:    0.0034    constr:    0.0000
atom:   44    charge:    0.8564    magn:   -0.0016    constr:    0.0000
atom:   45    charge:    0.8563    magn:   -0.0015    constr:    0.0000
atom:   46    charge:    2.7026    magn:    0.0035    constr:    0.0000
atom:   47    charge:    0.8565    magn:   -0.0015    constr:    0.0000
atom:   48    charge:    2.7026    magn:    0.0035    constr:    0.0000
atom:   49    charge:    0.8561    magn:   -0.0016    constr:    0.0000
atom:   50    charge:    2.7023    magn:    0.0035    constr:    0.0000
atom:   51    charge:    0.8563    magn:   -0.0015    constr:    0.0000
atom:   52    charge:    2.7023    magn:    0.0035    constr:    0.0000
atom:   53    charge:    0.8562    magn:   -0.0016    constr:    0.0000
atom:   54    charge:    2.7027    magn:    0.0035    constr:    0.0000
atom:   55    charge:    0.8563    magn:   -0.0016    constr:    0.0000
atom:   56    charge:    2.7025    magn:    0.0035    constr:    0.0000
atom:   57    charge:    0.8562    magn:   -0.0015    constr:    0.0000
atom:   58    charge:    2.7023    magn:    0.0035    constr:    0.0000
atom:   59    charge:    2.7026    magn:    0.0035    constr:    0.0000
atom:   60    charge:    0.8564    magn:   -0.0016    constr:    0.0000
atom:   61    charge:    2.7028    magn:    0.0034    constr:    0.0000
atom:   62    charge:    0.8562    magn:   -0.0015    constr:    0.0000
atom:   63    charge:    2.7023    magn:    0.0035    constr:    0.0000
atom:   64    charge:    0.8563    magn:   -0.0015    constr:    0.0000

total cpu time spent up to now is    19752.5 secs

total energy              =    -790.65897707 Ry
Harris-Foulkes estimate   =    -790.65890194 Ry
estimated scf accuracy    <       0.00005093 Ry

total magnetization       =     0.09 Bohr mag/cell
absolute magnetization    =     0.23 Bohr mag/cell

iteration #  8     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.99E-08,  avg # of iterations =  4.0

negative rho (up, down):  9.167E-04 9.147E-04

Magnetic moment per site:
atom:    1    charge:    1.6510    magn:    0.0007    constr:    0.0000
atom:    2    charge:    1.6495    magn:    0.0007    constr:    0.0000
atom:    3    charge:    1.6496    magn:    0.0007    constr:    0.0000
atom:    4    charge:    1.6484    magn:    0.0007    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0007    constr:    0.0000
atom:    6    charge:    1.6510    magn:    0.0007    constr:    0.0000
atom:    7    charge:    1.6503    magn:    0.0007    constr:    0.0000
atom:    8    charge:    1.6494    magn:    0.0007    constr:    0.0000
atom:    9    charge:    1.6489    magn:    0.0007    constr:    0.0000
atom:   10    charge:    1.6483    magn:    0.0007    constr:    0.0000
atom:   11    charge:    1.6484    magn:    0.0007    constr:    0.0000
atom:   12    charge:    1.6496    magn:    0.0007    constr:    0.0000
atom:   13    charge:    1.6502    magn:    0.0007    constr:    0.0000
atom:   14    charge:    1.6499    magn:    0.0007    constr:    0.0000
atom:   15    charge:    1.6502    magn:    0.0007    constr:    0.0000
atom:   16    charge:    1.6495    magn:    0.0007    constr:    0.0000
atom:   17    charge:    1.6508    magn:    0.0007    constr:    0.0000
atom:   18    charge:    1.6494    magn:    0.0007    constr:    0.0000
```

```
atom:   19    charge:    1.6513    magn:    0.0007    constr:    0.0000
atom:   20    charge:    1.6517    magn:    0.0007    constr:    0.0000
atom:   21    charge:    1.6510    magn:    0.0007    constr:    0.0000
atom:   22    charge:    1.6498    magn:    0.0007    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0007    constr:    0.0000
atom:   24    charge:    1.6502    magn:    0.0007    constr:    0.0000
atom:   25    charge:    1.6514    magn:    0.0007    constr:    0.0000
atom:   26    charge:    1.6514    magn:    0.0007    constr:    0.0000
atom:   27    charge:    1.6506    magn:    0.0007    constr:    0.0000
atom:   28    charge:    1.6509    magn:    0.0007    constr:    0.0000
atom:   29    charge:    1.6492    magn:    0.0007    constr:    0.0000
atom:   30    charge:    1.6508    magn:    0.0007    constr:    0.0000
atom:   31    charge:    1.6518    magn:    0.0007    constr:    0.0000
atom:   32    charge:    1.6517    magn:    0.0007    constr:    0.0000
atom:   33    charge:    0.8563    magn:   -0.0003    constr:    0.0000
atom:   34    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   35    charge:    0.8564    magn:   -0.0003    constr:    0.0000
atom:   36    charge:    2.7024    magn:    0.0007    constr:    0.0000
atom:   37    charge:    0.8563    magn:   -0.0003    constr:    0.0000
atom:   38    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   39    charge:    0.8564    magn:   -0.0003    constr:    0.0000
atom:   40    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   41    charge:    2.7027    magn:    0.0006    constr:    0.0000
atom:   42    charge:    0.8560    magn:   -0.0004    constr:    0.0000
atom:   43    charge:    2.7023    magn:    0.0007    constr:    0.0000
atom:   44    charge:    0.8564    magn:   -0.0003    constr:    0.0000
atom:   45    charge:    0.8562    magn:   -0.0003    constr:    0.0000
atom:   46    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   47    charge:    0.8564    magn:   -0.0003    constr:    0.0000
atom:   48    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   49    charge:    0.8561    magn:   -0.0004    constr:    0.0000
atom:   50    charge:    2.7024    magn:    0.0007    constr:    0.0000
atom:   51    charge:    0.8563    magn:   -0.0003    constr:    0.0000
atom:   52    charge:    2.7025    magn:    0.0007    constr:    0.0000
atom:   53    charge:    0.8561    magn:   -0.0003    constr:    0.0000
atom:   54    charge:    2.7027    magn:    0.0007    constr:    0.0000
atom:   55    charge:    0.8562    magn:   -0.0003    constr:    0.0000
atom:   56    charge:    2.7026    magn:    0.0007    constr:    0.0000
atom:   57    charge:    0.8562    magn:   -0.0003    constr:    0.0000
atom:   58    charge:    2.7025    magn:    0.0007    constr:    0.0000
atom:   59    charge:    2.7027    magn:    0.0007    constr:    0.0000
atom:   60    charge:    0.8563    magn:   -0.0003    constr:    0.0000
atom:   61    charge:    2.7028    magn:    0.0007    constr:    0.0000
atom:   62    charge:    0.8562    magn:   -0.0003    constr:    0.0000
atom:   63    charge:    2.7025    magn:    0.0007    constr:    0.0000
atom:   64    charge:    0.8563    magn:   -0.0003    constr:    0.0000

total cpu time spent up to now is    22718.1 secs

total energy              =    -790.65904536 Ry
Harris-Foulkes estimate   =    -790.65903705 Ry
estimated scf accuracy    <       0.00002507 Ry

total magnetization       =     0.07 Bohr mag/cell
absolute magnetization    =     0.12 Bohr mag/cell

iteration #  9     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  9.79E-09,  avg # of iterations =  4.0

negative rho (up, down):  9.159E-04 9.151E-04
```

```
 Magnetic moment per site:
 atom:    1    charge:    1.6510    magn:    0.0006    constr:    0.0000
 atom:    2    charge:    1.6495    magn:    0.0005    constr:    0.0000
 atom:    3    charge:    1.6496    magn:    0.0006    constr:    0.0000
 atom:    4    charge:    1.6484    magn:    0.0005    constr:    0.0000
 atom:    5    charge:    1.6502    magn:    0.0006    constr:    0.0000
 atom:    6    charge:    1.6510    magn:    0.0005    constr:    0.0000
 atom:    7    charge:    1.6503    magn:    0.0006    constr:    0.0000
 atom:    8    charge:    1.6494    magn:    0.0006    constr:    0.0000
 atom:    9    charge:    1.6489    magn:    0.0005    constr:    0.0000
 atom:   10    charge:    1.6483    magn:    0.0006    constr:    0.0000
 atom:   11    charge:    1.6484    magn:    0.0005    constr:    0.0000
 atom:   12    charge:    1.6496    magn:    0.0006    constr:    0.0000
 atom:   13    charge:    1.6502    magn:    0.0006    constr:    0.0000
 atom:   14    charge:    1.6499    magn:    0.0005    constr:    0.0000
 atom:   15    charge:    1.6502    magn:    0.0006    constr:    0.0000
 atom:   16    charge:    1.6495    magn:    0.0006    constr:    0.0000
 atom:   17    charge:    1.6509    magn:    0.0006    constr:    0.0000
 atom:   18    charge:    1.6494    magn:    0.0006    constr:    0.0000
 atom:   19    charge:    1.6513    magn:    0.0006    constr:    0.0000
 atom:   20    charge:    1.6517    magn:    0.0005    constr:    0.0000
 atom:   21    charge:    1.6510    magn:    0.0006    constr:    0.0000
 atom:   22    charge:    1.6498    magn:    0.0005    constr:    0.0000
 atom:   23    charge:    1.6509    magn:    0.0006    constr:    0.0000
 atom:   24    charge:    1.6502    magn:    0.0005    constr:    0.0000
 atom:   25    charge:    1.6514    magn:    0.0006    constr:    0.0000
 atom:   26    charge:    1.6514    magn:    0.0005    constr:    0.0000
 atom:   27    charge:    1.6506    magn:    0.0005    constr:    0.0000
 atom:   28    charge:    1.6509    magn:    0.0006    constr:    0.0000
 atom:   29    charge:    1.6492    magn:    0.0005    constr:    0.0000
 atom:   30    charge:    1.6508    magn:    0.0006    constr:    0.0000
 atom:   31    charge:    1.6518    magn:    0.0005    constr:    0.0000
 atom:   32    charge:    1.6517    magn:    0.0006    constr:    0.0000
 atom:   33    charge:    0.8562    magn:   -0.0001    constr:    0.0000
 atom:   34    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   35    charge:    0.8563    magn:   -0.0001    constr:    0.0000
 atom:   36    charge:    2.7026    magn:    0.0002    constr:    0.0000
 atom:   37    charge:    0.8562    magn:   -0.0001    constr:    0.0000
 atom:   38    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   39    charge:    0.8563    magn:   -0.0001    constr:    0.0000
 atom:   40    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   41    charge:    2.7028    magn:    0.0002    constr:    0.0000
 atom:   42    charge:    0.8559    magn:   -0.0001    constr:    0.0000
 atom:   43    charge:    2.7025    magn:    0.0002    constr:    0.0000
 atom:   44    charge:    0.8563    magn:   -0.0001    constr:    0.0000
 atom:   45    charge:    0.8562    magn:   -0.0001    constr:    0.0000
 atom:   46    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   47    charge:    0.8563    magn:   -0.0001    constr:    0.0000
 atom:   48    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   49    charge:    0.8560    magn:   -0.0001    constr:    0.0000
 atom:   50    charge:    2.7025    magn:    0.0002    constr:    0.0000
 atom:   51    charge:    0.8562    magn:   -0.0001    constr:    0.0000
 atom:   52    charge:    2.7025    magn:    0.0002    constr:    0.0000
 atom:   53    charge:    0.8560    magn:   -0.0001    constr:    0.0000
 atom:   54    charge:    2.7028    magn:    0.0002    constr:    0.0000
 atom:   55    charge:    0.8561    magn:   -0.0001    constr:    0.0000
 atom:   56    charge:    2.7027    magn:    0.0002    constr:    0.0000
 atom:   57    charge:    0.8561    magn:   -0.0001    constr:    0.0000
 atom:   58    charge:    2.7025    magn:    0.0002    constr:    0.0000
 atom:   59    charge:    2.7028    magn:    0.0002    constr:    0.0000
 atom:   60    charge:    0.8562    magn:   -0.0001    constr:    0.0000
 atom:   61    charge:    2.7029    magn:    0.0002    constr:    0.0000
```

```
atom:   62    charge:    0.8561    magn:   -0.0001    constr:    0.0000
atom:   63    charge:    2.7025    magn:    0.0002    constr:    0.0000
atom:   64    charge:    0.8562    magn:   -0.0001    constr:    0.0000

total cpu time spent up to now is    25321.2 secs

total energy              =    -790.65906060 Ry
Harris-Foulkes estimate   =    -790.65905994 Ry
estimated scf accuracy    <       0.00000180 Ry

total magnetization       =     0.05 Bohr mag/cell
absolute magnetization    =     0.06 Bohr mag/cell

iteration # 10     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  7.04E-10,  avg # of iterations =  3.4

negative rho (up, down):  9.152E-04 9.150E-04

Magnetic moment per site:
atom:    1    charge:    1.6510    magn:    0.0005    constr:    0.0000
atom:    2    charge:    1.6494    magn:    0.0004    constr:    0.0000
atom:    3    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:    4    charge:    1.6484    magn:    0.0005    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0005    constr:    0.0000
atom:    6    charge:    1.6510    magn:    0.0005    constr:    0.0000
atom:    7    charge:    1.6503    magn:    0.0005    constr:    0.0000
atom:    8    charge:    1.6494    magn:    0.0005    constr:    0.0000
atom:    9    charge:    1.6489    magn:    0.0005    constr:    0.0000
atom:   10    charge:    1.6483    magn:    0.0005    constr:    0.0000
atom:   11    charge:    1.6484    magn:    0.0005    constr:    0.0000
atom:   12    charge:    1.6496    magn:    0.0005    constr:    0.0000
atom:   13    charge:    1.6502    magn:    0.0005    constr:    0.0000
atom:   14    charge:    1.6499    magn:    0.0005    constr:    0.0000
atom:   15    charge:    1.6502    magn:    0.0005    constr:    0.0000
atom:   16    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0005    constr:    0.0000
atom:   18    charge:    1.6494    magn:    0.0005    constr:    0.0000
atom:   19    charge:    1.6513    magn:    0.0005    constr:    0.0000
atom:   20    charge:    1.6517    magn:    0.0005    constr:    0.0000
atom:   21    charge:    1.6510    magn:    0.0005    constr:    0.0000
atom:   22    charge:    1.6498    magn:    0.0005    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0005    constr:    0.0000
atom:   24    charge:    1.6503    magn:    0.0005    constr:    0.0000
atom:   25    charge:    1.6514    magn:    0.0005    constr:    0.0000
atom:   26    charge:    1.6514    magn:    0.0004    constr:    0.0000
atom:   27    charge:    1.6506    magn:    0.0005    constr:    0.0000
atom:   28    charge:    1.6509    magn:    0.0005    constr:    0.0000
atom:   29    charge:    1.6492    magn:    0.0005    constr:    0.0000
atom:   30    charge:    1.6508    magn:    0.0005    constr:    0.0000
atom:   31    charge:    1.6518    magn:    0.0005    constr:    0.0000
atom:   32    charge:    1.6517    magn:    0.0005    constr:    0.0000
atom:   33    charge:    0.8561    magn:   -0.0000    constr:    0.0000
atom:   34    charge:    2.7028    magn:    0.0001    constr:    0.0000
atom:   35    charge:    0.8562    magn:   -0.0000    constr:    0.0000
atom:   36    charge:    2.7026    magn:    0.0001    constr:    0.0000
atom:   37    charge:    0.8561    magn:   -0.0000    constr:    0.0000
atom:   38    charge:    2.7028    magn:    0.0001    constr:    0.0000
atom:   39    charge:    0.8563    magn:   -0.0000    constr:    0.0000
atom:   40    charge:    2.7027    magn:    0.0001    constr:    0.0000
atom:   41    charge:    2.7028    magn:    0.0001    constr:    0.0000
atom:   42    charge:    0.8559    magn:   -0.0000    constr:    0.0000
```

```
     atom:   43    charge:    2.7024    magn:    0.0001    constr:    0.0000
     atom:   44    charge:    0.8562    magn:   -0.0000    constr:    0.0000
     atom:   45    charge:    0.8561    magn:   -0.0000    constr:    0.0000
     atom:   46    charge:    2.7028    magn:    0.0001    constr:    0.0000
     atom:   47    charge:    0.8563    magn:   -0.0000    constr:    0.0000
     atom:   48    charge:    2.7028    magn:    0.0001    constr:    0.0000
     atom:   49    charge:    0.8559    magn:   -0.0000    constr:    0.0000
     atom:   50    charge:    2.7026    magn:    0.0001    constr:    0.0000
     atom:   51    charge:    0.8561    magn:   -0.0000    constr:    0.0000
     atom:   52    charge:    2.7027    magn:    0.0001    constr:    0.0000
     atom:   53    charge:    0.8560    magn:   -0.0000    constr:    0.0000
     atom:   54    charge:    2.7029    magn:    0.0001    constr:    0.0000
     atom:   55    charge:    0.8561    magn:   -0.0000    constr:    0.0000
     atom:   56    charge:    2.7028    magn:    0.0001    constr:    0.0000
     atom:   57    charge:    0.8560    magn:   -0.0000    constr:    0.0000
     atom:   58    charge:    2.7027    magn:    0.0001    constr:    0.0000
     atom:   59    charge:    2.7028    magn:    0.0001    constr:    0.0000
     atom:   60    charge:    0.8562    magn:   -0.0000    constr:    0.0000
     atom:   61    charge:    2.7029    magn:    0.0001    constr:    0.0000
     atom:   62    charge:    0.8560    magn:   -0.0000    constr:    0.0000
     atom:   63    charge:    2.7027    magn:    0.0001    constr:    0.0000
     atom:   64    charge:    0.8561    magn:   -0.0000    constr:    0.0000

     total cpu time spent up to now is    28071.6 secs

     End of self-consistent calculation

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


          k = 0.0000 0.0000 0.0000 ( 64705 PWs)   bands (ev):

   -21.5837 -21.4720 -20.1847 -20.1845 -20.1841 -20.1837 -20.1833 -20.1812
   -20.0348 -20.0345 -20.0334 -20.0293 -20.0284 -20.0282 -18.0861 -18.0851
   -18.0844 -18.0842 -18.0834 -18.0821 -17.9320 -17.9309 -17.9299 -17.0358
   -17.0347 -17.0339 -17.0336 -17.0310 -17.0293 -15.8727 -15.8676 -15.8655
   -15.1614 -15.1608 -15.1597 -12.3851 -12.3844 -12.3836 -12.0354 -12.0282
   -12.0216 -12.0193 -12.0133 -12.0094 -11.0277 -11.0276 -11.0275 -11.0269
   -11.0263 -11.0256 -10.7548 -10.7534 -10.7509 -10.7500 -10.7482 -10.7459
    -9.5968  -9.0361  -9.0360  -9.0359  -9.0356  -9.0351  -9.0341  -8.9541
    -8.8815  -8.8756  -8.8715  -8.8703  -8.8699  -8.8604  -8.1091  -8.1086
    -8.1081  -8.1078  -8.1071  -8.1067  -7.9947  -7.9924  -7.9852  -7.7097
    -7.7084  -7.7047  -7.7035  -7.7032  -7.7007  -7.2573  -7.2568  -7.2564
    -7.1808  -7.1806  -7.1804  -7.1796  -7.1789  -7.1765  -6.5067  -6.5060
    -6.5046  -6.5043  -6.4975  -6.4970  -5.9115  -5.9112  -5.9095  -5.9094
    -5.9086  -5.9068  -4.2963  -4.2915  -4.2725  -4.2720  -4.2699  -4.2664
    -4.2662  -4.2632  -4.2110  -4.2104  -4.2096  -4.2090  -4.2079  -4.2077
    -4.0367  -4.0365  -3.9515  -3.9507  -3.9503  -3.8178  -3.8167  -3.8155
     0.4508   0.4521   0.4539   1.3476   1.7541   1.7795   1.7960   1.7970
     1.8076   1.8162   1.8842   2.1190   2.2162   2.2164   2.2169   2.5855
     2.6804   3.4249   3.4253   3.4263   3.4264   3.4278   3.4280   3.4639
     3.4707   3.4756

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k = 0.0000 0.1925 0.0000 ( 64799 PWs)   bands (ev):

  -21.5402 -21.4348 -20.5648 -20.5029 -20.3554 -20.3545 -20.2458 -20.2453
  -19.9480 -19.9471 -19.7516 -19.7333 -19.7323 -19.4773 -18.4972 -18.4961
  -18.0751 -18.0741 -18.0533 -17.9424 -17.9414 -17.7252 -17.7226 -17.7175
  -17.7163 -16.9930 -16.9922 -16.5125 -16.2810 -16.2769 -16.0813 -16.0764
  -14.8791 -14.8779 -14.4517 -12.7500 -12.7425 -12.3972 -12.3928 -12.3200
  -12.3194 -12.2005 -11.4773 -11.4712 -11.4293 -11.4286 -11.2397 -11.2360
  -11.1755 -11.1749 -10.5804 -10.5798 -10.3730 -10.3668 -10.0364  -9.9949
   -9.9913  -9.5628  -9.4457  -9.4190  -9.4161  -9.4158  -9.1139  -8.9026
   -8.8615  -8.8608  -8.6220  -8.6217  -8.5165  -8.5159  -8.3219  -8.3086
   -8.2548  -8.1257  -8.1164  -7.9622  -7.9611  -7.9480  -7.7359  -7.7065
   -7.6247  -7.6244  -7.4174  -7.4165  -7.3543  -7.3525  -7.3518  -7.3503
   -7.2162  -7.1059  -7.0590  -6.9306  -6.8580  -6.8537  -6.8523  -6.8514
   -6.5788  -6.4065  -6.3975  -6.2933  -6.2072  -6.2061  -6.0345  -5.8004
   -5.7992  -5.4933  -5.0257  -5.0191  -4.8132  -4.8125  -4.4666  -4.3928
   -4.2453  -4.2443  -4.1916  -4.1909  -4.1907  -4.1446  -4.1156  -4.0927
   -3.9715  -3.9707  -3.8517  -3.8504  -3.6778  -3.6772  -3.4692  -3.4632
    0.5376   0.5395   0.8064   0.9058   0.9249   1.4086   1.6906   1.7005
    1.9446   2.1802   2.2891   2.2898   2.4607   2.6452   2.6645   2.6873
    2.7412   2.8387   2.8694   2.8697   3.1925   3.1938   3.3339   3.3346
    3.3804   3.5781

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k = 0.0000 0.3849 0.0000 ( 64790 PWs)   bands (ev):

  -21.4100 -21.3237 -20.8910 -20.8852 -20.4593 -20.4584 -20.3745 -20.3742
  -19.6520 -19.6510 -19.3514 -19.3501 -19.2850 -18.9124 -18.9113 -18.8430
```

```
 -18.3760 -18.3446 -18.3425 -18.0483 -18.0473 -17.9718 -17.9707 -17.4541
 -17.4529 -17.3488 -16.8714 -16.8699 -16.3995 -16.3962 -15.4881 -15.4831
 -14.3458 -14.3430 -13.5853 -13.5792 -13.4252 -13.0539 -13.0493 -12.1334
 -12.1328 -11.7230 -11.7223 -11.6951 -11.5005 -11.4999 -11.4790 -11.4758
 -11.1941 -11.0052 -10.9989 -10.1157 -10.1151 -10.0805 -10.0102  -9.9986
  -9.7064  -9.6986  -9.6422  -9.6419  -9.3664  -9.1359  -9.1355  -9.1114
  -9.1061  -8.7507  -8.7377  -8.4961  -8.4870  -8.4640  -8.4633  -8.1488
  -8.1149  -8.1129  -7.9039  -7.9032  -7.8210  -7.8176  -7.8123  -7.6211
  -7.6204  -7.5611  -7.5602  -7.4602  -7.4515  -7.3062  -7.2366  -7.2365
  -7.0951  -6.9020  -6.8977  -6.6765  -6.6756  -6.6741  -6.6265  -6.5063
  -6.4987  -6.4406  -6.4399  -6.3226  -6.1550  -5.9241  -5.8333  -5.8321
  -5.7442  -5.7266  -5.5229  -5.4036  -5.4030  -5.0694  -4.9635  -4.7608
  -4.6681  -4.6332  -4.6154  -4.3388  -4.1811  -4.1804  -4.1376  -4.1368
  -4.0261  -4.0252  -3.9398  -3.9390  -3.2733  -3.2727  -2.7407  -2.7345
   0.1243   0.1421   0.7745   0.7761   1.4361   1.4427   1.5905   1.6740
   2.1254   2.3078   2.3637   2.4566   2.4571   2.4930   2.4937   2.8241
   2.8451   2.9237   3.0200   3.0212   3.0924   3.0930   3.0960   3.1044
   3.5264   3.5520

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

          k = 0.0000-0.5774 0.0000 ( 64894 PWs)   bands (ev):

 -21.1959 -21.1906 -21.1403 -21.1392 -20.4941 -20.4932 -20.4174 -20.4172
 -19.3034 -19.3028 -19.3027 -19.3013 -18.8883 -18.8875 -18.8860 -18.8857
 -18.8117 -18.8104 -18.1323 -18.1309 -18.0111 -18.0107 -18.0103 -18.0087
 -17.3568 -17.3555 -16.6730 -16.6709 -16.6693 -16.6672 -14.8989 -14.8932
 -14.1966 -14.1947 -13.7254 -13.7218 -13.7209 -13.7173 -12.3333 -12.3278
 -11.8469 -11.8467 -11.8464 -11.8451 -11.8326 -11.8320 -11.5504 -11.5474
 -10.9614 -10.9606 -10.5255 -10.5235 -10.5179 -10.5151  -9.7165  -9.7162
  -9.6356  -9.6347  -9.6345  -9.6342  -9.1087  -9.1013  -9.0516  -9.0450
  -9.0417  -9.0354  -8.4988  -8.4970  -8.2524  -8.2474  -8.2346  -8.2304
  -8.1466  -8.1458  -8.0159  -8.0155  -8.0147  -8.0137  -7.6092  -7.6089
  -7.6082  -7.5928  -7.5832  -7.5821  -7.2660  -7.2657  -7.2649  -7.2641
  -7.0726  -7.0725  -6.8972  -6.8963  -6.6191  -6.6166  -6.3580  -6.3565
  -6.3521  -6.3502  -5.9537  -5.9532  -5.9531  -5.9519  -5.8798  -5.8785
  -5.7414  -5.7384  -5.5274  -5.5224  -5.3108  -5.3089  -5.2499  -5.2488
  -5.0736  -5.0632  -4.6716  -4.6705  -4.1012  -4.1007  -4.1005  -4.0989
  -4.0499  -4.0480  -4.0462  -4.0454  -3.1201  -3.1195  -2.3733  -2.3675
  -0.2607  -0.2429   1.1003   1.1014   1.1036   1.1050   1.8824   1.8990
   2.3000   2.3005   2.4248   2.4266   2.6666   2.6707   2.7827   2.7832
   2.7840   2.7850   2.7875   2.8029   2.9623   2.9636   3.1143   3.1308
```

```
    3.2255   3.2294

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k = 0.1667 0.2887 0.0000 ( 64766 PWs)   bands (ev):

  -21.4533 -21.3606 -20.7070 -20.7058 -20.6768 -20.6732 -20.0808 -20.0795
  -19.9049 -19.9028 -19.4972 -19.4960 -19.1394 -19.1371 -18.9368 -18.4599
  -18.4588 -18.3847 -18.1745 -18.1728 -17.8508 -17.7256 -17.7245 -17.6424
  -17.6412 -17.4315 -16.9060 -16.9040 -16.2031 -16.2012 -15.7644 -15.5150
  -15.0426 -13.9243 -13.9226 -13.3489 -13.3441 -13.1861 -12.3126 -12.0315
  -12.0264 -11.9673 -11.9657 -11.9134 -11.6580 -11.6575 -11.6144 -10.8613
  -10.8605 -10.6767 -10.6040 -10.6017 -10.5985 -10.5966  -9.9511  -9.8305
   -9.6049  -9.6041  -9.4609  -9.4528  -9.4313  -9.4088  -9.0854  -9.0848
   -8.8877  -8.8806  -8.8006  -8.5316  -8.4775  -8.4743  -8.2320  -8.2310
   -8.1766  -8.1754  -8.0483  -8.0378  -8.0354  -7.9028  -7.9007  -7.6618
   -7.5545  -7.5527  -7.2712  -7.2706  -7.2666  -7.2651  -7.2201  -7.2157
   -7.0374  -7.0361  -7.0070  -7.0058  -6.6585  -6.6580  -6.6553  -6.6537
   -6.5702  -6.5693  -6.2768  -6.2735  -6.2234  -6.2214  -5.9266  -5.9155
   -5.7565  -5.4399  -5.3704  -5.3697  -4.9492  -4.9486  -4.7911  -4.7563
   -4.7550  -4.5910  -4.4831  -4.3720  -4.3706  -4.3124  -4.3114  -4.2728
   -3.8378  -3.6837  -3.6826  -3.6559  -3.4657  -3.4631  -3.2427  -2.6845
    0.1323   0.4215   0.7888   0.7986   1.1873   1.1902   1.5301   2.0651
    2.2560   2.3024   2.4495   2.4636   2.4926   2.5937   2.6160   2.7368
    2.7380   2.7504   2.7508   2.7653   2.8629   3.1421   3.1448   3.3968
    3.4028   3.6626

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.1667 0.4811 0.0000 ( 64827 PWs)   bands (ev):

   -21.2799 -21.2131 -21.0203 -20.9939 -20.7777 -20.7612 -20.1471 -19.9893
   -19.7458 -19.4788 -19.3603 -19.1889 -19.0230 -18.9708 -18.8382 -18.7173
   -18.5622 -18.4654 -18.3881 -18.2895 -18.2187 -17.7858 -17.7458 -17.7183
   -17.5203 -17.4763 -17.2699 -17.2283 -16.0516 -15.8573 -15.4110 -14.7596
   -14.6550 -14.2286 -14.0287 -13.7970 -13.3264 -12.8609 -12.6869 -12.2380
   -12.1812 -11.9459 -11.9345 -11.7479 -11.7158 -11.6394 -11.6101 -11.3386
   -11.2521 -11.1301 -10.7044 -10.5277 -10.4901 -10.0683 -10.0521 -10.0290
    -9.8493  -9.4647  -9.3356  -9.2043  -9.1948  -9.1300  -8.8958  -8.8582
    -8.7457  -8.6377  -8.6021  -8.5987  -8.5891  -8.5705  -8.4544  -8.3634
    -8.2975  -8.0998  -7.9999  -7.8761  -7.8613  -7.8460  -7.8434  -7.7801
    -7.6471  -7.6019  -7.5951  -7.4981  -7.4781  -7.2385  -7.1298  -7.1103
    -7.0466  -7.0199  -6.8743  -6.8608  -6.8499  -6.5729  -6.4516  -6.3916
    -6.3671  -6.2342  -6.1718  -6.0353  -5.9597  -5.9033  -5.7906  -5.7736
    -5.6122  -5.5536  -5.3985  -5.3924  -5.3720  -5.2955  -5.1056  -5.0283
    -4.9512  -4.9458  -4.8906  -4.8084  -4.6461  -4.6103  -4.5650  -4.4938
    -3.7499  -3.7026  -3.5327  -3.4764  -3.3663  -2.9897  -2.8996  -1.9964
    -0.5518   0.1572   0.4597   0.6106   1.6357   1.7711   2.0807   2.1264
     2.2069   2.2726   2.3058   2.3521   2.3794   2.4889   2.5364   2.5469
     2.6660   2.9126   3.0032   3.0249   3.1060   3.1178   3.2004   3.2782
     3.3590   3.3828

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.3333 0.5774 0.0000 ( 64770 PWs)   bands (ev):

   -21.0678 -21.0635 -21.0593 -21.0311 -21.0305 -21.0291 -19.7785 -19.7774
   -19.7767 -19.5223 -19.5207 -19.5197 -18.7207 -18.7204 -18.7201 -18.7195
   -18.7189 -18.7174 -18.0108 -18.0105 -18.0092 -18.0080 -18.0077 -18.0067
   -17.6332 -17.6322 -17.6312 -17.2047 -15.4426 -15.4352 -15.4310 -14.7020
   -14.7012 -14.7000 -14.1481 -14.1412 -12.5901 -12.2531 -12.2507 -12.2493
   -12.2487 -12.2453 -12.2407 -12.1089 -12.1088 -12.1079 -11.6979 -10.9247
   -10.9240 -10.9238 -10.9235 -10.9232 -10.9219 -10.2099  -9.8976  -9.8950
    -9.8889  -9.1934  -9.1825  -9.1752  -8.9440  -8.9390  -8.9316  -8.6489
```

```
   -8.6479  -8.6478  -8.5783  -8.5780  -8.5776  -8.3487  -8.3479  -8.3457
   -8.1531  -8.1496  -8.1405  -8.1354  -8.1328  -8.1296  -7.9927  -7.9914
   -7.9903  -7.2971  -7.2968  -7.2966  -7.2961  -7.2955  -7.2948  -7.0969
   -7.0947  -7.0907  -6.9638  -6.9629  -6.9619  -6.6182  -6.6173  -6.6166
   -6.0468  -6.0425  -6.0354  -5.6182  -5.6168  -5.6165  -5.4552  -5.4499
   -5.4422  -5.3865  -5.3847  -5.3805  -5.3639  -5.3543  -5.3521  -5.1232
   -5.1229  -5.1224  -5.1216  -5.1208  -5.1196  -4.9309  -4.9304  -4.9302
   -3.5270  -3.5262  -3.5250  -3.1762  -3.1713  -3.1671  -2.8874  -1.2645
   -1.2615   0.2505   0.2546   0.2592   2.0579   2.0660   2.0881   2.2073
    2.3236   2.3246   2.3254   2.6031   2.6055   2.6070   2.7218   2.7248
    2.7264   2.7363   2.7408   2.7452   2.8485   2.8508   2.8563   3.2877
    3.2957   3.3161

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   0.7666
    0.6013   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k =-0.1667 0.0962 0.0000 ( 64799 PWs)   bands (ev):

  -21.5402 -21.4348 -20.5648 -20.5033 -20.3553 -20.3546 -20.2454 -20.2451
  -19.9479 -19.9472 -19.7516 -19.7328 -19.7325 -19.4780 -18.4971 -18.4962
  -18.0754 -18.0738 -18.0533 -17.9427 -17.9410 -17.7251 -17.7239 -17.7174
  -17.7164 -16.9910 -16.9905 -16.5153 -16.2814 -16.2793 -16.0774 -16.0760
  -14.8785 -14.8784 -14.4535 -12.7486 -12.7443 -12.3971 -12.3961 -12.3204
  -12.3190 -12.2005 -11.4737 -11.4690 -11.4292 -11.4286 -11.2371 -11.2349
  -11.1758 -11.1746 -10.5804 -10.5799 -10.3707 -10.3692 -10.0435  -9.9974
   -9.9948  -9.5516  -9.4440  -9.4232  -9.4161  -9.4158  -9.1139  -8.9026
   -8.8613  -8.8610  -8.6220  -8.6217  -8.5164  -8.5160  -8.3173  -8.3063
   -8.2586  -8.1256  -8.1234  -7.9611  -7.9608  -7.9409  -7.7422  -7.7065
   -7.6246  -7.6245  -7.4173  -7.4166  -7.3534  -7.3523  -7.3521  -7.3502
   -7.2161  -7.1060  -7.0576  -6.9252  -6.8616  -6.8598  -6.8523  -6.8516
   -6.5788  -6.4050  -6.4023  -6.2931  -6.2071  -6.2063  -6.0280  -5.8003
   -5.7994  -5.4932  -5.0251  -5.0200  -4.8131  -4.8125  -4.4700  -4.3894
   -4.2448  -4.2446  -4.1914  -4.1911  -4.1908  -4.1446  -4.1154  -4.0930
   -3.9715  -3.9707  -3.8515  -3.8500  -3.6777  -3.6773  -3.4690  -3.4640
    0.5387   0.5397   0.8043   0.9088   0.9234   1.4087   1.6915   1.6974
    1.9446   2.1802   2.2894   2.2897   2.4607   2.6451   2.6680   2.6861
    2.7412   2.8400   2.8695   2.8697   3.1920   3.1925   3.3343   3.3343
    3.3807   3.5782

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k = 0.1667 0.0962 0.0000 ( 64799 PWs)   bands (ev):

 -21.5402 -21.4348 -20.5648 -20.5028 -20.3555 -20.3544 -20.2459 -20.2455
 -19.9481 -19.9470 -19.7516 -19.7332 -19.7325 -19.4771 -18.4973 -18.4960
 -18.0746 -18.0746 -18.0532 -17.9419 -17.9418 -17.7249 -17.7225 -17.7176
 -17.7162 -16.9935 -16.9930 -16.5116 -16.2804 -16.2765 -16.0814 -16.0778
 -14.8789 -14.8779 -14.4513 -12.7500 -12.7428 -12.3960 -12.3926 -12.3197
 -12.3197 -12.2005 -11.4789 -11.4719 -11.4293 -11.4285 -11.2400 -11.2365
 -11.1752 -11.1752 -10.5805 -10.5798 -10.3725 -10.3677 -10.0342  -9.9941
  -9.9899  -9.5662  -9.4468  -9.4173  -9.4162  -9.4158  -9.1139  -8.9026
  -8.8614  -8.8609  -8.6221  -8.6217  -8.5166  -8.5159  -8.3236  -8.3084
  -8.2538  -8.1236  -8.1165  -7.9624  -7.9614  -7.9502  -7.7341  -7.7065
  -7.6247  -7.6244  -7.4174  -7.4163  -7.3549  -7.3524  -7.3519  -7.3501
  -7.2162  -7.1059  -7.0593  -6.9321  -6.8563  -6.8527  -6.8524  -6.8511
  -6.5788  -6.4054  -6.3980  -6.2933  -6.2072  -6.2061  -6.0363  -5.8004
  -5.7991  -5.4933  -5.0261  -5.0185  -4.8132  -4.8124  -4.4661  -4.3933
  -4.2452  -4.2446  -4.1914  -4.1910  -4.1909  -4.1445  -4.1156  -4.0923
  -3.9712  -3.9710  -3.8517  -3.8509  -3.6779  -3.6772  -3.4694  -3.4625
   0.5377   0.5395   0.8066   0.9039   0.9258   1.4086   1.6929   1.6996
   1.9446   2.1802   2.2893   2.2896   2.4608   2.6452   2.6619   2.6888
   2.7412   2.8382   2.8694   2.8697   3.1929   3.1940   3.3341   3.3344
   3.3803   3.5781

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000
```

```
          k =-0.3333 0.1925 0.0000 ( 64790 PWs)   bands (ev):

   -21.4100 -21.3237 -20.8912 -20.8852 -20.4592 -20.4585 -20.3742 -20.3738
   -19.6519 -19.6511 -19.3509 -19.3505 -19.2850 -18.9122 -18.9114 -18.8440
   -18.3760 -18.3442 -18.3434 -18.0486 -18.0470 -17.9721 -17.9704 -17.4540
   -17.4531 -17.3507 -16.8691 -16.8685 -16.3964 -16.3955 -15.4893 -15.4864
   -14.3446 -14.3440 -13.5841 -13.5809 -13.4281 -13.0528 -13.0518 -12.1337
   -12.1324 -11.7229 -11.7224 -11.6951 -11.5008 -11.4996 -11.4757 -11.4733
   -11.1990 -11.0009 -10.9962 -10.1156 -10.1152 -10.0806 -10.0038  -9.9967
    -9.7046  -9.7028  -9.6421  -9.6419  -9.3673  -9.1358  -9.1355  -9.1149
    -9.1116  -8.7509  -8.7375  -8.4955  -8.4933  -8.4638  -8.4636  -8.1487
    -8.1147  -8.1128  -7.9038  -7.9033  -7.8178  -7.8158  -7.8081  -7.6209
    -7.6207  -7.5610  -7.5603  -7.4615  -7.4571  -7.2985  -7.2365  -7.2365
    -7.0950  -6.9026  -6.9007  -6.6805  -6.6765  -6.6757  -6.6263  -6.5034
    -6.5010  -6.4405  -6.4399  -6.3251  -6.1551  -5.9242  -5.8332  -5.8323
    -5.7375  -5.7260  -5.5236  -5.4036  -5.4031  -5.0692  -4.9666  -4.7602
    -4.6644  -4.6334  -4.6154  -4.3386  -4.1809  -4.1804  -4.1374  -4.1369
    -4.0261  -4.0253  -3.9397  -3.9386  -3.2732  -3.2727  -2.7412  -2.7357
     0.1279   0.1412   0.7758   0.7758   1.4370   1.4408   1.5906   1.6703
     2.1254   2.3086   2.3639   2.4566   2.4570   2.4933   2.4935   2.8242
     2.8453   2.9237   3.0195   3.0199   3.0928   3.0928   3.0959   3.1043
     3.5316   3.5518

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.3333 0.1925 0.0000 ( 64790 PWs)   bands (ev):

   -21.4100 -21.3237 -20.8909 -20.8852 -20.4594 -20.4583 -20.3746 -20.3743
   -19.6521 -19.6509 -19.3512 -19.3502 -19.2850 -18.9124 -18.9112 -18.8427
   -18.3760 -18.3443 -18.3425 -18.0479 -18.0478 -17.9713 -17.9712 -17.4542
   -17.4528 -17.3481 -16.8718 -16.8708 -16.3997 -16.3973 -15.4873 -15.4822
   -14.3454 -14.3432 -13.5853 -13.5796 -13.4244 -13.0530 -13.0495 -12.1331
   -12.1331 -11.7230 -11.7222 -11.6951 -11.5002 -11.5002 -11.4800 -11.4765
   -11.1927 -11.0069 -10.9997 -10.1157 -10.1151 -10.0805 -10.0118  -9.9998
    -9.7053  -9.6993  -9.6422  -9.6419  -9.3662  -9.1359  -9.1354  -9.1100
    -9.1043  -8.7506  -8.7378  -8.4942  -8.4872  -8.4639  -8.4634  -8.1488
    -8.1151  -8.1128  -7.9040  -7.9031  -7.8213  -7.8183  -7.8136  -7.6210
    -7.6205  -7.5612  -7.5601  -7.4590  -7.4504  -7.3085  -7.2366  -7.2365
    -7.0951  -6.9014  -6.8973  -6.6766  -6.6755  -6.6724  -6.6265  -6.5061
    -6.4999  -6.4407  -6.4398  -6.3217  -6.1550  -5.9241  -5.8334  -5.8320
    -5.7461  -5.7271  -5.5223  -5.4036  -5.4030  -5.0694  -4.9631  -4.7608
```

```
  -4.6687  -4.6332  -4.6154  -4.3388  -4.1811  -4.1807  -4.1375  -4.1371
  -4.0258  -4.0255  -3.9399  -3.9394  -3.2734  -3.2726  -2.7406  -2.7335
   0.1220   0.1427   0.7747   0.7762   1.4376   1.4421   1.5905   1.6749
   2.1254   2.3075   2.3636   2.4566   2.4571   2.4931   2.4935   2.8240
   2.8450   2.9237   3.0204   3.0213   3.0925   3.0929   3.0960   3.1044
   3.5233   3.5532

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

         k = 0.5000-0.2887 0.0000 ( 64894 PWs)   bands (ev):

 -21.1954 -21.1914 -21.1404 -21.1392 -20.4940 -20.4933 -20.4171 -20.4167
 -19.3039 -19.3027 -19.3021 -19.3016 -18.8883 -18.8878 -18.8860 -18.8858
 -18.8116 -18.8105 -18.1335 -18.1325 -18.0116 -18.0104 -18.0103 -18.0084
 -17.3567 -17.3557 -16.6698 -16.6692 -16.6676 -16.6664 -14.9028 -14.8985
 -14.1943 -14.1931 -13.7235 -13.7226 -13.7205 -13.7195 -12.3364 -12.3324
 -11.8476 -11.8462 -11.8462 -11.8450 -11.8326 -11.8320 -11.5469 -11.5445
 -10.9615 -10.9606 -10.5199 -10.5188 -10.5153 -10.5128  -9.7164  -9.7163
  -9.6357  -9.6356  -9.6341  -9.6335  -9.1077  -9.1027  -9.0495  -9.0467
  -9.0444  -9.0415  -8.4989  -8.4969  -8.2673  -8.2634  -8.2373  -8.2341
  -8.1367  -8.1355  -8.0160  -8.0153  -8.0145  -8.0143  -7.6091  -7.6083
  -7.5998  -7.5879  -7.5823  -7.5812  -7.2661  -7.2658  -7.2650  -7.2639
  -7.0725  -7.0725  -6.8971  -6.8961  -6.6236  -6.6230  -6.3577  -6.3569
  -6.3455  -6.3427  -5.9541  -5.9532  -5.9525  -5.9521  -5.8797  -5.8787
  -5.7600  -5.7531  -5.5159  -5.5134  -5.3107  -5.3092  -5.2499  -5.2487
  -5.0687  -5.0608  -4.6714  -4.6704  -4.1017  -4.1010  -4.0996  -4.0990
  -4.0486  -4.0482  -4.0465  -4.0455  -3.1201  -3.1196  -2.3746  -2.3691
  -0.2563  -0.2433   1.1008   1.1023   1.1029   1.1047   1.8801   1.9016
   2.3000   2.3004   2.4242   2.4272   2.6659   2.6714   2.7826   2.7834
   2.7837   2.7840   2.7853   2.7962   2.9619   2.9626   3.1119   3.1330
   3.2250   3.2301

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

          k =-0.5000-0.2887 0.0000 ( 64894 PWs)   bands (ev):

 -21.1961 -21.1904 -21.1403 -21.1392 -20.4942 -20.4931 -20.4175 -20.4173
 -19.3034 -19.3031 -19.3021 -19.3017 -18.8880 -18.8872 -18.8864 -18.8857
 -18.8116 -18.8105 -18.1320 -18.1303 -18.0110 -18.0107 -18.0097 -18.0093
 -17.3569 -17.3554 -16.6739 -16.6721 -16.6695 -16.6676 -14.8976 -14.8909
 -14.1977 -14.1956 -13.7252 -13.7221 -13.7201 -13.7173 -12.3327 -12.3261
 -11.8471 -11.8464 -11.8461 -11.8454 -11.8327 -11.8319 -11.5515 -11.5481
 -10.9614 -10.9606 -10.5268 -10.5256 -10.5182 -10.5165  -9.7165  -9.7162
  -9.6354  -9.6352  -9.6343  -9.6342  -9.1091  -9.1008  -9.0504  -9.0446
  -9.0412  -9.0351  -8.4987  -8.4971  -8.2472  -8.2423  -8.2334  -8.2278
  -8.1509  -8.1499  -8.0160  -8.0155  -8.0145  -8.0140  -7.6128  -7.6092
  -7.6081  -7.5929  -7.5830  -7.5822  -7.2662  -7.2659  -7.2646  -7.2641
  -7.0726  -7.0725  -6.8971  -6.8964  -6.6180  -6.6151  -6.3587  -6.3570
  -6.3538  -6.3520  -5.9537  -5.9534  -5.9526  -5.9522  -5.8798  -5.8784
  -5.7357  -5.7331  -5.5312  -5.5259  -5.3108  -5.3089  -5.2498  -5.2489
  -5.0753  -5.0630  -4.6716  -4.6705  -4.1012  -4.1012  -4.0998  -4.0993
  -4.0510  -4.0482  -4.0467  -4.0444  -3.1202  -3.1195  -2.3729  -2.3662
  -0.2633  -0.2426   1.1010   1.1021   1.1037   1.1047   1.8835   1.8979
   2.3000   2.3005   2.4250   2.4265   2.6669   2.6704   2.7829   2.7832
   2.7842   2.7846   2.7879   2.8053   2.9624   2.9640   3.1154   3.1298
   3.2257   3.2290

     occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

          k =-0.1667 0.2887 0.0000 ( 64766 PWs)   bands (ev):

 -21.4534 -21.3606 -20.7069 -20.7059 -20.6776 -20.6725 -20.0804 -20.0800
 -19.9037 -19.9028 -19.4971 -19.4961 -19.1406 -19.1374 -18.9368 -18.4599
 -18.4587 -18.3863 -18.1738 -18.1736 -17.8507 -17.7256 -17.7245 -17.6413
```

```
 -17.6391 -17.4315 -16.9074 -16.9049 -16.2036 -16.1996 -15.7574 -15.5190
 -15.0439 -13.9266 -13.9244 -13.3544 -13.3462 -13.1811 -12.3126 -12.0296
 -12.0211 -11.9666 -11.9664 -11.9144 -11.6580 -11.6575 -11.6144 -10.8613
 -10.8605 -10.6742 -10.6087 -10.6028 -10.5955 -10.5914  -9.9511  -9.8305
  -9.6050  -9.6041  -9.4695  -9.4562  -9.4255  -9.4111  -9.0853  -9.0847
  -8.8838  -8.8783  -8.8008  -8.5402  -8.4774  -8.4728  -8.2320  -8.2312
  -8.1761  -8.1757  -8.0483  -8.0349  -8.0281  -7.9025  -7.9010  -7.6620
  -7.5556  -7.5530  -7.2711  -7.2706  -7.2635  -7.2581  -7.2264  -7.2175
  -7.0369  -7.0366  -7.0142  -7.0136  -6.6587  -6.6579  -6.6575  -6.6536
  -6.5702  -6.5690  -6.2754  -6.2751  -6.2232  -6.2216  -5.9290  -5.9086
  -5.7490  -5.4398  -5.3705  -5.3694  -4.9513  -4.9488  -4.7937  -4.7562
  -4.7552  -4.5882  -4.4833  -4.3717  -4.3709  -4.3120  -4.3118  -4.2726
  -3.8379  -3.6837  -3.6826  -3.6545  -3.4664  -3.4626  -3.2426  -2.6858
   0.1349   0.4220   0.7855   0.8006   1.1857   1.1883   1.5302   2.0652
   2.2560   2.3023   2.4471   2.4699   2.4928   2.5973   2.6123   2.7368
   2.7379   2.7504   2.7508   2.7655   2.8629   3.1427   3.1444   3.3978
   3.4018   3.6645

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k = 0.3333 0.0000 0.0000 ( 64766 PWs)   bands (ev):

 -21.4534 -21.3606 -20.7069 -20.7058 -20.6775 -20.6727 -20.0807 -20.0797
 -19.9041 -19.9028 -19.4972 -19.4960 -19.1404 -19.1372 -18.9368 -18.4599
 -18.4587 -18.3859 -18.1742 -18.1732 -17.8507 -17.7257 -17.7245 -17.6417
 -17.6395 -17.4315 -16.9076 -16.9041 -16.2040 -16.1995 -15.7594 -15.5180
 -15.0433 -13.9265 -13.9236 -13.3527 -13.3460 -13.1826 -12.3126 -12.0300
 -12.0222 -11.9669 -11.9662 -11.9139 -11.6580 -11.6575 -11.6144 -10.8613
 -10.8604 -10.6752 -10.6089 -10.6014 -10.5966 -10.5922  -9.9511  -9.8305
  -9.6050  -9.6041  -9.4673  -9.4558  -9.4270  -9.4102  -9.0854  -9.0847
  -8.8855  -8.8777  -8.8007  -8.5382  -8.4775  -8.4732  -8.2321  -8.2311
  -8.1763  -8.1755  -8.0483  -8.0372  -8.0283  -7.9026  -7.9009  -7.6619
  -7.5561  -7.5522  -7.2712  -7.2705  -7.2652  -7.2586  -7.2256  -7.2164
  -7.0372  -7.0363  -7.0128  -7.0118  -6.6586  -6.6579  -6.6576  -6.6529
  -6.5702  -6.5691  -6.2758  -6.2746  -6.2233  -6.2215  -5.9292  -5.9093
  -5.7508  -5.4398  -5.3705  -5.3695  -4.9509  -4.9488  -4.7935  -4.7562
  -4.7551  -4.5884  -4.4832  -4.3718  -4.3706  -4.3122  -4.3116  -4.2726
  -3.8379  -3.6837  -3.6826  -3.6551  -3.4661  -3.4627  -3.2426  -2.6853
   0.1340   0.4223   0.7866   0.7998   1.1858   1.1888   1.5302   2.0652
   2.2560   2.3024   2.4485   2.4678   2.4928   2.5962   2.6135   2.7368
   2.7380   2.7502   2.7509   2.7655   2.8629   3.1425   3.1445   3.3975
   3.4021   3.6638
```

```
     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.1667 0.4811 0.0000 ( 64827 PWs)   bands (ev):

   -21.2800 -21.2131 -21.0202 -20.9939 -20.7777 -20.7613 -20.1471 -19.9891
   -19.7458 -19.4777 -19.3603 -19.1889 -19.0230 -18.9721 -18.8382 -18.7189
   -18.5622 -18.4658 -18.3881 -18.2895 -18.2167 -17.7857 -17.7458 -17.7179
   -17.5203 -17.4749 -17.2699 -17.2304 -16.0541 -15.8530 -15.4087 -14.7635
   -14.6538 -14.2315 -14.0315 -13.7923 -13.3308 -12.8618 -12.6818 -12.2388
   -12.1812 -11.9459 -11.9345 -11.7470 -11.7158 -11.6394 -11.6067 -11.3386
   -11.2521 -11.1351 -10.7037 -10.5277 -10.4901 -10.0683 -10.0521 -10.0305
    -9.8420  -9.4560  -9.3356  -9.2080  -9.1948  -9.1381  -8.8969  -8.8673
    -8.7457  -8.6369  -8.6021  -8.5987  -8.5944  -8.5703  -8.4503  -8.3539
    -8.2975  -8.0999  -7.9999  -7.8761  -7.8601  -7.8461  -7.8369  -7.7835
    -7.6469  -7.6042  -7.5952  -7.4979  -7.4780  -7.2429  -7.1298  -7.1103
    -7.0437  -7.0198  -6.8743  -6.8610  -6.8542  -6.5729  -6.4552  -6.3916
    -6.3672  -6.2320  -6.1757  -6.0353  -5.9548  -5.9033  -5.7907  -5.7736
    -5.6044  -5.5536  -5.4038  -5.3919  -5.3720  -5.2957  -5.1056  -5.0284
    -4.9506  -4.9459  -4.8906  -4.8094  -4.6462  -4.6098  -4.5649  -4.4938
    -3.7499  -3.7026  -3.5314  -3.4774  -3.3663  -2.9897  -2.8993  -1.9975
    -0.5502   0.1565   0.4596   0.6110   1.6319   1.7712   2.0846   2.1263
     2.2064   2.2726   2.3059   2.3521   2.3794   2.4889   2.5363   2.5471
     2.6659   2.9126   3.0032   3.0250   3.1060   3.1177   3.2041   3.2784
     3.3588   3.3837

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.3333 0.3849 0.0000 ( 64827 PWs)   bands (ev):

   -21.2800 -21.2131 -21.0204 -20.9939 -20.7777 -20.7610 -20.1471 -19.9887
   -19.7458 -19.4783 -19.3603 -19.1889 -19.0230 -18.9720 -18.8382 -18.7181
   -18.5623 -18.4668 -18.3881 -18.2895 -18.2175 -17.7857 -17.7457 -17.7196
   -17.5203 -17.4740 -17.2699 -17.2282 -16.0508 -15.8520 -15.4130 -14.7649
   -14.6550 -14.2303 -14.0313 -13.7923 -13.3286 -12.8648 -12.6837 -12.2372
   -12.1812 -11.9459 -11.9345 -11.7516 -11.7158 -11.6394 -11.6046 -11.3386
   -11.2521 -11.1298 -10.6997 -10.5277 -10.4901 -10.0683 -10.0521 -10.0272
    -9.8467  -9.4544  -9.3356  -9.2080  -9.1947  -9.1377  -8.8961  -8.8654
    -8.7457  -8.6460  -8.6021  -8.5986  -8.5973  -8.5647  -8.4526  -8.3599
    -8.2975  -8.0999  -8.0000  -7.8761  -7.8535  -7.8467  -7.8461  -7.7855
    -7.6428  -7.5962  -7.5952  -7.4981  -7.4781  -7.2417  -7.1298  -7.1101
    -7.0460  -7.0199  -6.8742  -6.8609  -6.8505  -6.5729  -6.4551  -6.3917
    -6.3671  -6.2395  -6.1727  -6.0354  -5.9541  -5.9085  -5.7907  -5.7737
    -5.6044  -5.5537  -5.4015  -5.3918  -5.3721  -5.2957  -5.1037  -5.0285
    -4.9484  -4.9457  -4.8906  -4.8093  -4.6462  -4.6102  -4.5648  -4.4938
    -3.7499  -3.7026  -3.5312  -3.4767  -3.3663  -2.9897  -2.9005  -1.9983
    -0.5491   0.1581   0.4594   0.6104   1.6344   1.7711   2.0835   2.1245
     2.2048   2.2725   2.3060   2.3522   2.3794   2.4882   2.5364   2.5470
     2.6662   2.9125   3.0033   3.0248   3.1060   3.1178   3.2058   3.2783
     3.3585   3.3771

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.5000 0.0962 0.0000 ( 64827 PWs)   bands (ev):

   -21.2799 -21.2131 -21.0202 -20.9939 -20.7777 -20.7613 -20.1471 -19.9893
   -19.7458 -19.4778 -19.3603 -19.1889 -19.0230 -18.9718 -18.8382 -18.7187
   -18.5622 -18.4654 -18.3881 -18.2895 -18.2169 -17.7857 -17.7458 -17.7174
   -17.5203 -17.4756 -17.2699 -17.2306 -16.0546 -15.8545 -15.4077 -14.7619
   -14.6536 -14.2314 -14.0308 -13.7938 -13.3304 -12.8607 -12.6823 -12.2389
   -12.1812 -11.9459 -11.9345 -11.7458 -11.7158 -11.6394 -11.6081 -11.3386
   -11.2521 -11.1356 -10.7051 -10.5276 -10.4901 -10.0683 -10.0521 -10.0315
    -9.8424  -9.4586  -9.3356  -9.2071  -9.1948  -9.1363  -8.8968  -8.8659
    -8.7457  -8.6335  -8.6021  -8.5988  -8.5922  -8.5726  -8.4501  -8.3543
```

```
    -8.2975  -8.0999  -7.9999  -7.8761  -7.8625  -7.8461  -7.8352  -7.7820
    -7.6484  -7.6059  -7.5952  -7.4979  -7.4780  -7.2427  -7.1298  -7.1103
    -7.0437  -7.0198  -6.8743  -6.8609  -6.8539  -6.5729  -6.4543  -6.3916
    -6.3672  -6.2304  -6.1757  -6.0353  -5.9568  -5.9015  -5.7907  -5.7736
    -5.6064  -5.5535  -5.4029  -5.3926  -5.3720  -5.2956  -5.1060  -5.0284
    -4.9509  -4.9459  -4.8906  -4.8094  -4.6462  -4.6099  -4.5649  -4.4938
    -3.7499  -3.7026  -3.5321  -3.4775  -3.3663  -2.9897  -2.8987  -1.9966
    -0.5515   0.1557   0.4602   0.6113   1.6322   1.7711   2.0843   2.1271
     2.2066   2.2726   2.3059   2.3521   2.3795   2.4891   2.5363   2.5471
     2.6659   2.9126   3.0031   3.0251   3.1060   3.1177   3.2026   3.2783
     3.3588   3.3857

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.3333-0.3849 0.0000 ( 64827 PWs)   bands (ev):

   -21.2799 -21.2131 -21.0203 -20.9939 -20.7777 -20.7613 -20.1471 -19.9894
   -19.7458 -19.4786 -19.3603 -19.1889 -19.0230 -18.9709 -18.8382 -18.7175
   -18.5622 -18.4651 -18.3881 -18.2895 -18.2184 -17.7858 -17.7458 -17.7177
   -17.5203 -17.4766 -17.2699 -17.2291 -16.0528 -15.8576 -15.4094 -14.7590
   -14.6546 -14.2293 -14.0286 -13.7972 -13.3270 -12.8601 -12.6863 -12.2385
   -12.1812 -11.9459 -11.9345 -11.7465 -11.7158 -11.6394 -11.6109 -11.3386
   -11.2521 -11.1318 -10.7056 -10.5277 -10.4901 -10.0683 -10.0521 -10.0300
    -9.8480  -9.4654  -9.3356  -9.2044  -9.1948  -9.1302  -8.8960  -8.8590
    -8.7457  -8.6345  -8.6021  -8.5987  -8.5880  -8.5727  -8.4532  -8.3616
    -8.2975  -8.0998  -7.9999  -7.8761  -7.8634  -7.8460  -7.8403  -7.7792
    -7.6486  -7.6043  -7.5951  -7.4981  -7.4781  -7.2394  -7.1298  -7.1103
    -7.0458  -7.0199  -6.8743  -6.8608  -6.8506  -6.5728  -6.4516  -6.3916
    -6.3671  -6.2323  -6.1728  -6.0353  -5.9606  -5.9015  -5.7907  -5.7736
    -5.6121  -5.5535  -5.3988  -5.3927  -5.3720  -5.2955  -5.1061  -5.0283
    -4.9517  -4.9458  -4.8906  -4.8085  -4.6461  -4.6104  -4.5650  -4.4938
    -3.7499  -3.7026  -3.5328  -3.4769  -3.3663  -2.9897  -2.8989  -1.9959
    -0.5525   0.1562   0.4598   0.6113   1.6353   1.7711   2.0812   2.1272
     2.2069   2.2727   2.3058   2.3520   2.3794   2.4892   2.5364   2.5469
     2.6659   2.9126   3.0031   3.0250   3.1060   3.1178   3.1996   3.2781
     3.3589   3.3849

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.5000-0.0962 0.0000 ( 64827 PWs)   bands (ev):

   -21.2800 -21.2131 -21.0205 -20.9939 -20.7777 -20.7610 -20.1471 -19.9887
   -19.7458 -19.4786 -19.3603 -19.1889 -19.0230 -18.9716 -18.8382 -18.7177
   -18.5623 -18.4667 -18.3881 -18.2895 -18.2180 -17.7857 -17.7457 -17.7197
   -17.5203 -17.4743 -17.2699 -17.2277 -16.0501 -15.8532 -15.4136 -14.7639
   -14.6552 -14.2296 -14.0307 -13.7936 -13.3276 -12.8646 -12.6849 -12.2369
   -12.1812 -11.9459 -11.9345 -11.7518 -11.7158 -11.6394 -11.6053 -11.3386
   -11.2521 -11.1287 -10.6999 -10.5277 -10.4901 -10.0682 -10.0521 -10.0271
    -9.8484  -9.4564  -9.3356  -9.2070  -9.1947  -9.1358  -8.8959  -8.8632
    -8.7457  -8.6459  -8.6021  -8.5986  -8.5962  -8.5647  -8.4535  -8.3622
    -8.2976  -8.0999  -8.0000  -7.8761  -7.8539  -7.8480  -7.8461  -7.7850
    -7.6429  -7.5957  -7.5952  -7.4981  -7.4781  -7.2407  -7.1298  -7.1101
    -7.0467  -7.0199  -6.8742  -6.8609  -6.8495  -6.5729  -6.4542  -6.3917
    -6.3670  -6.2399  -6.1716  -6.0354  -5.9552  -5.9085  -5.7907  -5.7737
    -5.6065  -5.5537  -5.4003  -5.3922  -5.3721  -5.2956  -5.1038  -5.0284
    -4.9482  -4.9457  -4.8906  -4.8092  -4.6462  -4.6102  -4.5648  -4.4938
    -3.7499  -3.7026  -3.5318  -3.4763  -3.3663  -2.9897  -2.9006  -1.9979
    -0.5497   0.1584   0.4598   0.6100   1.6351   1.7711   2.0827   2.1245
     2.2050   2.2726   2.3059   2.3522   2.3793   2.4882   2.5364   2.5469
     2.6662   2.9125   3.0033   3.0248   3.1060   3.1178   3.2052   3.2782
     3.3585   3.3769

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000
```

```
 ------ SPIN DOWN ----------


          k = 0.0000 0.0000 0.0000 ( 64705 PWs)   bands (ev):

   -21.5815 -21.4717 -20.1843 -20.1841 -20.1837 -20.1834 -20.1830 -20.1809
   -20.0327 -20.0324 -20.0313 -20.0272 -20.0263 -20.0261 -18.0858 -18.0847
   -18.0840 -18.0838 -18.0830 -18.0817 -17.9316 -17.9305 -17.9295 -17.0338
   -17.0327 -17.0319 -17.0316 -17.0290 -17.0273 -15.8703 -15.8652 -15.8631
   -15.1602 -15.1596 -15.1585 -12.3851 -12.3843 -12.3835 -12.0336 -12.0264
   -12.0198 -12.0175 -12.0115 -12.0076 -11.0275 -11.0275 -11.0274 -11.0267
   -11.0261 -11.0254 -10.7541 -10.7526 -10.7502 -10.7493 -10.7474 -10.7452
    -9.5910  -9.0360  -9.0360  -9.0358  -9.0355  -9.0351  -9.0341  -8.9540
    -8.8802  -8.8743  -8.8702  -8.8690  -8.8686  -8.8590  -8.1090  -8.1084
    -8.1079  -8.1076  -8.1070  -8.1065  -7.9940  -7.9917  -7.9845  -7.7037
    -7.7024  -7.6986  -7.6975  -7.6972  -7.6946  -7.2572  -7.2566  -7.2562
    -7.1807  -7.1805  -7.1802  -7.1794  -7.1787  -7.1763  -6.5060  -6.5053
    -6.5039  -6.5035  -6.4967  -6.4963  -5.9113  -5.9110  -5.9094  -5.9092
    -5.9084  -5.9066  -4.2954  -4.2906  -4.2670  -4.2666  -4.2645  -4.2612
    -4.2609  -4.2582  -4.2095  -4.2088  -4.2079  -4.2070  -4.2062  -4.2060
    -4.0365  -4.0362  -3.9510  -3.9501  -3.9497  -3.8110  -3.8099  -3.8087
     0.4570   0.4584   0.4602   1.3481   1.7616   1.7870   1.8035   1.8045
     1.8150   1.8236   1.8847   2.1191   2.2157   2.2159   2.2164   2.5859
     2.6805   3.4246   3.4249   3.4259   3.4260   3.4274   3.4276   3.4646
     3.4712   3.4765

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.0000 0.1925 0.0000 ( 64799 PWs)   bands (ev):

   -21.5381 -21.4345 -20.5645 -20.5008 -20.3551 -20.3542 -20.2437 -20.2432
   -19.9477 -19.9467 -19.7513 -19.7312 -19.7303 -19.4752 -18.4968 -18.4957
   -18.0747 -18.0737 -18.0528 -17.9420 -17.9409 -17.7232 -17.7206 -17.7171
   -17.7159 -16.9910 -16.9902 -16.5105 -16.2790 -16.2749 -16.0791 -16.0742
   -14.8777 -14.8764 -14.4502 -12.7481 -12.7407 -12.3955 -12.3911 -12.3200
   -12.3193 -12.2005 -11.4756 -11.4695 -11.4291 -11.4284 -11.2388 -11.2352
   -11.1754 -11.1747 -10.5803 -10.5797 -10.3721 -10.3659 -10.0350  -9.9941
    -9.9905  -9.5579  -9.4443  -9.4167  -9.4161  -9.4158  -9.1137  -8.9025
    -8.8614  -8.8608  -8.6219  -8.6215  -8.5164  -8.5158  -8.3197  -8.3072
    -8.2497  -8.1250  -8.1157  -7.9563  -7.9551  -7.9471  -7.7346  -7.7063
    -7.6245  -7.6243  -7.4172  -7.4163  -7.3524  -7.3516  -7.3483  -7.3442
    -7.2160  -7.1057  -7.0531  -6.9299  -6.8572  -6.8530  -6.8521  -6.8511
```

```
  -6.5786  -6.4057  -6.3968  -6.2931  -6.2070  -6.2060  -6.0338  -5.8002
  -5.7990  -5.4931  -5.0193  -5.0127  -4.8127  -4.8121  -4.4658  -4.3921
  -4.2402  -4.2392  -4.1907  -4.1896  -4.1887  -4.1432  -4.1154  -4.0868
  -3.9710  -3.9701  -3.8449  -3.8436  -3.6773  -3.6767  -3.4625  -3.4565
   0.5439   0.5460   0.8129   0.9132   0.9322   1.4092   1.6980   1.7078
   1.9450   2.1802   2.2886   2.2893   2.4603   2.6455   2.6721   2.6948
   2.7413   2.8393   2.8689   2.8692   3.1931   3.1944   3.3336   3.3342
   3.3809   3.5787

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

          k = 0.0000 0.3849 0.0000 ( 64790 PWs)   bands (ev):

 -21.4078 -21.3234 -20.8891 -20.8847 -20.4590 -20.4581 -20.3724 -20.3721
 -19.6516 -19.6507 -19.3493 -19.3480 -19.2847 -18.9120 -18.9110 -18.8409
 -18.3756 -18.3425 -18.3404 -18.0479 -18.0469 -17.9714 -17.9703 -17.4537
 -17.4525 -17.3468 -16.8694 -16.8679 -16.3974 -16.3942 -15.4861 -15.4810
 -14.3442 -14.3414 -13.5836 -13.5775 -13.4236 -13.0523 -13.0477 -12.1333
 -12.1327 -11.7228 -11.7222 -11.6950 -11.5004 -11.4998 -11.4781 -11.4749
 -11.1927 -11.0037 -10.9974 -10.1155 -10.1150 -10.0804 -10.0088  -9.9972
  -9.7055  -9.6976  -9.6421  -9.6419  -9.3606  -9.1357  -9.1353  -9.1105
  -9.1052  -8.7504  -8.7319  -8.4953  -8.4862  -8.4639  -8.4632  -8.1486
  -8.1089  -8.1070  -7.9038  -7.9031  -7.8199  -7.8167  -7.8112  -7.6210
  -7.6203  -7.5609  -7.5600  -7.4594  -7.4507  -7.3055  -7.2364  -7.2363
  -7.0949  -6.8959  -6.8916  -6.6764  -6.6754  -6.6730  -6.6263  -6.5055
  -6.4979  -6.4404  -6.4396  -6.3164  -6.1548  -5.9239  -5.8331  -5.8319
  -5.7384  -5.7203  -5.5217  -5.4033  -5.4027  -5.0691  -4.9627  -4.7544
  -4.6673  -4.6330  -4.6149  -4.3385  -4.1775  -4.1768  -4.1342  -4.1333
  -4.0254  -4.0245  -3.9333  -3.9325  -3.2727  -3.2721  -2.7338  -2.7276
   0.1315   0.1493   0.7810   0.7828   1.4432   1.4498   1.5911   1.6807
   2.1258   2.3084   2.3638   2.4560   2.4564   2.4925   2.4932   2.8244
   2.8455   2.9238   3.0206   3.0218   3.0920   3.0926   3.0961   3.1041
   3.5333   3.5365

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k = 0.0000-0.5774 0.0000 ( 64894 PWs)   bands (ev):

 -21.1938 -21.1885 -21.1400 -21.1389 -20.4938 -20.4929 -20.4153 -20.4151
 -19.3031 -19.3025 -19.3024 -19.3010 -18.8862 -18.8854 -18.8840 -18.8837
 -18.8113 -18.8101 -18.1303 -18.1289 -18.0107 -18.0103 -18.0099 -18.0083
 -17.3564 -17.3551 -16.6710 -16.6689 -16.6673 -16.6652 -14.8967 -14.8909
 -14.1950 -14.1932 -13.7238 -13.7201 -13.7193 -13.7157 -12.3318 -12.3262
 -11.8468 -11.8466 -11.8463 -11.8450 -11.8325 -11.8318 -11.5494 -11.5465
 -10.9613 -10.9604 -10.5240 -10.5220 -10.5164 -10.5136  -9.7165  -9.7162
  -9.6354  -9.6346  -9.6343  -9.6340  -9.1029  -9.0954  -9.0507  -9.0441
  -9.0409  -9.0345  -8.4986  -8.4969  -8.2508  -8.2456  -8.2338  -8.2296
  -8.1415  -8.1407  -8.0158  -8.0154  -8.0146  -8.0136  -7.6090  -7.6083
  -7.6080  -7.5921  -7.5820  -7.5809  -7.2659  -7.2656  -7.2648  -7.2640
  -7.0724  -7.0723  -6.8970  -6.8962  -6.6182  -6.6157  -6.3518  -6.3503
  -6.3460  -6.3441  -5.9534  -5.9529  -5.9529  -5.9516  -5.8796  -5.8783
  -5.7400  -5.7370  -5.5214  -5.5165  -5.3105  -5.3087  -5.2495  -5.2484
  -5.0728  -5.0625  -4.6714  -4.6703  -4.0995  -4.0992  -4.0991  -4.0977
  -4.0443  -4.0426  -4.0402  -4.0396  -3.1195  -3.1189  -2.3663  -2.3605
  -0.2535  -0.2358   1.1071   1.1081   1.1105   1.1118   1.8830   1.8996
   2.2993   2.2998   2.4253   2.4271   2.6667   2.6708   2.7823   2.7827
   2.7836   2.7846   2.7945   2.8099   2.9629   2.9642   3.1147   3.1312
   3.2257   3.2295

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k = 0.1667 0.2887 0.0000 ( 64766 PWs)   bands (ev):

 -21.4512 -21.3604 -20.7066 -20.7055 -20.6747 -20.6711 -20.0805 -20.0792
```

```
-19.9029 -19.9007 -19.4968 -19.4957 -19.1373 -19.1350 -18.9364 -18.4595
-18.4584 -18.3827 -18.1741 -18.1724 -17.8503 -17.7252 -17.7241 -17.6404
-17.6392 -17.4310 -16.9040 -16.9019 -16.2011 -16.1992 -15.7620 -15.5130
-15.0414 -13.9227 -13.9210 -13.3472 -13.3424 -13.1841 -12.3126 -12.0299
-12.0249 -11.9672 -11.9657 -11.9127 -11.6579 -11.6574 -11.6142 -10.8612
-10.8603 -10.6750 -10.6026 -10.6003 -10.5975 -10.5956  -9.9510  -9.8305
 -9.6047  -9.6040  -9.4600  -9.4519  -9.4256  -9.4080  -9.0853  -9.0847
 -8.8864  -8.8792  -8.8005  -8.5308  -8.4715  -8.4684  -8.2319  -8.2309
 -8.1765  -8.1752  -8.0482  -8.0371  -8.0347  -7.9026  -7.9006  -7.6617
 -7.5484  -7.5466  -7.2711  -7.2705  -7.2658  -7.2643  -7.2190  -7.2145
 -7.0373  -7.0359  -7.0062  -7.0050  -6.6583  -6.6578  -6.6491  -6.6476
 -6.5700  -6.5691  -6.2766  -6.2733  -6.2231  -6.2211  -5.9254  -5.9147
 -5.7506  -5.4395  -5.3702  -5.3695  -4.9428  -4.9422  -4.7902  -4.7558
 -4.7545  -4.5903  -4.4828  -4.3663  -4.3649  -4.3110  -4.3100  -4.2726
 -3.8373  -3.6831  -3.6820  -3.6490  -3.4589  -3.4564  -3.2420  -2.6776
  0.1396   0.4278   0.7960   0.8057   1.1940   1.1968   1.5307   2.0656
  2.2555   2.3025   2.4567   2.4708   2.4921   2.5943   2.6166   2.7362
  2.7375   2.7500   2.7504   2.7657   2.8630   3.1426   3.1453   3.3970
  3.4029   3.6642

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000

       k = 0.1667 0.4811 0.0000 ( 64827 PWs)   bands (ev):

-21.2778 -21.2128 -21.0182 -20.9936 -20.7774 -20.7591 -20.1468 -19.9872
-19.7455 -19.4767 -19.3599 -19.1885 -19.0226 -18.9688 -18.8378 -18.7152
-18.5619 -18.4634 -18.3877 -18.2891 -18.2166 -17.7853 -17.7453 -17.7163
-17.5199 -17.4743 -17.2695 -17.2263 -16.0495 -15.8551 -15.4089 -14.7575
-14.6536 -14.2271 -14.0271 -13.7951 -13.3248 -12.8594 -12.6854 -12.2373
-12.1811 -11.9458 -11.9344 -11.7464 -11.7156 -11.6393 -11.6085 -11.3385
-11.2520 -11.1286 -10.7034 -10.5275 -10.4900 -10.0681 -10.0521 -10.0274
 -9.8484  -9.4631  -9.3354  -9.1986  -9.1947  -9.1291  -8.8899  -8.8574
 -8.7456  -8.6362  -8.6021  -8.5986  -8.5882  -8.5653  -8.4530  -8.3627
 -8.2974  -8.0997  -7.9998  -7.8759  -7.8606  -7.8459  -7.8425  -7.7793
 -7.6412  -7.6012  -7.5949  -7.4979  -7.4780  -7.2378  -7.1296  -7.1101
 -7.0405  -7.0198  -6.8741  -6.8607  -6.8487  -6.5726  -6.4454  -6.3914
 -6.3669  -6.2331  -6.1655  -6.0351  -5.9589  -5.8971  -5.7904  -5.7734
 -5.6063  -5.5533  -5.3974  -5.3914  -5.3718  -5.2952  -5.0992  -5.0281
 -4.9504  -4.9456  -4.8902  -4.8020  -4.6456  -4.6040  -4.5647  -4.4932
 -3.7493  -3.7021  -3.5258  -3.4696  -3.3657  -2.9890  -2.8927  -1.9894
 -0.5446   0.1642   0.4662   0.6175   1.6426   1.7717   2.0877   2.1273
  2.2135   2.2719   2.3063   2.3515   2.3788   2.4895   2.5359   2.5470
```

```
     2.6665   2.9127   3.0035   3.0254   3.1061   3.1175   3.2077   3.2782
     3.3594   3.5047

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.3333 0.5774 0.0000 ( 64770 PWs)   bands (ev):

   -21.0657 -21.0613 -21.0572 -21.0308 -21.0302 -21.0288 -19.7781 -19.7771
   -19.7764 -19.5203 -19.5186 -19.5176 -18.7204 -18.7200 -18.7197 -18.7191
   -18.7186 -18.7171 -18.0088 -18.0084 -18.0072 -18.0060 -18.0056 -18.0047
   -17.6327 -17.6318 -17.6308 -17.2043 -15.4403 -15.4329 -15.4287 -14.7006
   -14.6998 -14.6987 -14.1459 -14.1391 -12.5896 -12.2516 -12.2491 -12.2478
   -12.2471 -12.2437 -12.2392 -12.1088 -12.1087 -12.1078 -11.6977 -10.9246
   -10.9239 -10.9237 -10.9234 -10.9231 -10.9218 -10.2099  -9.8966  -9.8941
    -9.8880  -9.1917  -9.1809  -9.1737  -8.9381  -8.9333  -8.9260  -8.6488
    -8.6478  -8.6477  -8.5781  -8.5778  -8.5774  -8.3486  -8.3477  -8.3456
    -8.1524  -8.1488  -8.1397  -8.1346  -8.1321  -8.1288  -7.9919  -7.9906
    -7.9896  -7.2970  -7.2967  -7.2965  -7.2959  -7.2954  -7.2946  -7.0908
    -7.0886  -7.0846  -6.9637  -6.9627  -6.9618  -6.6180  -6.6170  -6.6163
    -6.0457  -6.0414  -6.0343  -5.6180  -5.6166  -5.6163  -5.4524  -5.4471
    -5.4394  -5.3802  -5.3784  -5.3742  -5.3594  -5.3500  -5.3479  -5.1228
    -5.1226  -5.1221  -5.1212  -5.1205  -5.1192  -4.9307  -4.9302  -4.9300
    -3.5265  -3.5257  -3.5245  -3.1693  -3.1644  -3.1601  -2.8867  -1.2574
    -1.2544   0.2573   0.2614   0.2659   2.0585   2.0666   2.0886   2.2065
     2.3230   2.3240   2.3248   2.6036   2.6061   2.6075   2.7289   2.7319
     2.7336   2.7433   2.7479   2.7523   2.8486   2.8509   2.8564   3.2880
     3.2961   3.3165

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   0.3811
   0.2510   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k =-0.1667 0.0962 0.0000 ( 64799 PWs)   bands (ev):

 -21.5381 -21.4345 -20.5645 -20.5012 -20.3550 -20.3543 -20.2433 -20.2430
 -19.9476 -19.9468 -19.7513 -19.7307 -19.7305 -19.4759 -18.4967 -18.4958
 -18.0750 -18.0734 -18.0529 -17.9423 -17.9406 -17.7230 -17.7219 -17.7169
 -17.7160 -16.9890 -16.9885 -16.5133 -16.2794 -16.2773 -16.0753 -16.0738
 -14.8770 -14.8769 -14.4519 -12.7468 -12.7425 -12.3954 -12.3943 -12.3204
 -12.3190 -12.2005 -11.4721 -11.4673 -11.4290 -11.4285 -11.2363 -11.2341
 -11.1757 -11.1745 -10.5802 -10.5797 -10.3698 -10.3683 -10.0421  -9.9965
  -9.9939  -9.5467  -9.4426  -9.4210  -9.4160  -9.4158  -9.1138  -8.9025
  -8.8613  -8.8610  -8.6218  -8.6215  -8.5164  -8.5159  -8.3152  -8.3050
  -8.2534  -8.1248  -8.1226  -7.9552  -7.9548  -7.9401  -7.7410  -7.7064
  -7.6244  -7.6243  -7.4172  -7.4164  -7.3522  -7.3520  -7.3474  -7.3441
  -7.2159  -7.1058  -7.0516  -6.9245  -6.8609  -6.8589  -6.8521  -6.8514
  -6.5786  -6.4043  -6.4016  -6.2930  -6.2069  -6.2062  -6.0272  -5.8001
  -5.7993  -5.4930  -5.0187  -5.0136  -4.8127  -4.8121  -4.4692  -4.3886
  -4.2398  -4.2396  -4.1909  -4.1894  -4.1889  -4.1432  -4.1152  -4.0871
  -3.9709  -3.9701  -3.8448  -3.8433  -3.6772  -3.6767  -3.4623  -3.4573
   0.5451   0.5461   0.8107   0.9161   0.9307   1.4092   1.6989   1.7048
   1.9450   2.1802   2.2889   2.2892   2.4602   2.6454   2.6756   2.6936
   2.7413   2.8406   2.8690   2.8692   3.1926   3.1931   3.3339   3.3339
   3.3812   3.5785

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k = 0.1667 0.0962 0.0000 ( 64799 PWs)   bands (ev):

 -21.5381 -21.4345 -20.5645 -20.5007 -20.3552 -20.3541 -20.2438 -20.2434
 -19.9478 -19.9467 -19.7513 -19.7311 -19.7304 -19.4750 -18.4969 -18.4956
 -18.0743 -18.0742 -18.0528 -17.9415 -17.9414 -17.7229 -17.7205 -17.7172
 -17.7157 -16.9915 -16.9910 -16.5095 -16.2784 -16.2745 -16.0792 -16.0756
 -14.8775 -14.8764 -14.4497 -12.7481 -12.7409 -12.3943 -12.3909 -12.3197
 -12.3197 -12.2004 -11.4772 -11.4701 -11.4292 -11.4284 -11.2392 -11.2357
 -11.1751 -11.1750 -10.5803 -10.5796 -10.3716 -10.3668 -10.0327  -9.9933
```

```
  -9.9891  -9.5614  -9.4454  -9.4161  -9.4157  -9.4149  -9.1137  -8.9025
  -8.8613  -8.8609  -8.6219  -8.6215  -8.5165  -8.5158  -8.3214  -8.3071
  -8.2488  -8.1229  -8.1158  -7.9566  -7.9554  -7.9492  -7.7328  -7.7063
  -7.6245  -7.6243  -7.4173  -7.4162  -7.3522  -7.3518  -7.3488  -7.3440
  -7.2160  -7.1057  -7.0534  -6.9314  -6.8555  -6.8522  -6.8519  -6.8507
  -6.5786  -6.4046  -6.3972  -6.2931  -6.2071  -6.2059  -6.0356  -5.8003
  -5.7989  -5.4931  -5.0197  -5.0122  -4.8128  -4.8120  -4.4653  -4.3926
  -4.2402  -4.2395  -4.1907  -4.1894  -4.1890  -4.1432  -4.1154  -4.0865
  -3.9707  -3.9704  -3.8449  -3.8442  -3.6773  -3.6766  -3.4627  -3.4558
   0.5440   0.5459   0.8131   0.9113   0.9332   1.4092   1.7002   1.7069
   1.9450   2.1802   2.2888   2.2891   2.4603   2.6456   2.6695   2.6963
   2.7414   2.8388   2.8689   2.8692   3.1936   3.1946   3.3337   3.3340
   3.3808   3.5785

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000

        k =-0.3333 0.1925 0.0000 ( 64790 PWs)   bands (ev):

 -21.4079 -21.3234 -20.8892 -20.8847 -20.4589 -20.4582 -20.3721 -20.3717
 -19.6515 -19.6508 -19.3488 -19.3485 -19.2847 -18.9119 -18.9111 -18.8419
 -18.3756 -18.3422 -18.3414 -18.0482 -18.0466 -17.9717 -17.9699 -17.4536
 -17.4526 -17.3486 -16.8671 -16.8665 -16.3944 -16.3934 -15.4873 -15.4844
 -14.3430 -14.3424 -13.5824 -13.5792 -13.4265 -13.0512 -13.0501 -12.1337
 -12.1323 -11.7228 -11.7222 -11.6950 -11.5007 -11.4995 -11.4747 -11.4724
 -11.1975 -10.9993 -10.9946 -10.1154 -10.1150 -10.0804 -10.0023  -9.9953
  -9.7037  -9.7019  -9.6421  -9.6419  -9.3614  -9.1356  -9.1353  -9.1141
  -9.1107  -8.7506  -8.7317  -8.4947  -8.4926  -8.4637  -8.4635  -8.1485
  -8.1087  -8.1069  -7.9037  -7.9032  -7.8166  -7.8145  -7.8074  -7.6208
  -7.6205  -7.5609  -7.5602  -7.4607  -7.4563  -7.2977  -7.2363  -7.2363
  -7.0948  -6.8965  -6.8946  -6.6794  -6.6763  -6.6756  -6.6262  -6.5027
  -6.5002  -6.4402  -6.4396  -6.3189  -6.1549  -5.9239  -5.8330  -5.8321
  -5.7316  -5.7197  -5.5225  -5.4032  -5.4028  -5.0690  -4.9657  -4.7537
  -4.6637  -4.6331  -4.6149  -4.3384  -4.1774  -4.1769  -4.1339  -4.1334
  -4.0253  -4.0245  -3.9332  -3.9321  -3.2726  -3.2721  -2.7342  -2.7288
   0.1350   0.1484   0.7824   0.7825   1.4442   1.4480   1.5912   1.6769
   2.1259   2.3092   2.3639   2.4560   2.4563   2.4928   2.4930   2.8245
   2.8457   2.9239   3.0201   3.0205   3.0923   3.0924   3.0960   3.1039
   3.5356   3.5595

   occupation numbers
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k = 0.3333 0.1925 0.0000 ( 64790 PWs)   bands (ev):

  -21.4078 -21.3234 -20.8890 -20.8847 -20.4591 -20.4580 -20.3725 -20.3722
  -19.6517 -19.6506 -19.3492 -19.3482 -19.2847 -18.9121 -18.9109 -18.8406
  -18.3756 -18.3423 -18.3405 -18.0475 -18.0474 -17.9709 -17.9708 -17.4538
  -17.4523 -17.3461 -16.8698 -16.8688 -16.3976 -16.3953 -15.4853 -15.4802
  -14.3439 -14.3417 -13.5835 -13.5779 -13.4228 -13.0514 -13.0479 -12.1330
  -12.1330 -11.7229 -11.7221 -11.6950 -11.5001 -11.5001 -11.4791 -11.4756
  -11.1912 -11.0053 -10.9982 -10.1155 -10.1149 -10.0804 -10.0103  -9.9984
   -9.7043  -9.6983  -9.6422  -9.6418  -9.3603  -9.1358  -9.1353  -9.1092
   -9.1034  -8.7503  -8.7320  -8.4934  -8.4864  -8.4638  -8.4633  -8.1487
   -8.1091  -8.1069  -7.9038  -7.9030  -7.8204  -7.8172  -7.8125  -7.6208
   -7.6204  -7.5610  -7.5599  -7.4582  -7.4497  -7.3078  -7.2364  -7.2363
   -7.0950  -6.8952  -6.8912  -6.6764  -6.6753  -6.6713  -6.6263  -6.5053
   -6.4991  -6.4405  -6.4396  -6.3155  -6.1548  -5.9239  -5.8332  -5.8318
   -5.7403  -5.7208  -5.5210  -5.4033  -5.4027  -5.0692  -4.9622  -4.7545
   -4.6680  -4.6330  -4.6149  -4.3385  -4.1774  -4.1770  -4.1341  -4.1336
   -4.0251  -4.0248  -3.9333  -3.9329  -3.2728  -3.2720  -2.7337  -2.7266
    0.1293   0.1499   0.7812   0.7828   1.4447   1.4492   1.5911   1.6817
    2.1258   2.3081   2.3637   2.4559   2.4565   2.4927   2.4930   2.8244
    2.8454   2.9238   3.0210   3.0220   3.0921   3.0925   3.0961   3.1041
    3.5306   3.5360

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
```

```
     0.0000   0.0000

          k = 0.5000-0.2887 0.0000 ( 64894 PWs)   bands (ev):

   -21.1932 -21.1893 -21.1401 -21.1389 -20.4937 -20.4929 -20.4150 -20.4146
   -19.3035 -19.3024 -19.3017 -19.3012 -18.8862 -18.8858 -18.8840 -18.8838
   -18.8113 -18.8102 -18.1314 -18.1304 -18.0112 -18.0100 -18.0099 -18.0080
   -17.3562 -17.3553 -16.6678 -16.6672 -16.6656 -16.6643 -14.9006 -14.8962
   -14.1928 -14.1916 -13.7219 -13.7210 -13.7189 -13.7179 -12.3349 -12.3308
   -11.8475 -11.8461 -11.8461 -11.8450 -11.8325 -11.8319 -11.5459 -11.5436
   -10.9613 -10.9605 -10.5184 -10.5173 -10.5138 -10.5113  -9.7164  -9.7162
    -9.6356  -9.6354  -9.6339  -9.6333  -9.1018  -9.0968  -9.0486  -9.0459
    -9.0436  -9.0406  -8.4988  -8.4968  -8.2654  -8.2615  -8.2365  -8.2332
    -8.1319  -8.1305  -8.0159  -8.0152  -8.0143  -8.0141  -7.6089  -7.6082
    -7.5991  -7.5871  -7.5810  -7.5800  -7.2660  -7.2657  -7.2648  -7.2638
    -7.0723  -7.0723  -6.8969  -6.8960  -6.6227  -6.6220  -6.3515  -6.3507
    -6.3395  -6.3368  -5.9538  -5.9529  -5.9522  -5.9518  -5.8795  -5.8785
    -5.7584  -5.7515  -5.5101  -5.5076  -5.3105  -5.3090  -5.2495  -5.2483
    -5.0679  -5.0600  -4.6712  -4.6702  -4.1001  -4.0993  -4.0983  -4.0978
    -4.0428  -4.0427  -4.0410  -4.0396  -3.1194  -3.1189  -2.3675  -2.3620
    -0.2493  -0.2363   1.1076   1.1092   1.1098   1.1116   1.8807   1.9022
     2.2993   2.2997   2.4247   2.4277   2.6660   2.6715   2.7821   2.7830
     2.7836   2.7847   2.7908   2.8031   2.9625   2.9632   3.1122   3.1333
     3.2252   3.2302

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.5000-0.2887 0.0000 ( 64894 PWs)   bands (ev):

   -21.1939 -21.1883 -21.1400 -21.1389 -20.4938 -20.4928 -20.4154 -20.4152
   -19.3031 -19.3028 -19.3017 -19.3013 -18.8860 -18.8851 -18.8843 -18.8837
   -18.8113 -18.8101 -18.1299 -18.1283 -18.0106 -18.0103 -18.0094 -18.0089
   -17.3565 -17.3550 -16.6719 -16.6701 -16.6675 -16.6655 -14.8954 -14.8887
   -14.1962 -14.1941 -13.7236 -13.7205 -13.7185 -13.7157 -12.3311 -12.3245
   -11.8470 -11.8463 -11.8460 -11.8454 -11.8326 -11.8318 -11.5506 -11.5472
   -10.9613 -10.9605 -10.5254 -10.5240 -10.5167 -10.5150  -9.7165  -9.7162
    -9.6352  -9.6350  -9.6342  -9.6340  -9.1033  -9.0949  -9.0495  -9.0438
    -9.0403  -9.0342  -8.4985  -8.4970  -8.2457  -8.2407  -8.2325  -8.2270
    -8.1458  -8.1447  -8.0158  -8.0153  -8.0144  -8.0138  -7.6121  -7.6091
    -7.6080  -7.5922  -7.5817  -7.5810  -7.2660  -7.2657  -7.2644  -7.2640
    -7.0724  -7.0723  -6.8969  -6.8962  -6.6172  -6.6143  -6.3525  -6.3508
    -6.3477  -6.3459  -5.9534  -5.9531  -5.9523  -5.9519  -5.8797  -5.8782
```

```
   -5.7344  -5.7317  -5.5252  -5.5199  -5.3106  -5.3087  -5.2495  -5.2485
   -5.0745  -5.0622  -4.6714  -4.6703  -4.0995  -4.0995  -4.0985  -4.0980
   -4.0455  -4.0427  -4.0408  -4.0385  -3.1195  -3.1188  -2.3660  -2.3593
   -0.2561  -0.2355   1.1077   1.1088   1.1105   1.1115   1.8841   1.8984
    2.2993   2.2998   2.4254   2.4270   2.6670   2.6705   2.7824   2.7828
    2.7838   2.7842   2.7949   2.8124   2.9630   2.9646   3.1157   3.1302
    3.2259   3.2292

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000

          k =-0.1667 0.2887 0.0000 ( 64766 PWs)   bands (ev):

  -21.4512 -21.3604 -20.7066 -20.7056 -20.6755 -20.6704 -20.0801 -20.0796
  -19.9016 -19.9007 -19.4968 -19.4958 -19.1385 -19.1354 -18.9364 -18.4595
  -18.4584 -18.3843 -18.1734 -18.1732 -17.8503 -17.7252 -17.7241 -17.6393
  -17.6371 -17.4310 -16.9054 -16.9029 -16.2016 -16.1976 -15.7551 -15.5170
  -15.0426 -13.9250 -13.9228 -13.3527 -13.3446 -13.1792 -12.3126 -12.0280
  -12.0195 -11.9666 -11.9664 -11.9136 -11.6579 -11.6574 -11.6142 -10.8612
  -10.8603 -10.6726 -10.6073 -10.6014 -10.5946 -10.5904  -9.9510  -9.8305
   -9.6048  -9.6039  -9.4687  -9.4553  -9.4198  -9.4101  -9.0853  -9.0847
   -8.8824  -8.8769  -8.8007  -8.5395  -8.4715  -8.4669  -8.2319  -8.2311
   -8.1760  -8.1755  -8.0482  -8.0342  -8.0274  -7.9024  -7.9008  -7.6618
   -7.5496  -7.5470  -7.2710  -7.2705  -7.2627  -7.2573  -7.2252  -7.2163
   -7.0367  -7.0364  -7.0134  -7.0128  -6.6585  -6.6577  -6.6514  -6.6474
   -6.5701  -6.5689  -6.2753  -6.2749  -6.2229  -6.2213  -5.9276  -5.9078
   -5.7433  -5.4395  -5.3703  -5.3692  -4.9450  -4.9424  -4.7929  -4.7557
   -4.7547  -4.5874  -4.4830  -4.3660  -4.3653  -4.3105  -4.3104  -4.2724
   -3.8373  -3.6831  -3.6820  -3.6477  -3.4596  -3.4558  -3.2420  -2.6789
    0.1422   0.4285   0.7927   0.8078   1.1923   1.1950   1.5308   2.0656
    2.2555   2.3024   2.4545   2.4772   2.4923   2.5980   2.6129   2.7363
    2.7374   2.7500   2.7504   2.7659   2.8630   3.1432   3.1448   3.3979
    3.4019   3.6641

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.3333 0.0000 0.0000 ( 64766 PWs)   bands (ev):

   -21.4512 -21.3604 -20.7066 -20.7055 -20.6754 -20.6706 -20.0804 -20.0793
   -19.9020 -19.9007 -19.4968 -19.4957 -19.1384 -19.1352 -18.9364 -18.4595
   -18.4583 -18.3839 -18.1738 -18.1728 -17.8503 -17.7253 -17.7241 -17.6397
   -17.6375 -17.4310 -16.9055 -16.9021 -16.2020 -16.1975 -15.7570 -15.5160
   -15.0421 -13.9249 -13.9220 -13.3510 -13.3444 -13.1806 -12.3126 -12.0284
   -12.0206 -11.9668 -11.9661 -11.9132 -11.6579 -11.6574 -11.6142 -10.8612
   -10.8603 -10.6735 -10.6074 -10.6001 -10.5956 -10.5913  -9.9509  -9.8305
    -9.6048  -9.6039  -9.4664  -9.4549  -9.4212  -9.4093  -9.0853  -9.0847
    -8.8842  -8.8763  -8.8006  -8.5374  -8.4716  -8.4672  -8.2319  -8.2310
    -8.1761  -8.1754  -8.0482  -8.0365  -8.0275  -7.9025  -7.9007  -7.6618
    -7.5501  -7.5462  -7.2711  -7.2704  -7.2645  -7.2578  -7.2245  -7.2152
    -7.0370  -7.0361  -7.0120  -7.0110  -6.6584  -6.6577  -6.6514  -6.6467
    -6.5700  -6.5689  -6.2757  -6.2744  -6.2230  -6.2212  -5.9279  -5.9085
    -5.7451  -5.4395  -5.3703  -5.3693  -4.9446  -4.9424  -4.7927  -4.7558
    -4.7546  -4.5876  -4.4830  -4.3661  -4.3650  -4.3107  -4.3101  -4.2724
    -3.8373  -3.6831  -3.6820  -3.6483  -3.4594  -3.4560  -3.2420  -2.6784
     0.1412   0.4287   0.7938   0.8069   1.1923   1.1955   1.5307   2.0656
     2.2555   2.3024   2.4558   2.4751   2.4922   2.5969   2.6141   2.7362
     2.7375   2.7498   2.7505   2.7658   2.8630   3.1430   3.1450   3.3977
     3.4022   3.6648

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.1667 0.4811 0.0000 ( 64827 PWs)   bands (ev):

   -21.2778 -21.2128 -21.0181 -20.9936 -20.7774 -20.7592 -20.1468 -19.9870
   -19.7455 -19.4757 -19.3600 -19.1885 -19.0226 -18.9701 -18.8378 -18.7168
```

```
-18.5619 -18.4637 -18.3877 -18.2891 -18.2147 -17.7853 -17.7454 -17.7159
-17.5199 -17.4729 -17.2695 -17.2283 -16.0521 -15.8508 -15.4066 -14.7615
-14.6523 -14.2299 -14.0300 -13.7904 -13.3292 -12.8602 -12.6802 -12.2381
-12.1811 -11.9458 -11.9344 -11.7454 -11.7156 -11.6393 -11.6051 -11.3385
-11.2520 -11.1336 -10.7028 -10.5275 -10.4900 -10.0682 -10.0521 -10.0290
 -9.8411  -9.4544  -9.3354  -9.2022  -9.1947  -9.1372  -8.8910  -8.8665
 -8.7455  -8.6354  -8.6020  -8.5986  -8.5936  -8.5651  -8.4489  -8.3531
 -8.2974  -8.0998  -7.9998  -7.8759  -7.8594  -7.8460  -7.8360  -7.7827
 -7.6410  -7.6034  -7.5950  -7.4978  -7.4779  -7.2421  -7.1296  -7.1101
 -7.0376  -7.0197  -6.8741  -6.8608  -6.8531  -6.5726  -6.4491  -6.3915
 -6.3669  -6.2309  -6.1695  -6.0351  -5.9540  -5.8970  -5.7904  -5.7734
 -5.5983  -5.5533  -5.4029  -5.3909  -5.3718  -5.2953  -5.0992  -5.0282
 -4.9498  -4.9456  -4.8902  -4.8031  -4.6457  -4.6035  -4.5646  -4.4931
 -3.7494  -3.7020  -3.5246  -3.4706  -3.3657  -2.9890  -2.8924  -1.9904
 -0.5431   0.1635   0.4663   0.6178   1.6387   1.7717   2.0917   2.1272
  2.2130   2.2719   2.3064   2.3516   2.3788   2.4895   2.5358   2.5472
  2.6664   2.9127   3.0035   3.0255   3.1062   3.1173   3.2115   3.2785
  3.3590   3.3908

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000

       k =-0.3333 0.3849 0.0000 ( 64827 PWs)   bands (ev):

-21.2779 -21.2128 -21.0183 -20.9936 -20.7774 -20.7589 -20.1467 -19.9866
-19.7455 -19.4762 -19.3600 -19.1885 -19.0227 -18.9699 -18.8378 -18.7161
-18.5619 -18.4648 -18.3877 -18.2891 -18.2155 -17.7853 -17.7453 -17.7176
-17.5199 -17.4720 -17.2695 -17.2262 -16.0487 -15.8498 -15.4109 -14.7628
-14.6535 -14.2288 -14.0297 -13.7904 -13.3270 -12.8632 -12.6821 -12.2364
-12.1811 -11.9458 -11.9344 -11.7501 -11.7156 -11.6393 -11.6030 -11.3385
-11.2520 -11.1283 -10.6987 -10.5276 -10.4899 -10.0681 -10.0521 -10.0256
 -9.8458  -9.4529  -9.3354  -9.2022  -9.1946  -9.1368  -8.8902  -8.8646
 -8.7455  -8.6442  -8.6020  -8.5985  -8.5965  -8.5597  -8.4512  -8.3592
 -8.2974  -8.0998  -7.9998  -7.8759  -7.8528  -7.8460  -7.8458  -7.7847
 -7.6370  -7.5955  -7.5950  -7.4979  -7.4779  -7.2409  -7.1296  -7.1100
 -7.0399  -7.0198  -6.8740  -6.8608  -6.8493  -6.5726  -6.4490  -6.3915
 -6.3668  -6.2385  -6.1664  -6.0351  -5.9533  -5.9022  -5.7904  -5.7735
 -5.5982  -5.5534  -5.4006  -5.3907  -5.3719  -5.2953  -5.0973  -5.0282
 -4.9476  -4.9455  -4.8902  -4.8030  -4.6457  -4.6039  -4.5646  -4.4932
 -3.7494  -3.7021  -3.5244  -3.4699  -3.3657  -2.9890  -2.8935  -1.9912
 -0.5420   0.1650   0.4661   0.6173   1.6413   1.7717   2.0906   2.1255
  2.2112   2.2718   2.3064   2.3517   2.3787   2.4888   2.5359   2.5470
  2.6667   2.9126   3.0036   3.0253   3.1062   3.1174   3.2132   3.2784
```

```
     3.3592   3.5044

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.5000 0.0962 0.0000 ( 64827 PWs)   bands (ev):

   -21.2778 -21.2128 -21.0181 -20.9936 -20.7774 -20.7592 -20.1468 -19.9872
   -19.7455 -19.4758 -19.3600 -19.1885 -19.0226 -18.9698 -18.8378 -18.7167
   -18.5619 -18.4633 -18.3877 -18.2891 -18.2149 -17.7853 -17.7454 -17.7154
   -17.5199 -17.4736 -17.2695 -17.2286 -16.0526 -15.8523 -15.4056 -14.7599
   -14.6521 -14.2298 -14.0293 -13.7918 -13.3288 -12.8591 -12.6807 -12.2383
   -12.1811 -11.9458 -11.9344 -11.7443 -11.7156 -11.6393 -11.6066 -11.3385
   -11.2520 -11.1341 -10.7042 -10.5275 -10.4900 -10.0682 -10.0521 -10.0299
    -9.8414  -9.4571  -9.3354  -9.2013  -9.1947  -9.1355  -8.8910  -8.8650
    -8.7455  -8.6321  -8.6020  -8.5986  -8.5914  -8.5673  -8.4487  -8.3535
    -8.2974  -8.0998  -7.9998  -7.8759  -7.8618  -7.8460  -7.8344  -7.7812
    -7.6425  -7.6052  -7.5950  -7.4978  -7.4779  -7.2420  -7.1296  -7.1101
    -7.0376  -7.0197  -6.8741  -6.8608  -6.8528  -6.5726  -6.4482  -6.3915
    -6.3670  -6.2292  -6.1695  -6.0350  -5.9560  -5.8952  -5.7904  -5.7734
    -5.6004  -5.5532  -5.4019  -5.3916  -5.3718  -5.2953  -5.0996  -5.0281
    -4.9501  -4.9457  -4.8902  -4.8030  -4.6456  -4.6036  -4.5647  -4.4931
    -3.7494  -3.7020  -3.5252  -3.4706  -3.3657  -2.9890  -2.8918  -1.9896
    -0.5443   0.1628   0.4668   0.6181   1.6390   1.7717   2.0914   2.1279
     2.2133   2.2719   2.3063   2.3516   2.3788   2.4898   2.5358   2.5472
     2.6664   2.9127   3.0035   3.0255   3.1062   3.1173   3.2100   3.2784
     3.3590   3.5044

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

```
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k =-0.3333-0.3849 0.0000 ( 64827 PWs)   bands (ev):

   -21.2777 -21.2128 -21.0181 -20.9936 -20.7774 -20.7592 -20.1468 -19.9873
   -19.7455 -19.4765 -19.3599 -19.1885 -19.0226 -18.9688 -18.8378 -18.7155
   -18.5619 -18.4631 -18.3877 -18.2891 -18.2164 -17.7853 -17.7453 -17.7157
   -17.5199 -17.4746 -17.2695 -17.2271 -16.0507 -15.8555 -15.4073 -14.7569
   -14.6532 -14.2277 -14.0270 -13.7952 -13.3254 -12.8585 -12.6847 -12.2378
   -12.1811 -11.9458 -11.9344 -11.7449 -11.7156 -11.6393 -11.6093 -11.3385
   -11.2520 -11.1303 -10.7046 -10.5275 -10.4900 -10.0681 -10.0521 -10.0284
    -9.8470  -9.4638  -9.3354  -9.1987  -9.1947  -9.1293  -8.8901  -8.8581
    -8.7456  -8.6331  -8.6020  -8.5986  -8.5872  -8.5675  -8.4518  -8.3608
    -8.2974  -8.0997  -7.9998  -7.8759  -7.8627  -7.8459  -7.8395  -7.7784
    -7.6426  -7.6036  -7.5949  -7.4979  -7.4780  -7.2386  -7.1296  -7.1101
    -7.0397  -7.0198  -6.8741  -6.8607  -6.8494  -6.5726  -6.4455  -6.3914
    -6.3669  -6.2312  -6.1666  -6.0351  -5.9598  -5.8952  -5.7904  -5.7734
    -5.6062  -5.5532  -5.3977  -5.3916  -5.3718  -5.2952  -5.0997  -5.0280
    -4.9509  -4.9456  -4.8902  -4.8021  -4.6456  -4.6041  -4.5648  -4.4932
    -3.7493  -3.7021  -3.5259  -3.4701  -3.3657  -2.9890  -2.8920  -1.9889
    -0.5452   0.1632   0.4664   0.6182   1.6421   1.7717   2.0882   2.1280
     2.2137   2.2719   2.3063   2.3515   2.3788   2.4898   2.5359   2.5470
     2.6664   2.9127   3.0035   3.0255   3.1061   3.1174   3.2070   3.2783
     3.3593   3.5047

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

          k = 0.5000-0.0962 0.0000 ( 64827 PWs)   bands (ev):

   -21.2778 -21.2128 -21.0183 -20.9936 -20.7774 -20.7589 -20.1467 -19.9866
   -19.7455 -19.4765 -19.3600 -19.1885 -19.0227 -18.9696 -18.8378 -18.7157
   -18.5619 -18.4647 -18.3877 -18.2891 -18.2160 -17.7853 -17.7453 -17.7177
   -17.5199 -17.4723 -17.2695 -17.2257 -16.0481 -15.8510 -15.4115 -14.7618
   -14.6537 -14.2281 -14.0291 -13.7917 -13.3260 -12.8630 -12.6833 -12.2362
   -12.1811 -11.9458 -11.9344 -11.7503 -11.7156 -11.6393 -11.6038 -11.3385
   -11.2520 -11.1272 -10.6989 -10.5276 -10.4900 -10.0681 -10.0521 -10.0255
    -9.8475  -9.4549  -9.3354  -9.2013  -9.1946  -9.1349  -8.8900  -8.8624
```

```
    -8.7455  -8.6441  -8.6020  -8.5985  -8.5954  -8.5597  -8.4521  -8.3615
    -8.2974  -8.0998  -7.9998  -7.8759  -7.8531  -7.8471  -7.8460  -7.7842
    -7.6370  -7.5950  -7.5949  -7.4979  -7.4779  -7.2399  -7.1296  -7.1100
    -7.0406  -7.0198  -6.8740  -6.8608  -6.8483  -6.5726  -6.4480  -6.3915
    -6.3668  -6.2388  -6.1654  -6.0351  -5.9544  -5.9022  -5.7904  -5.7735
    -5.6004  -5.5534  -5.3993  -5.3911  -5.3719  -5.2953  -5.0974  -5.0282
    -4.9474  -4.9455  -4.8902  -4.8028  -4.6457  -4.6039  -4.5646  -4.4932
    -3.7494  -3.7021  -3.5250  -3.4695  -3.3657  -2.9890  -2.8936  -1.9908
    -0.5426   0.1653   0.4664   0.6169   1.6420   1.7717   2.0898   2.1255
     2.2114   2.2718   2.3064   2.3516   2.3787   2.4888   2.5359   2.5470
     2.6667   2.9126   3.0036   3.0252   3.1061   3.1175   3.2125   3.2784
     3.3592   3.5045

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000

     the Fermi energy is    -1.2577 ev

!    total energy              =    -790.65906184 Ry
     Harris-Foulkes estimate   =    -790.65906159 Ry
     estimated scf accuracy    <       0.00000044 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =  -13600.96873166 Ry
     hartree contribution      =    6855.55987808 Ry
     xc contribution           =    -252.80940613 Ry
     ewald contribution        =    6207.55922825 Ry
     smearing contrib. (-TS)   =      -0.00003038 Ry

     total magnetization       =     0.04 Bohr mag/cell
     absolute magnetization    =     0.05 Bohr mag/cell

     convergence has been achieved in  10 iterations

     Forces acting on atoms (Ry/au):


     negative rho (up, down):  9.152E-04 9.150E-04
     atom    1 type  1   force =     0.00004926   -0.00006807    0.00011996
     atom    2 type  1   force =    -0.00000972    0.00003815    0.00009139
     atom    3 type  1   force =    -0.00004091    0.00015073   -0.00013535
     atom    4 type  1   force =    -0.00013891   -0.00012995   -0.00066842
```

```
atom    5 type  1   force =    -0.00010694    0.00004835   -0.00014797
atom    6 type  1   force =     0.00022111   -0.00008636   -0.00067393
atom    7 type  1   force =    -0.00018724    0.00018688    0.00049370
atom    8 type  1   force =    -0.00005650   -0.00000386   -0.00064025
atom    9 type  1   force =     0.00019698   -0.00018603    0.00073217
atom   10 type  1   force =     0.00000815    0.00002509    0.00050735
atom   11 type  1   force =    -0.00000252    0.00018330   -0.00069236
atom   12 type  1   force =    -0.00012979   -0.00007835   -0.00014987
atom   13 type  1   force =    -0.00007566    0.00006602   -0.00015843
atom   14 type  1   force =     0.00016645   -0.00012612   -0.00068059
atom   15 type  1   force =    -0.00021520    0.00013651    0.00049653
atom   16 type  1   force =    -0.00002198   -0.00005189   -0.00063185
atom   17 type  1   force =     0.00002660    0.00003741   -0.00011423
atom   18 type  1   force =     0.00004135   -0.00006456    0.00008570
atom   19 type  1   force =    -0.00017178    0.00007359   -0.00016109
atom   20 type  1   force =     0.00006086    0.00000660    0.00011151
atom   21 type  1   force =     0.00015013    0.00008027   -0.00007772
atom   22 type  1   force =     0.00005002   -0.00007609    0.00028286
atom   23 type  1   force =    -0.00000111    0.00012207    0.00003767
atom   24 type  1   force =    -0.00001570   -0.00008184    0.00011024
atom   25 type  1   force =    -0.00019513    0.00011853    0.00007889
atom   26 type  1   force =     0.00002308   -0.00002927    0.00026946
atom   27 type  1   force =     0.00003066    0.00003343    0.00012329
atom   28 type  1   force =    -0.00005387   -0.00001893    0.00005078
atom   29 type  1   force =     0.00004589   -0.00003348    0.00028067
atom   30 type  1   force =     0.00004128   -0.00014202   -0.00006838
atom   31 type  1   force =     0.00003398   -0.00004367    0.00011745
atom   32 type  1   force =    -0.00017664    0.00009343   -0.00013820
atom   33 type  2   force =    -0.00002398    0.00003410    0.00005169
atom   34 type  3   force =    -0.00028357    0.00020565   -0.00000771
atom   35 type  2   force =     0.00057122    0.00006502    0.00006853
atom   36 type  3   force =     0.00045121   -0.00006637   -0.00002877
atom   37 type  2   force =     0.00014157    0.00038434    0.00007053
atom   38 type  3   force =    -0.00009365   -0.00008800    0.00000955
atom   39 type  2   force =    -0.00008875   -0.00018042    0.00005854
atom   40 type  3   force =     0.00069385   -0.00002266    0.00004117
atom   41 type  3   force =    -0.00030077    0.00012150   -0.00001135
atom   42 type  2   force =    -0.00043641    0.00045627    0.00010504
atom   43 type  3   force =     0.00028876   -0.00029388   -0.00003423
atom   44 type  2   force =     0.00041559   -0.00070251    0.00007551
atom   45 type  2   force =    -0.00050571   -0.00050402    0.00008384
atom   46 type  3   force =     0.00004260    0.00017475   -0.00000162
atom   47 type  2   force =     0.00003316    0.00020101    0.00006184
atom   48 type  3   force =     0.00041604   -0.00051469    0.00003945
atom   49 type  2   force =    -0.00001915   -0.00015447    0.00003552
atom   50 type  3   force =    -0.00026499    0.00025860    0.00004907
atom   51 type  2   force =     0.00017645    0.00003856    0.00005004
atom   52 type  3   force =    -0.00002359   -0.00063208    0.00002939
atom   53 type  2   force =    -0.00002633    0.00069682    0.00004681
atom   54 type  3   force =    -0.00050480   -0.00012948    0.00002187
atom   55 type  2   force =     0.00009023   -0.00031454    0.00004344
atom   56 type  3   force =    -0.00031746   -0.00016991    0.00001559
atom   57 type  2   force =     0.00039614   -0.00010360    0.00005217
atom   58 type  3   force =    -0.00042307    0.00023765    0.00002448
atom   59 type  3   force =     0.00012586    0.00022662    0.00000796
atom   60 type  2   force =     0.00022556    0.00019568    0.00004719
atom   61 type  3   force =    -0.00020983    0.00041286    0.00001802
atom   62 type  2   force =    -0.00062699   -0.00015081    0.00004709
atom   63 type  3   force =     0.00046957    0.00027852    0.00003248
atom   64 type  2   force =     0.00006505   -0.00014039    0.00004593
The non-local contrib.  to forces
atom    1 type  1   force =    -0.00080701    0.00039906   -0.00577275
```

```
atom    2 type  1   force =    -0.00049662    0.00018818    0.00284279
atom    3 type  1   force =     0.00020131    0.00066938    0.00712847
atom    4 type  1   force =    -0.00058885   -0.00075923    0.00303346
atom    5 type  1   force =    -0.00002417   -0.00081917    0.00280461
atom    6 type  1   force =    -0.00005643   -0.00008582    0.00434620
atom    7 type  1   force =    -0.00057252   -0.00062697    0.00064561
atom    8 type  1   force =     0.00030116   -0.00060833   -0.00735470
atom    9 type  1   force =     0.00077003   -0.00046233    0.00511414
atom   10 type  1   force =    -0.00015455    0.00005325    0.01216684
atom   11 type  1   force =     0.00027264    0.00063876    0.00461248
atom   12 type  1   force =    -0.00058703   -0.00032531    0.00700644
atom   13 type  1   force =     0.00062723    0.00036643    0.00467023
atom   14 type  1   force =     0.00024413    0.00008465    0.00503742
atom   15 type  1   force =    -0.00004867    0.00073819    0.00263875
atom   16 type  1   force =     0.00093221   -0.00012771   -0.00843609
atom   17 type  1   force =    -0.00037014    0.00012020   -0.00090203
atom   18 type  1   force =    -0.00008517    0.00020910   -0.01357749
atom   19 type  1   force =     0.00069108    0.00037710   -0.00943369
atom   20 type  1   force =    -0.00001040    0.00015574    0.00296269
atom   21 type  1   force =     0.00007188    0.00067787   -0.00273240
atom   22 type  1   force =    -0.00110792   -0.00043430   -0.00664970
atom   23 type  1   force =     0.00088124    0.00008438    0.00239488
atom   24 type  1   force =    -0.00009018   -0.00072265   -0.00160657
atom   25 type  1   force =     0.00016160    0.00011616   -0.00388086
atom   26 type  1   force =    -0.00047794    0.00013124    0.00806059
atom   27 type  1   force =     0.00061719    0.00065201    0.00019746
atom   28 type  1   force =     0.00022657   -0.00079100    0.00239100
atom   29 type  1   force =    -0.00016774    0.00106191   -0.00377905
atom   30 type  1   force =    -0.00052777   -0.00019042   -0.00479965
atom   31 type  1   force =    -0.00010613   -0.00012736    0.00398760
atom   32 type  1   force =     0.00001258   -0.00047404   -0.01157143
atom   33 type  2   force =    -0.00007290    0.00008578    0.00005035
atom   34 type  3   force =    -0.00072438    0.00049797   -0.00024095
atom   35 type  2   force =     0.00015286    0.00011905    0.00005660
atom   36 type  3   force =     0.00064517   -0.00026525   -0.00040109
atom   37 type  2   force =     0.00011868    0.00021128    0.00005556
atom   38 type  3   force =    -0.00021274   -0.00027331   -0.00014096
atom   39 type  2   force =    -0.00011731   -0.00021082    0.00005244
atom   40 type  3   force =     0.00123965   -0.00009476    0.00003903
atom   41 type  3   force =    -0.00038643    0.00007542   -0.00031644
atom   42 type  2   force =    -0.00035477    0.00030740    0.00006708
atom   43 type  3   force =     0.00049723   -0.00034026   -0.00045204
atom   44 type  2   force =     0.00007269   -0.00035409    0.00005812
atom   45 type  2   force =    -0.00033176   -0.00032657    0.00005849
atom   46 type  3   force =     0.00017810    0.00045025   -0.00020703
atom   47 type  2   force =     0.00008312    0.00018689    0.00005524
atom   48 type  3   force =     0.00084596   -0.00094988    0.00002163
atom   49 type  2   force =     0.00002849   -0.00016448    0.00004160
atom   50 type  3   force =    -0.00046551    0.00050541    0.00010254
atom   51 type  2   force =     0.00002079    0.00010971    0.00004758
atom   52 type  3   force =    -0.00003089   -0.00081080   -0.00001182
atom   53 type  2   force =    -0.00006017    0.00060847    0.00004327
atom   54 type  3   force =    -0.00093067   -0.00025170   -0.00005421
atom   55 type  2   force =    -0.00011714   -0.00025668    0.00004325
atom   56 type  3   force =    -0.00047009   -0.00028787   -0.00009071
atom   57 type  2   force =     0.00037393   -0.00012577    0.00004823
atom   58 type  3   force =    -0.00063332    0.00035710   -0.00005046
atom   59 type  3   force =     0.00027710    0.00036205   -0.00014346
atom   60 type  2   force =     0.00007309    0.00032885    0.00004533
atom   61 type  3   force =    -0.00042595    0.00073160   -0.00008518
atom   62 type  2   force =    -0.00059861   -0.00014495    0.00004313
atom   63 type  3   force =     0.00060443    0.00035705    0.00000486
```

```
atom   64 type  2   force =    -0.00005262   -0.00004837    0.00004651
The ionic contribution  to forces
atom    1 type  1   force =     0.02189222   -0.01202711   15.33036975
atom    2 type  1   force =    -0.00302845    0.00235347   14.30388877
atom    3 type  1   force =    -0.01862268   -0.01289340   14.14554304
atom    4 type  1   force =    -0.01792104   -0.00559952   13.52177230
atom    5 type  1   force =    -0.00384083    0.00187692   14.33272805
atom    6 type  1   force =     0.00155497    0.00856025   14.79054750
atom    7 type  1   force =     0.01515820    0.01319467   14.88456766
atom    8 type  1   force =    -0.03145960    0.01492335   16.07835200
atom    9 type  1   force =     0.01248033   -0.01208131   13.86765328
atom   10 type  1   force =     0.01820207   -0.01667703   12.94243175
atom   11 type  1   force =    -0.00876392    0.01910094   13.23201832
atom   12 type  1   force =    -0.00088795    0.02652608   13.94503274
atom   13 type  1   force =     0.00555228    0.01247764   13.90538507
atom   14 type  1   force =    -0.00294499   -0.00569758   14.42421435
atom   15 type  1   force =     0.00744284   -0.01722112   14.65701412
atom   16 type  1   force =    -0.03518748    0.01997629   16.01374980
atom   17 type  1   force =    -0.00297523    0.00650604   16.41635022
atom   18 type  1   force =     0.00905856   -0.01444982   16.47699454
atom   19 type  1   force =    -0.01475055   -0.01062101   15.34375553
atom   20 type  1   force =     0.00085349    0.00338210   15.51743065
atom   21 type  1   force =     0.00825545   -0.01202098   15.88145397
atom   22 type  1   force =     0.02826353    0.01359297   15.51198897
atom   23 type  1   force =     0.00689184    0.00532953   15.76988542
atom   24 type  1   force =     0.00480850    0.01491066   15.17420257
atom   25 type  1   force =    -0.01016179    0.00127046   15.21580347
atom   26 type  1   force =    -0.00040122   -0.00208486   15.20201663
atom   27 type  1   force =    -0.01525459   -0.01132522   14.87267673
atom   28 type  1   force =     0.00179196   -0.00769625   15.56077753
atom   29 type  1   force =     0.00231482   -0.02742698   15.27538696
atom   30 type  1   force =     0.02102384   -0.00529369   15.90349821
atom   31 type  1   force =    -0.00007692   -0.00514570   15.58576418
atom   32 type  1   force =     0.00073262    0.01428014   15.57712008
atom   33 type  2   force =    -0.01552198    0.00905442  -11.23249144
atom   34 type  3   force =    -0.04875172    0.02315325  -18.76762440
atom   35 type  2   force =    -0.03394108   -0.00532228  -11.26468288
atom   36 type  3   force =    -0.02879979   -0.02859533  -18.80829055
atom   37 type  2   force =    -0.01033597   -0.02400589  -11.26052224
atom   38 type  3   force =     0.01613513   -0.04253040  -18.74444262
atom   39 type  2   force =     0.02457410   -0.02624447  -11.24442910
atom   40 type  3   force =     0.03371401   -0.01317261  -18.68933323
atom   41 type  3   force =     0.04793842   -0.03632046  -18.78655918
atom   42 type  2   force =     0.00495368   -0.00841340  -11.29827313
atom   43 type  3   force =     0.00309188    0.02996438  -18.82227707
atom   44 type  2   force =    -0.01720019    0.02852050  -11.27076081
atom   45 type  2   force =     0.01495987    0.02048883  -11.27269523
atom   46 type  3   force =     0.04893225    0.00466413  -18.76206826
atom   47 type  2   force =     0.03479517   -0.01415463  -11.25046363
atom   48 type  3   force =     0.03274118   -0.02867019  -18.69303528
atom   49 type  2   force =     0.01207423   -0.00735376  -11.20249322
atom   50 type  3   force =    -0.01762589    0.01554511  -18.67225602
atom   51 type  2   force =     0.01713542    0.00104243  -11.23437497
atom   52 type  3   force =    -0.00251637   -0.00671919  -18.70834035
atom   53 type  2   force =    -0.00630435   -0.01028404  -11.21740157
atom   54 type  3   force =    -0.05174315   -0.01955291  -18.71475667
atom   55 type  2   force =    -0.02611494   -0.00649038  -11.21854097
atom   56 type  3   force =    -0.03256039   -0.01618917  -18.72729974
atom   57 type  2   force =    -0.00034580    0.00653512  -11.23541856
atom   58 type  3   force =     0.01453925    0.00049051  -18.72078956
atom   59 type  3   force =     0.00242434    0.04714588  -18.74109145
atom   60 type  2   force =    -0.00763227    0.03217845  -11.22450513
```

```
atom   61 type  3   force =    -0.01656853    0.05877454  -18.72478658
atom   62 type  2   force =     0.00033580    0.01395849  -11.21737627
atom   63 type  3   force =    -0.00015957    0.01174996  -18.70464876
atom   64 type  2   force =     0.00777702   -0.00924682  -11.22834528
The local contribution  to forces
atom    1 type  1   force =    -0.02108510    0.01168900  -15.32432728
atom    2 type  1   force =     0.00356854   -0.00238209  -14.30646540
atom    3 type  1   force =     0.01837547    0.01235822  -14.15262468
atom    4 type  1   force =     0.01848650    0.00620451  -13.52527672
atom    5 type  1   force =     0.00378804   -0.00117279  -14.33549668
atom    6 type  1   force =    -0.00124016   -0.00863638  -14.79539975
atom    7 type  1   force =    -0.01470596   -0.01242599  -14.88454381
atom    8 type  1   force =     0.03114443   -0.01434491  -16.07148882
atom    9 type  1   force =    -0.01300527    0.01238177  -13.87183833
atom   10 type  1   force =    -0.01789602    0.01671569  -12.95387971
atom   11 type  1   force =     0.00860966   -0.01947051  -13.23711131
atom   12 type  1   force =     0.00148484   -0.02611924  -13.95199927
atom   13 type  1   force =    -0.00620150   -0.01268029  -13.91001413
atom   14 type  1   force =     0.00283143    0.00557385  -14.42975360
atom   15 type  1   force =    -0.00762071    0.01665964  -14.65897455
atom   16 type  1   force =     0.03414017   -0.01995531  -16.00579138
atom   17 type  1   force =     0.00335490   -0.00667301  -16.41542115
atom   18 type  1   force =    -0.00898465    0.01404907  -16.46318857
atom   19 type  1   force =     0.01375785    0.01036727  -15.33433850
atom   20 type  1   force =    -0.00088976   -0.00342927  -15.52014157
atom   21 type  1   force =    -0.00829173    0.01139632  -15.87865209
atom   22 type  1   force =    -0.02714331   -0.01330394  -15.50489614
atom   23 type  1   force =    -0.00783732   -0.00546233  -15.77209035
atom   24 type  1   force =    -0.00473040   -0.01445060  -15.17232732
atom   25 type  1   force =     0.00973180   -0.00135215  -15.21169435
atom   26 type  1   force =     0.00081537    0.00192373  -15.20966793
atom   27 type  1   force =     0.01469093    0.01069027  -14.87258385
atom   28 type  1   force =    -0.00203408    0.00844087  -15.56296403
atom   29 type  1   force =    -0.00201789    0.02639553  -15.27116606
atom   30 type  1   force =    -0.02038231    0.00539648  -15.89862586
atom   31 type  1   force =     0.00022386    0.00531068  -15.58949688
atom   32 type  1   force =    -0.00093962   -0.01369553  -15.56554624
atom   33 type  2   force =     0.01541128   -0.00899663   11.23243853
atom   34 type  3   force =     0.04893540   -0.02327887   18.76770708
atom   35 type  2   force =     0.03420616    0.00533018   11.26463885
atom   36 type  3   force =     0.02850076    0.02868017   18.80850534
atom   37 type  2   force =     0.01028358    0.02405555   11.26048450
atom   38 type  3   force =    -0.01607938    0.04236074   18.74446471
atom   39 type  2   force =    -0.02463584    0.02613327   11.24439256
atom   40 type  3   force =    -0.03428116    0.01302629   18.68922231
atom   41 type  3   force =    -0.04782519    0.03627490   18.78672978
atom   42 type  2   force =    -0.00513600    0.00857994   11.29825507
atom   43 type  3   force =    -0.00331944   -0.02978812   18.82255502
atom   44 type  2   force =     0.01737979   -0.02877874   11.27073222
atom   45 type  2   force =    -0.01509872   -0.02054307   11.27267578
atom   46 type  3   force =    -0.04879188   -0.00469167   18.76215134
atom   47 type  2   force =    -0.03479234    0.01425750   11.25042835
atom   48 type  3   force =    -0.03297965    0.02916384   18.69292908
atom   49 type  2   force =    -0.01213430    0.00733873   11.20243941
atom   50 type  3   force =     0.01789104   -0.01581726   18.67208629
atom   51 type  2   force =    -0.01692957   -0.00096997   11.23433437
atom   52 type  3   force =     0.00254760    0.00710576   18.70825105
atom   53 type  2   force =     0.00631209    0.01052041   11.21734562
atom   54 type  3   force =     0.05207772    0.01972056   18.71468467
atom   55 type  2   force =     0.02628009    0.00640891   11.21848746
atom   56 type  3   force =     0.03275445    0.01610405   18.72727617
atom   57 type  2   force =     0.00043288   -0.00652489   11.23538059
```

```
atom   58 type  3   force =    -0.01419798   -0.00061148   18.72074938
atom   59 type  3   force =    -0.00237323   -0.04715181   18.74112859
atom   60 type  2   force =     0.00775460   -0.03225429   11.22446415
atom   61 type  3   force =     0.01663783   -0.05901950   18.72476854
atom   62 type  2   force =    -0.00054569   -0.01401620   11.21733069
atom   63 type  3   force =    -0.00014111   -0.01188036   18.70455616
atom   64 type  2   force =    -0.00774531    0.00906932   11.22830015
The core correction contribution to forces
atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
atom    3 type  1   force =     0.00000000    0.00000000    0.00000000
atom    4 type  1   force =     0.00000000    0.00000000    0.00000000
atom    5 type  1   force =     0.00000000    0.00000000    0.00000000
atom    6 type  1   force =     0.00000000    0.00000000    0.00000000
atom    7 type  1   force =     0.00000000    0.00000000    0.00000000
atom    8 type  1   force =     0.00000000    0.00000000    0.00000000
atom    9 type  1   force =     0.00000000    0.00000000    0.00000000
atom   10 type  1   force =     0.00000000    0.00000000    0.00000000
atom   11 type  1   force =     0.00000000    0.00000000    0.00000000
atom   12 type  1   force =     0.00000000    0.00000000    0.00000000
atom   13 type  1   force =     0.00000000    0.00000000    0.00000000
atom   14 type  1   force =     0.00000000    0.00000000    0.00000000
atom   15 type  1   force =     0.00000000    0.00000000    0.00000000
atom   16 type  1   force =     0.00000000    0.00000000    0.00000000
atom   17 type  1   force =     0.00000000    0.00000000    0.00000000
atom   18 type  1   force =     0.00000000    0.00000000    0.00000000
atom   19 type  1   force =     0.00000000    0.00000000    0.00000000
atom   20 type  1   force =     0.00000000    0.00000000    0.00000000
atom   21 type  1   force =     0.00000000    0.00000000    0.00000000
atom   22 type  1   force =     0.00000000    0.00000000    0.00000000
atom   23 type  1   force =     0.00000000    0.00000000    0.00000000
atom   24 type  1   force =     0.00000000    0.00000000    0.00000000
atom   25 type  1   force =     0.00000000    0.00000000    0.00000000
atom   26 type  1   force =     0.00000000    0.00000000    0.00000000
atom   27 type  1   force =     0.00000000    0.00000000    0.00000000
atom   28 type  1   force =     0.00000000    0.00000000    0.00000000
atom   29 type  1   force =     0.00000000    0.00000000    0.00000000
atom   30 type  1   force =     0.00000000    0.00000000    0.00000000
atom   31 type  1   force =     0.00000000    0.00000000    0.00000000
atom   32 type  1   force =     0.00000000    0.00000000    0.00000000
atom   33 type  2   force =     0.00006274   -0.00002663   -0.00001845
atom   34 type  3   force =     0.00000582   -0.00000417   -0.00000039
atom   35 type  2   force =     0.00005412   -0.00003185   -0.00002727
atom   36 type  3   force =    -0.00000804    0.00000139    0.00000045
atom   37 type  2   force =     0.00005224   -0.00003245   -0.00002206
atom   38 type  3   force =     0.00000215    0.00000221   -0.00000065
atom   39 type  2   force =     0.00006539   -0.00001275   -0.00002405
atom   40 type  3   force =    -0.00001279    0.00000029   -0.00000132
atom   41 type  3   force =     0.00000558   -0.00000224   -0.00000018
atom   42 type  2   force =     0.00007570   -0.00003585   -0.00002067
atom   43 type  3   force =    -0.00000537    0.00000504    0.00000047
atom   44 type  2   force =     0.00005994   -0.00000609   -0.00002680
atom   45 type  2   force =     0.00007361   -0.00000661   -0.00001966
atom   46 type  3   force =    -0.00000101   -0.00000392   -0.00000035
atom   47 type  2   force =     0.00005610   -0.00003102   -0.00002486
atom   48 type  3   force =    -0.00000774    0.00000946   -0.00000136
atom   49 type  2   force =     0.00005837   -0.00001451   -0.00001485
atom   50 type  3   force =     0.00000538   -0.00000524   -0.00000177
atom   51 type  2   force =     0.00006426   -0.00002701   -0.00002147
atom   52 type  3   force =     0.00000084    0.00001077   -0.00000114
atom   53 type  2   force =     0.00006451   -0.00004983   -0.00001336
atom   54 type  3   force =     0.00000988    0.00000224   -0.00000133
```

```
     atom   55 type  2   force =     0.00006722   -0.00001319   -0.00001677
     atom   56 type  3   force =     0.00000662    0.00000283   -0.00000115
     atom   57 type  2   force =     0.00004296   -0.00001616   -0.00002032
     atom   58 type  3   force =     0.00000801   -0.00000460   -0.00000076
     atom   59 type  3   force =    -0.00000187   -0.00000480   -0.00000097
     atom   60 type  2   force =     0.00005983   -0.00003783   -0.00001767
     atom   61 type  3   force =     0.00000432   -0.00000820   -0.00000121
     atom   62 type  2   force =     0.00008821   -0.00001709   -0.00001309
     atom   63 type  3   force =    -0.00000774   -0.00000528   -0.00000109
     atom   64 type  2   force =     0.00006472   -0.00002559   -0.00002026
     The Hubbard contrib.    to forces
     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    3 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    4 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    5 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    6 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    7 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    8 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    9 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   10 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   11 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   12 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   13 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   14 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   15 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   16 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   17 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   18 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   19 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   20 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   21 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   22 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   23 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   24 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   25 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   26 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   27 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   28 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   29 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   30 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   31 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   32 type  1   force =     0.00000000    0.00000000    0.00000000
     atom   33 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   34 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   35 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   36 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   37 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   38 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   39 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   40 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   41 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   42 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   43 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   44 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   45 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   46 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   47 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   48 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   49 type  2   force =     0.00000000    0.00000000    0.00000000
     atom   50 type  3   force =     0.00000000    0.00000000    0.00000000
     atom   51 type  2   force =     0.00000000    0.00000000    0.00000000
```

```
atom   52 type  3   force =     0.00000000    0.00000000    0.00000000
atom   53 type  2   force =     0.00000000    0.00000000    0.00000000
atom   54 type  3   force =     0.00000000    0.00000000    0.00000000
atom   55 type  2   force =     0.00000000    0.00000000    0.00000000
atom   56 type  3   force =     0.00000000    0.00000000    0.00000000
atom   57 type  2   force =     0.00000000    0.00000000    0.00000000
atom   58 type  3   force =     0.00000000    0.00000000    0.00000000
atom   59 type  3   force =     0.00000000    0.00000000    0.00000000
atom   60 type  2   force =     0.00000000    0.00000000    0.00000000
atom   61 type  3   force =     0.00000000    0.00000000    0.00000000
atom   62 type  2   force =     0.00000000    0.00000000    0.00000000
atom   63 type  3   force =     0.00000000    0.00000000    0.00000000
atom   64 type  2   force =     0.00000000    0.00000000    0.00000000
The SCF correction term to forces
atom    1 type  1   force =     0.00005492   -0.00012945   -0.00015952
atom    2 type  1   force =    -0.00004742   -0.00012186   -0.00018454
atom    3 type  1   force =     0.00001076    0.00001610   -0.00019195
atom    4 type  1   force =    -0.00010974    0.00002385   -0.00020723
atom    5 type  1   force =    -0.00002421    0.00016296   -0.00019371
atom    6 type  1   force =    -0.00003149    0.00007516   -0.00017763
atom    7 type  1   force =    -0.00006118    0.00004473   -0.00018553
atom    8 type  1   force =    -0.00003671    0.00002558   -0.00015848
atom    9 type  1   force =    -0.00004233   -0.00002459   -0.00020668
atom   10 type  1   force =    -0.00013758   -0.00006726   -0.00022129
atom   11 type  1   force =    -0.00011513   -0.00008632   -0.00022160
atom   12 type  1   force =    -0.00013388   -0.00016031   -0.00019953
atom   13 type  1   force =    -0.00004789   -0.00009820   -0.00020936
atom   14 type  1   force =     0.00004164   -0.00008749   -0.00018853
atom   15 type  1   force =     0.00001713   -0.00004064   -0.00019156
atom   16 type  1   force =     0.00009890    0.00005440   -0.00016395
atom   17 type  1   force =     0.00002285    0.00008374   -0.00015104
atom   18 type  1   force =     0.00005839    0.00012665   -0.00015254
atom   19 type  1   force =     0.00013561   -0.00005020   -0.00015420
atom   20 type  1   force =     0.00011331   -0.00010241   -0.00015003
atom   21 type  1   force =     0.00012030    0.00002663   -0.00015695
atom   22 type  1   force =     0.00004350    0.00006874   -0.00017004
atom   23 type  1   force =     0.00006891    0.00017006   -0.00016204
atom   24 type  1   force =     0.00000215    0.00018031   -0.00016821
atom   25 type  1   force =     0.00007904    0.00008362   -0.00015913
atom   26 type  1   force =     0.00009264    0.00000019   -0.00014959
atom   27 type  1   force =    -0.00001710    0.00001594   -0.00017681
atom   28 type  1   force =    -0.00003255    0.00002700   -0.00016349
atom   29 type  1   force =    -0.00007753   -0.00006438   -0.00017095
atom   30 type  1   force =    -0.00006670   -0.00005483   -0.00015083
atom   31 type  1   force =    -0.00000105   -0.00008172   -0.00014721
atom   32 type  1   force =     0.00002355   -0.00001759   -0.00015037
atom   33 type  2   force =     0.00010266   -0.00008327    0.00006294
atom   34 type  3   force =     0.00025708   -0.00016297    0.00014119
atom   35 type  2   force =     0.00010493   -0.00003052    0.00007347
atom   36 type  3   force =     0.00011888    0.00011221    0.00014732
atom   37 type  2   force =     0.00002881    0.00015541    0.00006501
atom   38 type  3   force =     0.00006696    0.00035232    0.00011931
atom   39 type  2   force =     0.00003069    0.00015391    0.00005693
atom   40 type  3   force =     0.00003990    0.00021769    0.00010462
atom   41 type  3   force =    -0.00002737    0.00009345    0.00012489
atom   42 type  2   force =     0.00003076    0.00001774    0.00006692
atom   43 type  3   force =     0.00003023   -0.00013535    0.00012962
atom   44 type  2   force =     0.00010912   -0.00008454    0.00006301
atom   45 type  2   force =    -0.00010294   -0.00011704    0.00005469
atom   46 type  3   force =    -0.00026908   -0.00024448    0.00011292
atom   47 type  2   force =    -0.00010311   -0.00005816    0.00005698
atom   48 type  3   force =    -0.00017795   -0.00006835    0.00011561
```

```
     atom   49 type  2   force =    -0.00004016    0.00003911    0.00005281
     atom   50 type  3   force =    -0.00006424    0.00003014    0.00010827
     atom   51 type  2   force =    -0.00010868   -0.00011703    0.00005477
     atom   52 type  3   force =    -0.00001900   -0.00021906    0.00012188
     atom   53 type  2   force =    -0.00003263   -0.00009863    0.00006308
     atom   54 type  3   force =     0.00008719   -0.00004811    0.00013965
     atom   55 type  2   force =    -0.00001923    0.00003636    0.00006071
     atom   56 type  3   force =    -0.00004228    0.00019981    0.00012125
     atom   57 type  2   force =    -0.00010206    0.00002767    0.00005246
     atom   58 type  3   force =    -0.00013326    0.00000569    0.00010611
     atom   59 type  3   force =    -0.00019471   -0.00012514    0.00010548
     atom   60 type  2   force =    -0.00002391   -0.00001993    0.00005074
     atom   61 type  3   force =     0.00014827   -0.00006602    0.00011268
     atom   62 type  2   force =     0.00009906    0.00006850    0.00005286
     atom   63 type  3   force =     0.00017933    0.00005671    0.00011154
     atom   64 type  2   force =     0.00002701    0.00011063    0.00005504

     Total force =     0.003467     Total SCF correction =     0.001631
     SCF correction compared to forces is large: reduce conv_thr to get better values


     entering subroutine stress ...


     negative rho (up, down):  9.152E-04 9.150E-04
          total   stress  (Ry/bohr**3)                   (kbar)     P=   89.44
  0.00091485   0.00000112  -0.00000000        134.58      0.17     -0.00
  0.00000112   0.00091550  -0.00000000          0.17    134.67     -0.00
 -0.00000000  -0.00000000  -0.00000644         -0.00     -0.00     -0.95

     kinetic stress (kbar)   2986.23      0.08      0.00
                               0.08   2986.31     -0.00
                               0.00     -0.00   3317.50

     local   stress (kbar)-135334.57     -4.49      0.00
                              -4.49-135336.92     -0.01
                               0.00     -0.01 135670.99

     nonloc. stress (kbar)    516.54     -0.04     -0.00
                              -0.04    516.52      0.00
                              -0.00      0.00    469.95

     hartree stress (kbar)  66066.32      1.68      0.00
                               1.68  66067.22      0.00
                               0.00      0.00 -65641.93

     exc-cor stress (kbar)   -566.08      0.00     -0.00
                               0.00   -566.08      0.00
                              -0.00      0.00   -595.13

     corecor stress (kbar)   -167.56     -0.00     -0.00
                              -0.00   -167.56      0.00
                              -0.00      0.00   -160.16

     ewald   stress (kbar)  66633.69      2.94     -0.01
                               2.94  66635.18      0.01
                              -0.01      0.01 -73062.17

     hubbard stress (kbar)      0.00      0.00      0.00
                               0.00      0.00      0.00
                               0.00      0.00      0.00
```

```
london  stress (kbar)      0.00      0.00      0.00
                           0.00      0.00      0.00
                           0.00      0.00      0.00

XDM     stress (kbar)      0.00      0.00      0.00
                           0.00      0.00      0.00
                           0.00      0.00      0.00

dft-nl  stress (kbar)      0.00      0.00      0.00
                           0.00      0.00      0.00
                           0.00      0.00      0.00


Writing output data file A.save

init_run     :    927.03s CPU    933.78s WALL (       1 calls)
electrons    :  26918.73s CPU  27137.78s WALL (       1 calls)
forces       :    620.52s CPU    623.84s WALL (       1 calls)
stress       :    941.34s CPU    945.08s WALL (       1 calls)

Called by init_run:
wfcinit      :    896.50s CPU    902.69s WALL (       1 calls)
potinit      :      3.66s CPU      3.81s WALL (       1 calls)

Called by electrons:
c_bands      :  24348.29s CPU  24548.91s WALL (      10 calls)
sum_band     :   2354.28s CPU   2370.72s WALL (      10 calls)
v_of_rho     :     35.20s CPU     36.12s WALL (      11 calls)
v_h          :      0.94s CPU      0.96s WALL (      11 calls)
v_xc         :     40.36s CPU     41.39s WALL (      13 calls)
newd         :    189.14s CPU    190.08s WALL (      11 calls)
mix_rho      :      4.00s CPU      4.07s WALL (      10 calls)

Called by c_bands:
init_us_2    :     39.21s CPU     40.77s WALL (     920 calls)
cegterg      :  24238.11s CPU  24433.89s WALL (     400 calls)

Called by sum_band:
sum_band:bec :      1.54s CPU      1.49s WALL (     400 calls)
addusdens    :    202.62s CPU    204.00s WALL (      10 calls)

Called by *egterg:
h_psi        :  11600.00s CPU  11666.86s WALL (    2681 calls)
s_psi        :   3895.92s CPU   3912.68s WALL (    2681 calls)
g_psi        :     10.92s CPU     11.13s WALL (    2241 calls)
cdiaghg      :   1809.91s CPU   1818.10s WALL (    2641 calls)
cegterg:over :   3279.87s CPU   3295.18s WALL (    2241 calls)
cegterg:upda :   2347.42s CPU   2366.31s WALL (    2241 calls)
cegterg:last :   1149.84s CPU   1156.59s WALL (     400 calls)
cdiaghg:chol :    125.58s CPU    126.16s WALL (    2641 calls)
cdiaghg:inve :     14.58s CPU     14.67s WALL (    2641 calls)
cdiaghg:para :    592.88s CPU    595.16s WALL (    5282 calls)

Called by h_psi:
h_psi:vloc   :   3907.48s CPU   3937.64s WALL (    2681 calls)
h_psi:vnl    :   7678.89s CPU   7714.33s WALL (    2681 calls)
add_vuspsi   :   3912.23s CPU   3928.63s WALL (    2681 calls)

General routines
calbec       :   5334.80s CPU   5361.11s WALL (    3161 calls)
fft          :     33.71s CPU     34.12s WALL (     375 calls)
```

```
     ffts          :      0.66s CPU      0.68s WALL (      42 calls)
     fftw          :   3539.59s CPU   3562.95s WALL (  429932 calls)
     interpolate   :      3.67s CPU      3.75s WALL (      42 calls)
     davcio        :      0.02s CPU      1.57s WALL (      40 calls)

     Parallel routines
     fft_scatter   :   1392.88s CPU   1404.67s WALL (  430349 calls)

     PWSCF         :     8h10m CPU        8h14m WALL


   This run was terminated on:  20: 2: 1   4Apr2021

=------------------------------------------------------------------------------=
   JOB DONE.
=------------------------------------------------------------------------------=
```