```
     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)  1.0713 (a.u.) for type    2
     new r_m :   0.0595 (alat units)  1.0713 (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      =           63
     number of atomic types    =            3
     number of electrons       =       251.00
     number of Kohn-Sham states=          151
     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            1.000
   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) = (  -0.3722366   0.7921448   1.5717944  )
         2           C   tau(   2) = (  -0.2473910   0.7200609   1.5623360  )
         3           C   tau(   3) = (  -0.2474691   0.5756022   1.5610312  )
         4           C   tau(   4) = (  -0.1224131   0.5034014   1.5544232  )
         5           C   tau(   5) = (  -0.1223507   0.3591490   1.5624812  )
         6           C   tau(   6) = (   0.0027140   0.2869869   1.5670464  )
         7           C   tau(   7) = (   0.1277598   0.3591986   1.5678954  )
         8           C   tau(   8) = (   0.2525712   0.2870861   1.5787682  )
         9           C   tau(   9) = (   0.1278261   0.5033923   1.5585775  )
        10           C   tau(  10) = (   0.0027784   0.5755650   1.5496533  )
        11           C   tau(  11) = (   0.0026970   0.7201590   1.5516657  )
        12           C   tau(  12) = (  -0.1223559   0.7923673   1.5590329  )
        13           C   tau(  13) = (   0.1277243   0.7922839   1.5584105  )
        14           C   tau(  14) = (   0.2527637   0.7200073   1.5635029  )
        15           C   tau(  15) = (   0.2527600   0.5755851   1.5658214  )
        16           C   tau(  16) = (   0.3775331   0.5035898   1.5780416  )
        17           C   tau(  17) = (   0.3776073   0.3592204   1.5826716  )
        18           C   tau(  18) = (   0.5027720   0.2869211   1.5823397  )
        19           C   tau(  19) = (   0.3776161   0.7921545   1.5714407  )
        20           C   tau(  20) = (   0.5026977   0.7200094   1.5742757  )
        21           C   tau(  21) = (   0.5027163   0.5757032   1.5773054  )
        22           C   tau(  22) = (   0.6278477   0.5035633   1.5734387  )
        23           C   tau(  23) = (   0.6277604   0.3591888   1.5767155  )
        24           C   tau(  24) = (   0.7527168   0.2870625   1.5705363  )
        25           C   tau(  25) = (   0.7526731   0.1426533   1.5707759  )
        26           C   tau(  26) = (   0.8776915   0.0704882   1.5715804  )
        27           C   tau(  27) = (   0.6276478   0.0704597   1.5677269  )
        28           C   tau(  28) = (   0.5027069   0.1426034   1.5746730  )
        29           C   tau(  29) = (   0.3777180   0.0703653   1.5713549  )
        30           C   tau(  30) = (   0.2527097   0.1426003   1.5773581  )
        31           C   tau(  31) = (   0.1277070   0.0704739   1.5750269  )
        32           C   tau(  32) = (   0.0026672   0.1427206   1.5735489  )
        33           B   tau(  33) = (  -0.3723011   0.7921796   0.7500309  )
        34           N   tau(  34) = (  -0.2461847   0.7193662   0.7499639  )
        35           B   tau(  35) = (  -0.2428711   0.5746819   0.7500392  )
        36           N   tau(  36) = (  -0.1133046   0.5034055   0.7499748  )
        37           B   tau(  37) = (  -0.1218726   0.3594202   0.7500545  )
        38           N   tau(  38) = (   0.0071152   0.2948555   0.7499757  )
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      39           B   tau(  39) = (   0.1276926   0.3823671   0.7499907  )
      40           N   tau(  40) = (   0.2482812   0.2948563   0.7499761  )
      41           B   tau(  41) = (   0.0227395   0.5641029   0.7499910  )
      42           N   tau(  42) = (   0.0072803   0.7122660   0.7499745  )
      43           B   tau(  43) = (  -0.1192267   0.7888341   0.7500393  )
      44           B   tau(  44) = (   0.1276920   0.7916782   0.7500547  )
      45           N   tau(  45) = (   0.2481032   0.7122564   0.7499754  )
      46           B   tau(  46) = (   0.2326013   0.5640775   0.7499908  )
      47           N   tau(  47) = (   0.3686860   0.5033988   0.7499761  )
      48           B   tau(  48) = (   0.3772666   0.3594145   0.7500536  )
      49           N   tau(  49) = (   0.5022326   0.2872664   0.7499647  )
      50           B   tau(  50) = (   0.3746145   0.7888222   0.7500385  )
      51           N   tau(  51) = (   0.5015730   0.7193626   0.7499646  )
      52           B   tau(  52) = (   0.4982326   0.5746846   0.7500385  )
      53           N   tau(  53) = (   0.6276871   0.5042160   0.7499734  )
      54           B   tau(  54) = (   0.6276989   0.3595746   0.7500331  )
      55           N   tau(  55) = (   0.7531637   0.2872632   0.7499646  )
      56           B   tau(  56) = (   0.7530631   0.1424499   0.7500344  )
      57           N   tau(  57) = (   0.8783197   0.0701337   0.7499731  )
      58           N   tau(  58) = (   0.6277023   0.0699528   0.7499645  )
      59           B   tau(  59) = (   0.5023447   0.1424555   0.7500334  )
      60           N   tau(  60) = (   0.3770736   0.0701437   0.7499734  )
      61           B   tau(  61) = (   0.2513216   0.1470238   0.7500386  )
      62           N   tau(  62) = (   0.1276966   0.0717912   0.7499647  )
      63           B   tau(  63) = (   0.0040635   0.1470100   0.7500383  )

   Crystallographic axes

     site n.     atom                  positions (cryst. coord.)
         1           C   tau(   1) = (  0.0851085  0.9146901  0.5239315  )
         2           C   tau(   2) = (  0.1683364  0.8314548  0.5207787  )
         3           C   tau(   3) = (  0.0848550  0.6646481  0.5203437  )
         4           C   tau(   4) = (  0.1682258  0.5812779  0.5181411  )
         5           C   tau(   5) = (  0.0850041  0.4147095  0.5208271  )
         6           C   tau(   6) = (  0.1684059  0.3313840  0.5223488  )
         7           C   tau(   7) = (  0.3351432  0.4147669  0.5226318  )
         8           C   tau(   8) = (  0.4183205  0.3314984  0.5262561  )
         9           C   tau(   9) = (  0.4184598  0.5812674  0.5195258  )
        10           C   tau(  10) = (  0.3350811  0.6646053  0.5165511  )
        11           C   tau(  11) = (  0.4184810  0.8315680  0.5172219  )
        12           C   tau(  12) = (  0.3351176  0.9149469  0.5196776  )
        13           C   tau(  13) = (  0.5851496  0.9148507  0.5194702  )
        14           C   tau(  14) = (  0.6684601  0.8313928  0.5211676  )
        15           C   tau(  15) = (  0.5850742  0.6646284  0.5219405  )
        16           C   tau(  16) = (  0.6682808  0.5814954  0.5260139  )
        17           C   tau(  17) = (  0.5850033  0.4147920  0.5275572  )
        18           C   tau(  18) = (  0.6684259  0.3313080  0.5274466  )
        19           C   tau(  19) = (  0.8349667  0.9147012  0.5238136  )
        20           C   tau(  20) = (  0.9183954  0.8313952  0.5247586  )
        21           C   tau(  21) = (  0.8350987  0.6647648  0.5257685  )
        22           C   tau(  22) = (  0.9185801  0.5814648  0.5244796  )
        23           C   tau(  23) = (  0.8351382  0.4147555  0.5255719  )
        24           C   tau(  24) = (  0.9184524  0.3314712  0.5235121  )
        25           C   tau(  25) = (  0.8350340  0.1647218  0.5235920  )
        26           C   tau(  26) = (  0.9183879  0.0813927  0.5238601  )
        27           C   tau(  27) = (  0.6683277  0.0813598  0.5225756  )
        28           C   tau(  28) = (  0.5850391  0.1646643  0.5248910  )
        29           C   tau(  29) = (  0.4183435  0.0812509  0.5237850  )
        30           C   tau(  30) = (  0.3350401  0.1646607  0.5257860  )
        31           C   tau(  31) = (  0.1683951  0.0813763  0.5250090  )
        32           C   tau(  32) = (  0.0850669  0.1647995  0.5245163  )
        33           B   tau(  33) = (  0.0850640  0.9147302  0.2500103  )
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     34           N   tau(  34) = (  0.1691416  0.8306526  0.2499880  )
     35           B   tau(  35) = (  0.0889216  0.6635855  0.2500131  )
     36           N   tau(  36) = (  0.1773367  0.5812827  0.2499916  )
     37           B   tau(  37) = (  0.0856388  0.4150228  0.2500182  )
     38           N   tau(  38) = (  0.1773501  0.3404698  0.2499919  )
     39           B   tau(  39) = (  0.3484523  0.4415195  0.2499969  )
     40           N   tau(  40) = (  0.4185166  0.3404708  0.2499920  )
     41           B   tau(  41) = (  0.3484244  0.6513699  0.2499970  )
     42           N   tau(  42) = (  0.4185072  0.8224539  0.2499915  )
     43           B   tau(  43) = (  0.3362069  0.9108671  0.2500131  )
     44           B   tau(  44) = (  0.5847677  0.9141513  0.2500182  )
     45           N   tau(  45) = (  0.6593247  0.8224429  0.2499918  )
     46           B   tau(  46) = (  0.5582716  0.6513406  0.2499969  )
     47           N   tau(  47) = (  0.6593235  0.5812749  0.2499920  )
     48           B   tau(  48) = (  0.5847747  0.4150161  0.2500179  )
     49           N   tau(  49) = (  0.6680860  0.3317067  0.2499882  )
     50           B   tau(  50) = (  0.8300412  0.9108534  0.2500128  )
     51           N   tau(  51) = (  0.9168972  0.8306483  0.2499882  )
     52           B   tau(  52) = (  0.8300269  0.6635886  0.2500128  )
     53           N   tau(  53) = (  0.9187963  0.5822185  0.2499911  )
     54           B   tau(  54) = (  0.8352994  0.4152010  0.2500110  )
     55           N   tau(  55) = (  0.9190152  0.3317030  0.2499882  )
     56           B   tau(  56) = (  0.8353066  0.1644870  0.2500115  )
     57           N   tau(  57) = (  0.9188114  0.0809834  0.2499910  )
     58           N   tau(  58) = (  0.6680895  0.0807745  0.2499882  )
     59           B   tau(  59) = (  0.5845914  0.1644935  0.2500111  )
     60           N   tau(  60) = (  0.4175711  0.0809950  0.2499911  )
     61           B   tau(  61) = (  0.3362059  0.1697685  0.2500129  )
     62           N   tau(  62) = (  0.1691453  0.0828974  0.2499882  )
     63           B   tau(  63) = (  0.0889398  0.1697525  0.2500128  )

  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
     k(   28) = (  -0.1666667   0.0962250   0.0000000), wk =   0.0555556
     k(   29) = (   0.1666667   0.0962250   0.0000000), wk =   0.0555556
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     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         18.76 Mb     (    8143,  151)
      NL pseudopotentials             62.62 Mb     (    8143,  504)
      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        75.05 Mb     (    8143,  604)
   Each subspace H/S matrix        1.39 Mb     (     302,  302)
   Each <psi_i|beta_j> matrix      1.16 Mb     (     504,  151)
   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):   -0.000334
Check: negative starting charge=(component2):   -0.000288

starting charge  250.99369, renormalised to  251.00000

negative rho (up, down):  3.340E-04 2.881E-04
Starting wfc are  252 randomized atomic wfcs

total cpu time spent up to now is     1120.1 secs

per-process dynamical memory:  1007.1 Mb

Self-consistent Calculation

iteration #  1     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  2.2

negative rho (up, down):  4.844E-04 7.045E-04

Magnetic moment per site:
atom:    1    charge:    1.6730    magn:    0.2632    constr:    0.0000
atom:    2    charge:    1.6715    magn:    0.2628    constr:    0.0000
atom:    3    charge:    1.6712    magn:    0.2630    constr:    0.0000
atom:    4    charge:    1.6700    magn:    0.2627    constr:    0.0000
atom:    5    charge:    1.6719    magn:    0.2630    constr:    0.0000
atom:    6    charge:    1.6732    magn:    0.2631    constr:    0.0000
atom:    7    charge:    1.6721    magn:    0.2630    constr:    0.0000
atom:    8    charge:    1.6712    magn:    0.2631    constr:    0.0000
atom:    9    charge:    1.6707    magn:    0.2629    constr:    0.0000
atom:   10    charge:    1.6694    magn:    0.2632    constr:    0.0000
atom:   11    charge:    1.6699    magn:    0.2629    constr:    0.0000
atom:   12    charge:    1.6711    magn:    0.2631    constr:    0.0000
atom:   13    charge:    1.6719    magn:    0.2632    constr:    0.0000
atom:   14    charge:    1.6718    magn:    0.2629    constr:    0.0000
atom:   15    charge:    1.6720    magn:    0.2630    constr:    0.0000
atom:   16    charge:    1.6712    magn:    0.2631    constr:    0.0000
atom:   17    charge:    1.6728    magn:    0.2629    constr:    0.0000
atom:   18    charge:    1.6709    magn:    0.2634    constr:    0.0000
atom:   19    charge:    1.6733    magn:    0.2632    constr:    0.0000
atom:   20    charge:    1.6740    magn:    0.2632    constr:    0.0000
atom:   21    charge:    1.6730    magn:    0.2630    constr:    0.0000
atom:   22    charge:    1.6717    magn:    0.2631    constr:    0.0000
atom:   23    charge:    1.6730    magn:    0.2629    constr:    0.0000
atom:   24    charge:    1.6723    magn:    0.2631    constr:    0.0000
atom:   25    charge:    1.6736    magn:    0.2631    constr:    0.0000
atom:   26    charge:    1.6738    magn:    0.2630    constr:    0.0000
atom:   27    charge:    1.6726    magn:    0.2631    constr:    0.0000
atom:   28    charge:    1.6730    magn:    0.2629    constr:    0.0000
atom:   29    charge:    1.6710    magn:    0.2629    constr:    0.0000
atom:   30    charge:    1.6727    magn:    0.2631    constr:    0.0000
```

```
atom:   31    charge:    1.6741    magn:    0.2631    constr:    0.0000
atom:   32    charge:    1.6738    magn:    0.2633    constr:    0.0000
atom:   33    charge:    0.7444    magn:    0.2119    constr:    0.0000
atom:   34    charge:    2.9346    magn:   -0.0403    constr:    0.0000
atom:   35    charge:    0.7318    magn:    0.2122    constr:    0.0000
atom:   36    charge:    2.9068    magn:   -0.0479    constr:    0.0000
atom:   37    charge:    0.7845    magn:    0.2197    constr:    0.0000
atom:   38    charge:    2.9071    magn:   -0.0479    constr:    0.0000
atom:   39    charge:    0.6453    magn:    0.2267    constr:    0.0000
atom:   40    charge:    2.9075    magn:   -0.0479    constr:    0.0000
atom:   41    charge:    0.6449    magn:    0.2267    constr:    0.0000
atom:   42    charge:    2.9068    magn:   -0.0479    constr:    0.0000
atom:   43    charge:    0.7319    magn:    0.2122    constr:    0.0000
atom:   44    charge:    0.7846    magn:    0.2197    constr:    0.0000
atom:   45    charge:    2.9071    magn:   -0.0479    constr:    0.0000
atom:   46    charge:    0.6453    magn:    0.2267    constr:    0.0000
atom:   47    charge:    2.9074    magn:   -0.0479    constr:    0.0000
atom:   48    charge:    0.7848    magn:    0.2198    constr:    0.0000
atom:   49    charge:    2.9363    magn:   -0.0387    constr:    0.0000
atom:   50    charge:    0.7311    magn:    0.2121    constr:    0.0000
atom:   51    charge:    2.9355    magn:   -0.0403    constr:    0.0000
atom:   52    charge:    0.7318    magn:    0.2122    constr:    0.0000
atom:   53    charge:    2.9095    magn:   -0.0468    constr:    0.0000
atom:   54    charge:    0.7639    magn:    0.2142    constr:    0.0000
atom:   55    charge:    2.9356    magn:   -0.0387    constr:    0.0000
atom:   56    charge:    0.7638    magn:    0.2141    constr:    0.0000
atom:   57    charge:    2.9089    magn:   -0.0468    constr:    0.0000
atom:   58    charge:    2.9357    magn:   -0.0387    constr:    0.0000
atom:   59    charge:    0.7639    magn:    0.2141    constr:    0.0000
atom:   60    charge:    2.9095    magn:   -0.0468    constr:    0.0000
atom:   61    charge:    0.7319    magn:    0.2122    constr:    0.0000
atom:   62    charge:    2.9355    magn:   -0.0403    constr:    0.0000
atom:   63    charge:    0.7311    magn:    0.2121    constr:    0.0000

total cpu time spent up to now is     3773.5 secs

total energy              =    -765.36120447 Ry
Harris-Foulkes estimate   =    -767.92673564 Ry
estimated scf accuracy    <      14.26351315 Ry

total magnetization       =     3.78 Bohr mag/cell
absolute magnetization    =    10.34 Bohr mag/cell

iteration #  2     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.68E-03,  avg # of iterations =  3.9

negative rho (up, down):  5.158E-04 6.926E-04

Magnetic moment per site:
atom:    1    charge:    1.6590    magn:    0.1492    constr:    0.0000
atom:    2    charge:    1.6578    magn:    0.1489    constr:    0.0000
atom:    3    charge:    1.6579    magn:    0.1491    constr:    0.0000
atom:    4    charge:    1.6570    magn:    0.1489    constr:    0.0000
atom:    5    charge:    1.6584    magn:    0.1491    constr:    0.0000
atom:    6    charge:    1.6592    magn:    0.1490    constr:    0.0000
atom:    7    charge:    1.6587    magn:    0.1490    constr:    0.0000
atom:    8    charge:    1.6576    magn:    0.1491    constr:    0.0000
atom:    9    charge:    1.6577    magn:    0.1490    constr:    0.0000
atom:   10    charge:    1.6572    magn:    0.1492    constr:    0.0000
atom:   11    charge:    1.6571    magn:    0.1489    constr:    0.0000
atom:   12    charge:    1.6581    magn:    0.1491    constr:    0.0000
```

```
atom:   13    charge:    1.6586    magn:    0.1491    constr:    0.0000
atom:   14    charge:    1.6581    magn:    0.1490    constr:    0.0000
atom:   15    charge:    1.6586    magn:    0.1490    constr:    0.0000
atom:   16    charge:    1.6577    magn:    0.1491    constr:    0.0000
atom:   17    charge:    1.6589    magn:    0.1489    constr:    0.0000
atom:   18    charge:    1.6576    magn:    0.1493    constr:    0.0000
atom:   19    charge:    1.6591    magn:    0.1491    constr:    0.0000
atom:   20    charge:    1.6596    magn:    0.1491    constr:    0.0000
atom:   21    charge:    1.6590    magn:    0.1490    constr:    0.0000
atom:   22    charge:    1.6580    magn:    0.1491    constr:    0.0000
atom:   23    charge:    1.6589    magn:    0.1489    constr:    0.0000
atom:   24    charge:    1.6583    magn:    0.1491    constr:    0.0000
atom:   25    charge:    1.6593    magn:    0.1491    constr:    0.0000
atom:   26    charge:    1.6592    magn:    0.1490    constr:    0.0000
atom:   27    charge:    1.6587    magn:    0.1491    constr:    0.0000
atom:   28    charge:    1.6590    magn:    0.1489    constr:    0.0000
atom:   29    charge:    1.6574    magn:    0.1490    constr:    0.0000
atom:   30    charge:    1.6588    magn:    0.1491    constr:    0.0000
atom:   31    charge:    1.6597    magn:    0.1490    constr:    0.0000
atom:   32    charge:    1.6595    magn:    0.1492    constr:    0.0000
atom:   33    charge:    0.8326    magn:    0.1394    constr:    0.0000
atom:   34    charge:    2.6680    magn:   -0.0630    constr:    0.0000
atom:   35    charge:    0.8190    magn:    0.1390    constr:    0.0000
atom:   36    charge:    2.6337    magn:   -0.0702    constr:    0.0000
atom:   37    charge:    0.8633    magn:    0.1435    constr:    0.0000
atom:   38    charge:    2.6340    magn:   -0.0702    constr:    0.0000
atom:   39    charge:    0.7736    magn:    0.1558    constr:    0.0000
atom:   40    charge:    2.6342    magn:   -0.0702    constr:    0.0000
atom:   41    charge:    0.7732    magn:    0.1558    constr:    0.0000
atom:   42    charge:    2.6337    magn:   -0.0702    constr:    0.0000
atom:   43    charge:    0.8192    magn:    0.1390    constr:    0.0000
atom:   44    charge:    0.8634    magn:    0.1434    constr:    0.0000
atom:   45    charge:    2.6340    magn:   -0.0702    constr:    0.0000
atom:   46    charge:    0.7734    magn:    0.1559    constr:    0.0000
atom:   47    charge:    2.6343    magn:   -0.0702    constr:    0.0000
atom:   48    charge:    0.8636    magn:    0.1435    constr:    0.0000
atom:   49    charge:    2.6765    magn:   -0.0604    constr:    0.0000
atom:   50    charge:    0.8182    magn:    0.1390    constr:    0.0000
atom:   51    charge:    2.6690    magn:   -0.0630    constr:    0.0000
atom:   52    charge:    0.8190    magn:    0.1390    constr:    0.0000
atom:   53    charge:    2.6545    magn:   -0.0706    constr:    0.0000
atom:   54    charge:    0.8472    magn:    0.1399    constr:    0.0000
atom:   55    charge:    2.6759    magn:   -0.0604    constr:    0.0000
atom:   56    charge:    0.8469    magn:    0.1399    constr:    0.0000
atom:   57    charge:    2.6539    magn:   -0.0706    constr:    0.0000
atom:   58    charge:    2.6760    magn:   -0.0604    constr:    0.0000
atom:   59    charge:    0.8472    magn:    0.1399    constr:    0.0000
atom:   60    charge:    2.6545    magn:   -0.0706    constr:    0.0000
atom:   61    charge:    0.8192    magn:    0.1390    constr:    0.0000
atom:   62    charge:    2.6690    magn:   -0.0630    constr:    0.0000
atom:   63    charge:    0.8182    magn:    0.1389    constr:    0.0000

total cpu time spent up to now is     6323.5 secs

total energy              =    -768.27323476 Ry
Harris-Foulkes estimate   =    -770.72158681 Ry
estimated scf accuracy    <       5.57560885 Ry

total magnetization       =     1.11 Bohr mag/cell
absolute magnetization    =     5.71 Bohr mag/cell

iteration #  3     ecut=    40.00 Ry     beta=0.70
```

```
Davidson diagonalization with overlap
ethr =  2.22E-03,  avg # of iterations =  7.8

negative rho (up, down):  6.042E-04 6.986E-04

Magnetic moment per site:
atom:    1    charge:    1.6597    magn:    0.0798    constr:    0.0000
atom:    2    charge:    1.6578    magn:    0.0793    constr:    0.0000
atom:    3    charge:    1.6579    magn:    0.0796    constr:    0.0000
atom:    4    charge:    1.6566    magn:    0.0797    constr:    0.0000
atom:    5    charge:    1.6582    magn:    0.0795    constr:    0.0000
atom:    6    charge:    1.6593    magn:    0.0795    constr:    0.0000
atom:    7    charge:    1.6582    magn:    0.0794    constr:    0.0000
atom:    8    charge:    1.6579    magn:    0.0797    constr:    0.0000
atom:    9    charge:    1.6569    magn:    0.0795    constr:    0.0000
atom:   10    charge:    1.6567    magn:    0.0803    constr:    0.0000
atom:   11    charge:    1.6567    magn:    0.0799    constr:    0.0000
atom:   12    charge:    1.6579    magn:    0.0797    constr:    0.0000
atom:   13    charge:    1.6584    magn:    0.0796    constr:    0.0000
atom:   14    charge:    1.6580    magn:    0.0794    constr:    0.0000
atom:   15    charge:    1.6581    magn:    0.0794    constr:    0.0000
atom:   16    charge:    1.6580    magn:    0.0798    constr:    0.0000
atom:   17    charge:    1.6598    magn:    0.0800    constr:    0.0000
atom:   18    charge:    1.6587    magn:    0.0806    constr:    0.0000
atom:   19    charge:    1.6601    magn:    0.0800    constr:    0.0000
atom:   20    charge:    1.6604    magn:    0.0797    constr:    0.0000
atom:   21    charge:    1.6595    magn:    0.0796    constr:    0.0000
atom:   22    charge:    1.6584    magn:    0.0797    constr:    0.0000
atom:   23    charge:    1.6597    magn:    0.0797    constr:    0.0000
atom:   24    charge:    1.6586    magn:    0.0795    constr:    0.0000
atom:   25    charge:    1.6599    magn:    0.0795    constr:    0.0000
atom:   26    charge:    1.6605    magn:    0.0800    constr:    0.0000
atom:   27    charge:    1.6589    magn:    0.0795    constr:    0.0000
atom:   28    charge:    1.6596    magn:    0.0796    constr:    0.0000
atom:   29    charge:    1.6576    magn:    0.0795    constr:    0.0000
atom:   30    charge:    1.6593    magn:    0.0796    constr:    0.0000
atom:   31    charge:    1.6607    magn:    0.0798    constr:    0.0000
atom:   32    charge:    1.6608    magn:    0.0803    constr:    0.0000
atom:   33    charge:    0.8474    magn:    0.0844    constr:    0.0000
atom:   34    charge:    2.6739    magn:   -0.0652    constr:    0.0000
atom:   35    charge:    0.8335    magn:    0.0843    constr:    0.0000
atom:   36    charge:    2.6341    magn:   -0.0726    constr:    0.0000
atom:   37    charge:    0.8655    magn:    0.0859    constr:    0.0000
atom:   38    charge:    2.6345    magn:   -0.0726    constr:    0.0000
atom:   39    charge:    0.7148    magn:    0.0900    constr:    0.0000
atom:   40    charge:    2.6349    magn:   -0.0726    constr:    0.0000
atom:   41    charge:    0.7144    magn:    0.0900    constr:    0.0000
atom:   42    charge:    2.6342    magn:   -0.0726    constr:    0.0000
atom:   43    charge:    0.8336    magn:    0.0843    constr:    0.0000
atom:   44    charge:    0.8655    magn:    0.0858    constr:    0.0000
atom:   45    charge:    2.6345    magn:   -0.0727    constr:    0.0000
atom:   46    charge:    0.7147    magn:    0.0901    constr:    0.0000
atom:   47    charge:    2.6349    magn:   -0.0727    constr:    0.0000
atom:   48    charge:    0.8658    magn:    0.0859    constr:    0.0000
atom:   49    charge:    2.6787    magn:   -0.0636    constr:    0.0000
atom:   50    charge:    0.8327    magn:    0.0843    constr:    0.0000
atom:   51    charge:    2.6750    magn:   -0.0652    constr:    0.0000
atom:   52    charge:    0.8335    magn:    0.0844    constr:    0.0000
atom:   53    charge:    2.6571    magn:   -0.0707    constr:    0.0000
atom:   54    charge:    0.8595    magn:    0.0845    constr:    0.0000
atom:   55    charge:    2.6780    magn:   -0.0636    constr:    0.0000
atom:   56    charge:    0.8593    magn:    0.0845    constr:    0.0000
```

```
atom:   57    charge:    2.6565    magn:   -0.0707    constr:    0.0000
atom:   58    charge:    2.6781    magn:   -0.0635    constr:    0.0000
atom:   59    charge:    0.8595    magn:    0.0845    constr:    0.0000
atom:   60    charge:    2.6570    magn:   -0.0707    constr:    0.0000
atom:   61    charge:    0.8336    magn:    0.0843    constr:    0.0000
atom:   62    charge:    2.6750    magn:   -0.0652    constr:    0.0000
atom:   63    charge:    0.8327    magn:    0.0843    constr:    0.0000

total cpu time spent up to now is     8987.9 secs

total energy              =    -769.48846068 Ry
Harris-Foulkes estimate   =    -770.08302997 Ry
estimated scf accuracy    <       1.48993293 Ry

total magnetization       =     0.89 Bohr mag/cell
absolute magnetization    =     3.74 Bohr mag/cell

iteration #  4     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.94E-04,  avg # of iterations =  8.9

negative rho (up, down):  6.559E-04 7.233E-04

Magnetic moment per site:
atom:    1    charge:    1.6517    magn:    0.0433    constr:    0.0000
atom:    2    charge:    1.6503    magn:    0.0426    constr:    0.0000
atom:    3    charge:    1.6502    magn:    0.0429    constr:    0.0000
atom:    4    charge:    1.6491    magn:    0.0431    constr:    0.0000
atom:    5    charge:    1.6507    magn:    0.0428    constr:    0.0000
atom:    6    charge:    1.6517    magn:    0.0428    constr:    0.0000
atom:    7    charge:    1.6507    magn:    0.0427    constr:    0.0000
atom:    8    charge:    1.6499    magn:    0.0431    constr:    0.0000
atom:    9    charge:    1.6495    magn:    0.0428    constr:    0.0000
atom:   10    charge:    1.6491    magn:    0.0437    constr:    0.0000
atom:   11    charge:    1.6492    magn:    0.0433    constr:    0.0000
atom:   12    charge:    1.6503    magn:    0.0430    constr:    0.0000
atom:   13    charge:    1.6508    magn:    0.0429    constr:    0.0000
atom:   14    charge:    1.6505    magn:    0.0427    constr:    0.0000
atom:   15    charge:    1.6506    magn:    0.0426    constr:    0.0000
atom:   16    charge:    1.6501    magn:    0.0433    constr:    0.0000
atom:   17    charge:    1.6518    magn:    0.0433    constr:    0.0000
atom:   18    charge:    1.6503    magn:    0.0443    constr:    0.0000
atom:   19    charge:    1.6521    magn:    0.0436    constr:    0.0000
atom:   20    charge:    1.6526    magn:    0.0430    constr:    0.0000
atom:   21    charge:    1.6516    magn:    0.0429    constr:    0.0000
atom:   22    charge:    1.6504    magn:    0.0431    constr:    0.0000
atom:   23    charge:    1.6519    magn:    0.0430    constr:    0.0000
atom:   24    charge:    1.6508    magn:    0.0429    constr:    0.0000
atom:   25    charge:    1.6522    magn:    0.0429    constr:    0.0000
atom:   26    charge:    1.6527    magn:    0.0434    constr:    0.0000
atom:   27    charge:    1.6511    magn:    0.0428    constr:    0.0000
atom:   28    charge:    1.6518    magn:    0.0428    constr:    0.0000
atom:   29    charge:    1.6497    magn:    0.0429    constr:    0.0000
atom:   30    charge:    1.6514    magn:    0.0430    constr:    0.0000
atom:   31    charge:    1.6528    magn:    0.0431    constr:    0.0000
atom:   32    charge:    1.6527    magn:    0.0439    constr:    0.0000
atom:   33    charge:    0.8448    magn:    0.0536    constr:    0.0000
atom:   34    charge:    2.6877    magn:   -0.0619    constr:    0.0000
atom:   35    charge:    0.8318    magn:    0.0549    constr:    0.0000
atom:   36    charge:    2.6629    magn:   -0.0631    constr:    0.0000
atom:   37    charge:    0.8651    magn:    0.0551    constr:    0.0000
atom:   38    charge:    2.6632    magn:   -0.0632    constr:    0.0000
```

```
atom:   39    charge:    0.7260    magn:    0.0724    constr:    0.0000
atom:   40    charge:    2.6638    magn:   -0.0631    constr:    0.0000
atom:   41    charge:    0.7260    magn:    0.0728    constr:    0.0000
atom:   42    charge:    2.6630    magn:   -0.0631    constr:    0.0000
atom:   43    charge:    0.8318    magn:    0.0549    constr:    0.0000
atom:   44    charge:    0.8652    magn:    0.0550    constr:    0.0000
atom:   45    charge:    2.6632    magn:   -0.0633    constr:    0.0000
atom:   46    charge:    0.7260    magn:    0.0724    constr:    0.0000
atom:   47    charge:    2.6637    magn:   -0.0631    constr:    0.0000
atom:   48    charge:    0.8655    magn:    0.0551    constr:    0.0000
atom:   49    charge:    2.6924    magn:   -0.0605    constr:    0.0000
atom:   50    charge:    0.8309    magn:    0.0549    constr:    0.0000
atom:   51    charge:    2.6887    magn:   -0.0619    constr:    0.0000
atom:   52    charge:    0.8317    magn:    0.0549    constr:    0.0000
atom:   53    charge:    2.6689    magn:   -0.0654    constr:    0.0000
atom:   54    charge:    0.8579    magn:    0.0538    constr:    0.0000
atom:   55    charge:    2.6917    magn:   -0.0605    constr:    0.0000
atom:   56    charge:    0.8578    magn:    0.0538    constr:    0.0000
atom:   57    charge:    2.6683    magn:   -0.0654    constr:    0.0000
atom:   58    charge:    2.6918    magn:   -0.0605    constr:    0.0000
atom:   59    charge:    0.8579    magn:    0.0537    constr:    0.0000
atom:   60    charge:    2.6689    magn:   -0.0654    constr:    0.0000
atom:   61    charge:    0.8318    magn:    0.0549    constr:    0.0000
atom:   62    charge:    2.6887    magn:   -0.0618    constr:    0.0000
atom:   63    charge:    0.8309    magn:    0.0548    constr:    0.0000

total cpu time spent up to now is    11801.4 secs

total energy              =    -769.23537067 Ry
Harris-Foulkes estimate   =    -770.39406922 Ry
estimated scf accuracy    <       4.96697431 Ry

total magnetization       =     1.93 Bohr mag/cell
absolute magnetization    =     3.59 Bohr mag/cell

iteration #  5     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.94E-04,  avg # of iterations = 12.4

negative rho (up, down):  6.279E-04 7.139E-04

Magnetic moment per site:
atom:    1    charge:    1.6522    magn:    0.0219    constr:    0.0000
atom:    2    charge:    1.6511    magn:    0.0213    constr:    0.0000
atom:    3    charge:    1.6512    magn:    0.0216    constr:    0.0000
atom:    4    charge:    1.6501    magn:    0.0216    constr:    0.0000
atom:    5    charge:    1.6518    magn:    0.0215    constr:    0.0000
atom:    6    charge:    1.6526    magn:    0.0214    constr:    0.0000
atom:    7    charge:    1.6521    magn:    0.0214    constr:    0.0000
atom:    8    charge:    1.6507    magn:    0.0218    constr:    0.0000
atom:    9    charge:    1.6510    magn:    0.0215    constr:    0.0000
atom:   10    charge:    1.6502    magn:    0.0221    constr:    0.0000
atom:   11    charge:    1.6501    magn:    0.0218    constr:    0.0000
atom:   12    charge:    1.6512    magn:    0.0217    constr:    0.0000
atom:   13    charge:    1.6519    magn:    0.0216    constr:    0.0000
atom:   14    charge:    1.6516    magn:    0.0214    constr:    0.0000
atom:   15    charge:    1.6521    magn:    0.0213    constr:    0.0000
atom:   16    charge:    1.6508    magn:    0.0219    constr:    0.0000
atom:   17    charge:    1.6518    magn:    0.0218    constr:    0.0000
atom:   18    charge:    1.6501    magn:    0.0227    constr:    0.0000
atom:   19    charge:    1.6523    magn:    0.0221    constr:    0.0000
atom:   20    charge:    1.6528    magn:    0.0216    constr:    0.0000
```

```
atom:   21    charge:    1.6522    magn:    0.0216    constr:    0.0000
atom:   22    charge:    1.6510    magn:    0.0218    constr:    0.0000
atom:   23    charge:    1.6520    magn:    0.0216    constr:    0.0000
atom:   24    charge:    1.6516    magn:    0.0216    constr:    0.0000
atom:   25    charge:    1.6526    magn:    0.0216    constr:    0.0000
atom:   26    charge:    1.6524    magn:    0.0219    constr:    0.0000
atom:   27    charge:    1.6520    magn:    0.0215    constr:    0.0000
atom:   28    charge:    1.6522    magn:    0.0215    constr:    0.0000
atom:   29    charge:    1.6505    magn:    0.0216    constr:    0.0000
atom:   30    charge:    1.6520    magn:    0.0216    constr:    0.0000
atom:   31    charge:    1.6529    magn:    0.0217    constr:    0.0000
atom:   32    charge:    1.6526    magn:    0.0223    constr:    0.0000
atom:   33    charge:    0.8345    magn:    0.0338    constr:    0.0000
atom:   34    charge:    2.6876    magn:   -0.0513    constr:    0.0000
atom:   35    charge:    0.8213    magn:    0.0352    constr:    0.0000
atom:   36    charge:    2.6676    magn:   -0.0501    constr:    0.0000
atom:   37    charge:    0.8609    magn:    0.0352    constr:    0.0000
atom:   38    charge:    2.6679    magn:   -0.0502    constr:    0.0000
atom:   39    charge:    0.7326    magn:    0.0535    constr:    0.0000
atom:   40    charge:    2.6683    magn:   -0.0500    constr:    0.0000
atom:   41    charge:    0.7325    magn:    0.0539    constr:    0.0000
atom:   42    charge:    2.6677    magn:   -0.0501    constr:    0.0000
atom:   43    charge:    0.8214    magn:    0.0352    constr:    0.0000
atom:   44    charge:    0.8609    magn:    0.0352    constr:    0.0000
atom:   45    charge:    2.6680    magn:   -0.0502    constr:    0.0000
atom:   46    charge:    0.7326    magn:    0.0535    constr:    0.0000
atom:   47    charge:    2.6683    magn:   -0.0500    constr:    0.0000
atom:   48    charge:    0.8612    magn:    0.0352    constr:    0.0000
atom:   49    charge:    2.6947    magn:   -0.0500    constr:    0.0000
atom:   50    charge:    0.8205    magn:    0.0352    constr:    0.0000
atom:   51    charge:    2.6886    magn:   -0.0513    constr:    0.0000
atom:   52    charge:    0.8213    magn:    0.0353    constr:    0.0000
atom:   53    charge:    2.6713    magn:   -0.0532    constr:    0.0000
atom:   54    charge:    0.8501    magn:    0.0340    constr:    0.0000
atom:   55    charge:    2.6940    magn:   -0.0501    constr:    0.0000
atom:   56    charge:    0.8500    magn:    0.0340    constr:    0.0000
atom:   57    charge:    2.6706    magn:   -0.0532    constr:    0.0000
atom:   58    charge:    2.6941    magn:   -0.0500    constr:    0.0000
atom:   59    charge:    0.8501    magn:    0.0339    constr:    0.0000
atom:   60    charge:    2.6713    magn:   -0.0532    constr:    0.0000
atom:   61    charge:    0.8214    magn:    0.0353    constr:    0.0000
atom:   62    charge:    2.6886    magn:   -0.0512    constr:    0.0000
atom:   63    charge:    0.8205    magn:    0.0352    constr:    0.0000

total cpu time spent up to now is    14432.3 secs

total energy              =    -770.00810017 Ry
Harris-Foulkes estimate   =    -770.08538113 Ry
estimated scf accuracy    <       0.46839871 Ry

total magnetization       =     0.22 Bohr mag/cell
absolute magnetization    =     1.86 Bohr mag/cell

iteration #  6     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.87E-04,  avg # of iterations =  9.2

negative rho (up, down):  6.589E-04 7.184E-04

Magnetic moment per site:
atom:    1    charge:    1.6515    magn:    0.0085    constr:    0.0000
atom:    2    charge:    1.6501    magn:    0.0081    constr:    0.0000
```

```
atom:    3    charge:    1.6501    magn:    0.0083    constr:    0.0000
atom:    4    charge:    1.6486    magn:    0.0083    constr:    0.0000
atom:    5    charge:    1.6506    magn:    0.0082    constr:    0.0000
atom:    6    charge:    1.6515    magn:    0.0082    constr:    0.0000
atom:    7    charge:    1.6508    magn:    0.0082    constr:    0.0000
atom:    8    charge:    1.6499    magn:    0.0084    constr:    0.0000
atom:    9    charge:    1.6494    magn:    0.0082    constr:    0.0000
atom:   10    charge:    1.6483    magn:    0.0085    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0084    constr:    0.0000
atom:   12    charge:    1.6500    magn:    0.0083    constr:    0.0000
atom:   13    charge:    1.6506    magn:    0.0083    constr:    0.0000
atom:   14    charge:    1.6503    magn:    0.0082    constr:    0.0000
atom:   15    charge:    1.6507    magn:    0.0081    constr:    0.0000
atom:   16    charge:    1.6499    magn:    0.0085    constr:    0.0000
atom:   17    charge:    1.6510    magn:    0.0083    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0089    constr:    0.0000
atom:   19    charge:    1.6515    magn:    0.0086    constr:    0.0000
atom:   20    charge:    1.6522    magn:    0.0083    constr:    0.0000
atom:   21    charge:    1.6515    magn:    0.0083    constr:    0.0000
atom:   22    charge:    1.6503    magn:    0.0084    constr:    0.0000
atom:   23    charge:    1.6513    magn:    0.0082    constr:    0.0000
atom:   24    charge:    1.6509    magn:    0.0083    constr:    0.0000
atom:   25    charge:    1.6520    magn:    0.0083    constr:    0.0000
atom:   26    charge:    1.6517    magn:    0.0084    constr:    0.0000
atom:   27    charge:    1.6512    magn:    0.0083    constr:    0.0000
atom:   28    charge:    1.6515    magn:    0.0082    constr:    0.0000
atom:   29    charge:    1.6498    magn:    0.0083    constr:    0.0000
atom:   30    charge:    1.6513    magn:    0.0083    constr:    0.0000
atom:   31    charge:    1.6522    magn:    0.0083    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0087    constr:    0.0000
atom:   33    charge:    0.8319    magn:    0.0199    constr:    0.0000
atom:   34    charge:    2.6921    magn:   -0.0337    constr:    0.0000
atom:   35    charge:    0.8180    magn:    0.0206    constr:    0.0000
atom:   36    charge:    2.6600    magn:   -0.0306    constr:    0.0000
atom:   37    charge:    0.8618    magn:    0.0244    constr:    0.0000
atom:   38    charge:    2.6603    magn:   -0.0306    constr:    0.0000
atom:   39    charge:    0.7273    magn:    0.0459    constr:    0.0000
atom:   40    charge:    2.6606    magn:   -0.0306    constr:    0.0000
atom:   41    charge:    0.7270    magn:    0.0461    constr:    0.0000
atom:   42    charge:    2.6600    magn:   -0.0306    constr:    0.0000
atom:   43    charge:    0.8181    magn:    0.0206    constr:    0.0000
atom:   44    charge:    0.8619    magn:    0.0243    constr:    0.0000
atom:   45    charge:    2.6604    magn:   -0.0307    constr:    0.0000
atom:   46    charge:    0.7273    magn:    0.0459    constr:    0.0000
atom:   47    charge:    2.6606    magn:   -0.0306    constr:    0.0000
atom:   48    charge:    0.8621    magn:    0.0243    constr:    0.0000
atom:   49    charge:    2.6984    magn:   -0.0326    constr:    0.0000
atom:   50    charge:    0.8172    magn:    0.0206    constr:    0.0000
atom:   51    charge:    2.6930    magn:   -0.0337    constr:    0.0000
atom:   52    charge:    0.8180    magn:    0.0206    constr:    0.0000
atom:   53    charge:    2.6734    magn:   -0.0366    constr:    0.0000
atom:   54    charge:    0.8482    magn:    0.0208    constr:    0.0000
atom:   55    charge:    2.6977    magn:   -0.0326    constr:    0.0000
atom:   56    charge:    0.8480    magn:    0.0208    constr:    0.0000
atom:   57    charge:    2.6728    magn:   -0.0367    constr:    0.0000
atom:   58    charge:    2.6978    magn:   -0.0326    constr:    0.0000
atom:   59    charge:    0.8481    magn:    0.0208    constr:    0.0000
atom:   60    charge:    2.6734    magn:   -0.0366    constr:    0.0000
atom:   61    charge:    0.8181    magn:    0.0206    constr:    0.0000
atom:   62    charge:    2.6931    magn:   -0.0337    constr:    0.0000
atom:   63    charge:    0.8171    magn:    0.0206    constr:    0.0000
```

```
     total cpu time spent up to now is    16405.9 secs

     total energy              =    -770.07788386 Ry
     Harris-Foulkes estimate   =    -770.07421330 Ry
     estimated scf accuracy    <       0.01614515 Ry

     total magnetization       =     1.11 Bohr mag/cell
     absolute magnetization    =     2.03 Bohr mag/cell

     iteration #  7     ecut=    40.00 Ry     beta=0.70
     Davidson diagonalization with overlap
     c_bands:  2 eigenvalues not converged
     c_bands:  1 eigenvalues not converged
     c_bands:  2 eigenvalues not converged
     ethr =  6.43E-06,  avg # of iterations = 13.0

     negative rho (up, down):  6.857E-04 7.254E-04

     Magnetic moment per site:
     atom:    1    charge:    1.6512    magn:    0.0029    constr:    0.0000
     atom:    2    charge:    1.6497    magn:    0.0027    constr:    0.0000
     atom:    3    charge:    1.6498    magn:    0.0028    constr:    0.0000
     atom:    4    charge:    1.6488    magn:    0.0028    constr:    0.0000
     atom:    5    charge:    1.6504    magn:    0.0027    constr:    0.0000
     atom:    6    charge:    1.6512    magn:    0.0027    constr:    0.0000
     atom:    7    charge:    1.6506    magn:    0.0027    constr:    0.0000
     atom:    8    charge:    1.6496    magn:    0.0028    constr:    0.0000
     atom:    9    charge:    1.6494    magn:    0.0027    constr:    0.0000
     atom:   10    charge:    1.6488    magn:    0.0030    constr:    0.0000
     atom:   11    charge:    1.6488    magn:    0.0028    constr:    0.0000
     atom:   12    charge:    1.6499    magn:    0.0028    constr:    0.0000
     atom:   13    charge:    1.6505    magn:    0.0028    constr:    0.0000
     atom:   14    charge:    1.6501    magn:    0.0027    constr:    0.0000
     atom:   15    charge:    1.6505    magn:    0.0027    constr:    0.0000
     atom:   16    charge:    1.6497    magn:    0.0029    constr:    0.0000
     atom:   17    charge:    1.6509    magn:    0.0027    constr:    0.0000
     atom:   18    charge:    1.6496    magn:    0.0031    constr:    0.0000
     atom:   19    charge:    1.6515    magn:    0.0029    constr:    0.0000
     atom:   20    charge:    1.6517    magn:    0.0027    constr:    0.0000
     atom:   21    charge:    1.6510    magn:    0.0027    constr:    0.0000
     atom:   22    charge:    1.6499    magn:    0.0028    constr:    0.0000
     atom:   23    charge:    1.6509    magn:    0.0027    constr:    0.0000
     atom:   24    charge:    1.6504    magn:    0.0028    constr:    0.0000
     atom:   25    charge:    1.6515    magn:    0.0027    constr:    0.0000
     atom:   26    charge:    1.6515    magn:    0.0028    constr:    0.0000
     atom:   27    charge:    1.6508    magn:    0.0028    constr:    0.0000
     atom:   28    charge:    1.6510    magn:    0.0027    constr:    0.0000
     atom:   29    charge:    1.6493    magn:    0.0028    constr:    0.0000
     atom:   30    charge:    1.6509    magn:    0.0028    constr:    0.0000
     atom:   31    charge:    1.6518    magn:    0.0027    constr:    0.0000
     atom:   32    charge:    1.6519    magn:    0.0030    constr:    0.0000
     atom:   33    charge:    0.8339    magn:    0.0107    constr:    0.0000
     atom:   34    charge:    2.6878    magn:   -0.0172    constr:    0.0000
     atom:   35    charge:    0.8202    magn:    0.0108    constr:    0.0000
     atom:   36    charge:    2.6612    magn:   -0.0156    constr:    0.0000
     atom:   37    charge:    0.8607    magn:    0.0170    constr:    0.0000
     atom:   38    charge:    2.6615    magn:   -0.0156    constr:    0.0000
     atom:   39    charge:    0.7240    magn:    0.0415    constr:    0.0000
     atom:   40    charge:    2.6620    magn:   -0.0155    constr:    0.0000
     atom:   41    charge:    0.7237    magn:    0.0416    constr:    0.0000
     atom:   42    charge:    2.6613    magn:   -0.0156    constr:    0.0000
     atom:   43    charge:    0.8203    magn:    0.0108    constr:    0.0000
```

```
atom:   44    charge:    0.8608    magn:    0.0170    constr:    0.0000
atom:   45    charge:    2.6615    magn:   -0.0156    constr:    0.0000
atom:   46    charge:    0.7241    magn:    0.0415    constr:    0.0000
atom:   47    charge:    2.6619    magn:   -0.0155    constr:    0.0000
atom:   48    charge:    0.8611    magn:    0.0170    constr:    0.0000
atom:   49    charge:    2.6926    magn:   -0.0169    constr:    0.0000
atom:   50    charge:    0.8194    magn:    0.0108    constr:    0.0000
atom:   51    charge:    2.6887    magn:   -0.0172    constr:    0.0000
atom:   52    charge:    0.8202    magn:    0.0108    constr:    0.0000
atom:   53    charge:    2.6712    magn:   -0.0211    constr:    0.0000
atom:   54    charge:    0.8487    magn:    0.0118    constr:    0.0000
atom:   55    charge:    2.6919    magn:   -0.0169    constr:    0.0000
atom:   56    charge:    0.8486    magn:    0.0118    constr:    0.0000
atom:   57    charge:    2.6705    magn:   -0.0212    constr:    0.0000
atom:   58    charge:    2.6920    magn:   -0.0169    constr:    0.0000
atom:   59    charge:    0.8487    magn:    0.0118    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0211    constr:    0.0000
atom:   61    charge:    0.8203    magn:    0.0108    constr:    0.0000
atom:   62    charge:    2.6887    magn:   -0.0171    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0108    constr:    0.0000

total cpu time spent up to now is    19383.6 secs

total energy              =    -770.08452069 Ry
Harris-Foulkes estimate   =    -770.08231023 Ry
estimated scf accuracy    <       0.00365044 Ry

total magnetization       =     1.11 Bohr mag/cell
absolute magnetization    =     1.57 Bohr mag/cell

iteration #  8     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
c_bands:  1 eigenvalues not converged
ethr =  1.45E-06,  avg # of iterations =  6.6

negative rho (up, down):  7.005E-04 7.286E-04

Magnetic moment per site:
atom:    1    charge:    1.6513    magn:    0.0014    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0013    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0013    constr:    0.0000
atom:    4    charge:    1.6483    magn:    0.0014    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0013    constr:    0.0000
atom:    6    charge:    1.6511    magn:    0.0013    constr:    0.0000
atom:    7    charge:    1.6504    magn:    0.0013    constr:    0.0000
atom:    8    charge:    1.6496    magn:    0.0014    constr:    0.0000
atom:    9    charge:    1.6489    magn:    0.0013    constr:    0.0000
atom:   10    charge:    1.6482    magn:    0.0015    constr:    0.0000
atom:   11    charge:    1.6483    magn:    0.0014    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0014    constr:    0.0000
atom:   13    charge:    1.6502    magn:    0.0014    constr:    0.0000
atom:   14    charge:    1.6499    magn:    0.0013    constr:    0.0000
atom:   15    charge:    1.6502    magn:    0.0013    constr:    0.0000
atom:   16    charge:    1.6497    magn:    0.0014    constr:    0.0000
atom:   17    charge:    1.6510    magn:    0.0013    constr:    0.0000
atom:   18    charge:    1.6496    magn:    0.0016    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0014    constr:    0.0000
atom:   20    charge:    1.6519    magn:    0.0013    constr:    0.0000
atom:   21    charge:    1.6512    magn:    0.0013    constr:    0.0000
atom:   22    charge:    1.6500    magn:    0.0014    constr:    0.0000
atom:   23    charge:    1.6512    magn:    0.0013    constr:    0.0000
atom:   24    charge:    1.6505    magn:    0.0013    constr:    0.0000
```

```
atom:   25    charge:    1.6516    magn:    0.0013    constr:    0.0000
atom:   26    charge:    1.6517    magn:    0.0013    constr:    0.0000
atom:   27    charge:    1.6508    magn:    0.0013    constr:    0.0000
atom:   28    charge:    1.6512    magn:    0.0012    constr:    0.0000
atom:   29    charge:    1.6494    magn:    0.0013    constr:    0.0000
atom:   30    charge:    1.6510    magn:    0.0013    constr:    0.0000
atom:   31    charge:    1.6521    magn:    0.0013    constr:    0.0000
atom:   32    charge:    1.6519    magn:    0.0015    constr:    0.0000
atom:   33    charge:    0.8344    magn:    0.0055    constr:    0.0000
atom:   34    charge:    2.6877    magn:   -0.0059    constr:    0.0000
atom:   35    charge:    0.8206    magn:    0.0054    constr:    0.0000
atom:   36    charge:    2.6592    magn:   -0.0057    constr:    0.0000
atom:   37    charge:    0.8610    magn:    0.0131    constr:    0.0000
atom:   38    charge:    2.6596    magn:   -0.0057    constr:    0.0000
atom:   39    charge:    0.7238    magn:    0.0394    constr:    0.0000
atom:   40    charge:    2.6599    magn:   -0.0057    constr:    0.0000
atom:   41    charge:    0.7234    magn:    0.0394    constr:    0.0000
atom:   42    charge:    2.6592    magn:   -0.0057    constr:    0.0000
atom:   43    charge:    0.8207    magn:    0.0053    constr:    0.0000
atom:   44    charge:    0.8610    magn:    0.0131    constr:    0.0000
atom:   45    charge:    2.6596    magn:   -0.0057    constr:    0.0000
atom:   46    charge:    0.7238    magn:    0.0394    constr:    0.0000
atom:   47    charge:    2.6599    magn:   -0.0057    constr:    0.0000
atom:   48    charge:    0.8613    magn:    0.0131    constr:    0.0000
atom:   49    charge:    2.6949    magn:   -0.0062    constr:    0.0000
atom:   50    charge:    0.8198    magn:    0.0054    constr:    0.0000
atom:   51    charge:    2.6887    magn:   -0.0059    constr:    0.0000
atom:   52    charge:    0.8206    magn:    0.0054    constr:    0.0000
atom:   53    charge:    2.6705    magn:   -0.0105    constr:    0.0000
atom:   54    charge:    0.8495    magn:    0.0069    constr:    0.0000
atom:   55    charge:    2.6942    magn:   -0.0062    constr:    0.0000
atom:   56    charge:    0.8493    magn:    0.0069    constr:    0.0000
atom:   57    charge:    2.6698    magn:   -0.0105    constr:    0.0000
atom:   58    charge:    2.6943    magn:   -0.0062    constr:    0.0000
atom:   59    charge:    0.8495    magn:    0.0069    constr:    0.0000
atom:   60    charge:    2.6704    magn:   -0.0105    constr:    0.0000
atom:   61    charge:    0.8207    magn:    0.0054    constr:    0.0000
atom:   62    charge:    2.6888    magn:   -0.0059    constr:    0.0000
atom:   63    charge:    0.8198    magn:    0.0054    constr:    0.0000

total cpu time spent up to now is    21855.1 secs

total energy              =    -770.08586651 Ry
Harris-Foulkes estimate   =    -770.08550759 Ry
estimated scf accuracy    <       0.00143645 Ry

total magnetization       =     1.10 Bohr mag/cell
absolute magnetization    =     1.34 Bohr mag/cell

iteration #  9     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  5.72E-07,  avg # of iterations =  6.4

negative rho (up, down):  7.056E-04 7.278E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0009    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0009    constr:    0.0000
atom:    3    charge:    1.6498    magn:    0.0009    constr:    0.0000
atom:    4    charge:    1.6486    magn:    0.0009    constr:    0.0000
atom:    5    charge:    1.6503    magn:    0.0009    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0009    constr:    0.0000
```

```
atom:    7    charge:    1.6506    magn:    0.0009    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0009    constr:    0.0000
atom:    9    charge:    1.6493    magn:    0.0009    constr:    0.0000
atom:   10    charge:    1.6485    magn:    0.0010    constr:    0.0000
atom:   11    charge:    1.6486    magn:    0.0010    constr:    0.0000
atom:   12    charge:    1.6498    magn:    0.0009    constr:    0.0000
atom:   13    charge:    1.6504    magn:    0.0009    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0009    constr:    0.0000
atom:   15    charge:    1.6505    magn:    0.0009    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0010    constr:    0.0000
atom:   17    charge:    1.6508    magn:    0.0009    constr:    0.0000
atom:   18    charge:    1.6493    magn:    0.0010    constr:    0.0000
atom:   19    charge:    1.6513    magn:    0.0010    constr:    0.0000
atom:   20    charge:    1.6517    magn:    0.0009    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0009    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0009    constr:    0.0000
atom:   23    charge:    1.6509    magn:    0.0009    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0009    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0009    constr:    0.0000
atom:   26    charge:    1.6514    magn:    0.0009    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0009    constr:    0.0000
atom:   28    charge:    1.6510    magn:    0.0009    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0009    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0009    constr:    0.0000
atom:   31    charge:    1.6518    magn:    0.0009    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0010    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0031    constr:    0.0000
atom:   34    charge:    2.6887    magn:   -0.0000    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0028    constr:    0.0000
atom:   36    charge:    2.6594    magn:   -0.0005    constr:    0.0000
atom:   37    charge:    0.8613    magn:    0.0112    constr:    0.0000
atom:   38    charge:    2.6597    magn:   -0.0005    constr:    0.0000
atom:   39    charge:    0.7238    magn:    0.0384    constr:    0.0000
atom:   40    charge:    2.6601    magn:   -0.0005    constr:    0.0000
atom:   41    charge:    0.7235    magn:    0.0384    constr:    0.0000
atom:   42    charge:    2.6594    magn:   -0.0005    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0028    constr:    0.0000
atom:   44    charge:    0.8614    magn:    0.0112    constr:    0.0000
atom:   45    charge:    2.6597    magn:   -0.0005    constr:    0.0000
atom:   46    charge:    0.7239    magn:    0.0384    constr:    0.0000
atom:   47    charge:    2.6600    magn:   -0.0005    constr:    0.0000
atom:   48    charge:    0.8616    magn:    0.0112    constr:    0.0000
atom:   49    charge:    2.6941    magn:   -0.0009    constr:    0.0000
atom:   50    charge:    0.8195    magn:    0.0028    constr:    0.0000
atom:   51    charge:    2.6897    magn:   -0.0000    constr:    0.0000
atom:   52    charge:    0.8203    magn:    0.0028    constr:    0.0000
atom:   53    charge:    2.6712    magn:   -0.0048    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0046    constr:    0.0000
atom:   55    charge:    2.6934    magn:   -0.0009    constr:    0.0000
atom:   56    charge:    0.8490    magn:    0.0046    constr:    0.0000
atom:   57    charge:    2.6706    magn:   -0.0048    constr:    0.0000
atom:   58    charge:    2.6935    magn:   -0.0009    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0046    constr:    0.0000
atom:   60    charge:    2.6712    magn:   -0.0048    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0028    constr:    0.0000
atom:   62    charge:    2.6897    magn:   -0.0000    constr:    0.0000
atom:   63    charge:    0.8195    magn:    0.0028    constr:    0.0000

total cpu time spent up to now is    24111.0 secs

total energy              =    -770.08631297 Ry
Harris-Foulkes estimate   =    -770.08627745 Ry
```

```
     estimated scf accuracy    <       0.00026056 Ry

     total magnetization       =     1.05 Bohr mag/cell
     absolute magnetization    =     1.19 Bohr mag/cell

     iteration # 10     ecut=    40.00 Ry     beta=0.70
     Davidson diagonalization with overlap
     ethr =  1.04E-07,  avg # of iterations =  3.4

     negative rho (up, down):  7.048E-04 7.258E-04

     Magnetic moment per site:
     atom:    1    charge:    1.6512    magn:    0.0006    constr:    0.0000
     atom:    2    charge:    1.6497    magn:    0.0006    constr:    0.0000
     atom:    3    charge:    1.6497    magn:    0.0006    constr:    0.0000
     atom:    4    charge:    1.6484    magn:    0.0006    constr:    0.0000
     atom:    5    charge:    1.6502    magn:    0.0006    constr:    0.0000
     atom:    6    charge:    1.6511    magn:    0.0006    constr:    0.0000
     atom:    7    charge:    1.6504    magn:    0.0006    constr:    0.0000
     atom:    8    charge:    1.6495    magn:    0.0006    constr:    0.0000
     atom:    9    charge:    1.6491    magn:    0.0006    constr:    0.0000
     atom:   10    charge:    1.6483    magn:    0.0007    constr:    0.0000
     atom:   11    charge:    1.6484    magn:    0.0006    constr:    0.0000
     atom:   12    charge:    1.6497    magn:    0.0006    constr:    0.0000
     atom:   13    charge:    1.6503    magn:    0.0006    constr:    0.0000
     atom:   14    charge:    1.6499    magn:    0.0006    constr:    0.0000
     atom:   15    charge:    1.6503    magn:    0.0006    constr:    0.0000
     atom:   16    charge:    1.6496    magn:    0.0006    constr:    0.0000
     atom:   17    charge:    1.6509    magn:    0.0006    constr:    0.0000
     atom:   18    charge:    1.6495    magn:    0.0007    constr:    0.0000
     atom:   19    charge:    1.6514    magn:    0.0006    constr:    0.0000
     atom:   20    charge:    1.6519    magn:    0.0006    constr:    0.0000
     atom:   21    charge:    1.6511    magn:    0.0006    constr:    0.0000
     atom:   22    charge:    1.6499    magn:    0.0006    constr:    0.0000
     atom:   23    charge:    1.6511    magn:    0.0006    constr:    0.0000
     atom:   24    charge:    1.6504    magn:    0.0006    constr:    0.0000
     atom:   25    charge:    1.6516    magn:    0.0006    constr:    0.0000
     atom:   26    charge:    1.6515    magn:    0.0006    constr:    0.0000
     atom:   27    charge:    1.6507    magn:    0.0006    constr:    0.0000
     atom:   28    charge:    1.6511    magn:    0.0006    constr:    0.0000
     atom:   29    charge:    1.6493    magn:    0.0006    constr:    0.0000
     atom:   30    charge:    1.6509    magn:    0.0006    constr:    0.0000
     atom:   31    charge:    1.6520    magn:    0.0006    constr:    0.0000
     atom:   32    charge:    1.6518    magn:    0.0006    constr:    0.0000
     atom:   33    charge:    0.8340    magn:    0.0023    constr:    0.0000
     atom:   34    charge:    2.6884    magn:    0.0016    constr:    0.0000
     atom:   35    charge:    0.8203    magn:    0.0019    constr:    0.0000
     atom:   36    charge:    2.6598    magn:    0.0010    constr:    0.0000
     atom:   37    charge:    0.8612    magn:    0.0104    constr:    0.0000
     atom:   38    charge:    2.6601    magn:    0.0010    constr:    0.0000
     atom:   39    charge:    0.7240    magn:    0.0378    constr:    0.0000
     atom:   40    charge:    2.6605    magn:    0.0010    constr:    0.0000
     atom:   41    charge:    0.7237    magn:    0.0378    constr:    0.0000
     atom:   42    charge:    2.6598    magn:    0.0010    constr:    0.0000
     atom:   43    charge:    0.8203    magn:    0.0019    constr:    0.0000
     atom:   44    charge:    0.8612    magn:    0.0104    constr:    0.0000
     atom:   45    charge:    2.6601    magn:    0.0010    constr:    0.0000
     atom:   46    charge:    0.7241    magn:    0.0378    constr:    0.0000
     atom:   47    charge:    2.6605    magn:    0.0010    constr:    0.0000
     atom:   48    charge:    0.8615    magn:    0.0104    constr:    0.0000
     atom:   49    charge:    2.6942    magn:    0.0005    constr:    0.0000
     atom:   50    charge:    0.8194    magn:    0.0019    constr:    0.0000
```

```
atom:   51    charge:    2.6894    magn:    0.0016    constr:    0.0000
atom:   52    charge:    0.8202    magn:    0.0019    constr:    0.0000
atom:   53    charge:    2.6712    magn:   -0.0030    constr:    0.0000
atom:   54    charge:    0.8490    magn:    0.0038    constr:    0.0000
atom:   55    charge:    2.6935    magn:    0.0005    constr:    0.0000
atom:   56    charge:    0.8489    magn:    0.0038    constr:    0.0000
atom:   57    charge:    2.6705    magn:   -0.0030    constr:    0.0000
atom:   58    charge:    2.6936    magn:    0.0005    constr:    0.0000
atom:   59    charge:    0.8490    magn:    0.0038    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0030    constr:    0.0000
atom:   61    charge:    0.8203    magn:    0.0019    constr:    0.0000
atom:   62    charge:    2.6894    magn:    0.0017    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0019    constr:    0.0000

total cpu time spent up to now is    26270.0 secs

total energy              =    -770.08635894 Ry
Harris-Foulkes estimate   =    -770.08639978 Ry
estimated scf accuracy    <       0.00037121 Ry

total magnetization       =     0.98 Bohr mag/cell
absolute magnetization    =     1.09 Bohr mag/cell

iteration # 11     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
c_bands:  3 eigenvalues not converged
ethr =  1.04E-07,  avg # of iterations =  1.9

negative rho (up, down):  7.048E-04 7.250E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0005    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0005    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0005    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0005    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0005    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0005    constr:    0.0000
atom:    7    charge:    1.6504    magn:    0.0005    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:    9    charge:    1.6492    magn:    0.0005    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0005    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0005    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0005    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0005    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0005    constr:    0.0000
atom:   15    charge:    1.6503    magn:    0.0005    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0005    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0004    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0005    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0005    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0005    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0005    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0004    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0005    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0005    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0005    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0005    constr:    0.0000
atom:   28    charge:    1.6510    magn:    0.0004    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0005    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0005    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0005    constr:    0.0000
```

```
atom:   32    charge:    1.6518    magn:    0.0005    constr:    0.0000
atom:   33    charge:    0.8340    magn:    0.0018    constr:    0.0000
atom:   34    charge:    2.6883    magn:    0.0027    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0015    constr:    0.0000
atom:   36    charge:    2.6598    magn:    0.0018    constr:    0.0000
atom:   37    charge:    0.8611    magn:    0.0100    constr:    0.0000
atom:   38    charge:    2.6602    magn:    0.0018    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0376    constr:    0.0000
atom:   40    charge:    2.6605    magn:    0.0018    constr:    0.0000
atom:   41    charge:    0.7237    magn:    0.0376    constr:    0.0000
atom:   42    charge:    2.6599    magn:    0.0018    constr:    0.0000
atom:   43    charge:    0.8203    magn:    0.0015    constr:    0.0000
atom:   44    charge:    0.8611    magn:    0.0100    constr:    0.0000
atom:   45    charge:    2.6602    magn:    0.0018    constr:    0.0000
atom:   46    charge:    0.7241    magn:    0.0376    constr:    0.0000
atom:   47    charge:    2.6605    magn:    0.0018    constr:    0.0000
atom:   48    charge:    0.8614    magn:    0.0100    constr:    0.0000
atom:   49    charge:    2.6944    magn:    0.0013    constr:    0.0000
atom:   50    charge:    0.8194    magn:    0.0015    constr:    0.0000
atom:   51    charge:    2.6893    magn:    0.0027    constr:    0.0000
atom:   52    charge:    0.8202    magn:    0.0015    constr:    0.0000
atom:   53    charge:    2.6710    magn:   -0.0020    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0034    constr:    0.0000
atom:   55    charge:    2.6938    magn:    0.0013    constr:    0.0000
atom:   56    charge:    0.8489    magn:    0.0034    constr:    0.0000
atom:   57    charge:    2.6704    magn:   -0.0020    constr:    0.0000
atom:   58    charge:    2.6938    magn:    0.0013    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0034    constr:    0.0000
atom:   60    charge:    2.6710    magn:   -0.0020    constr:    0.0000
atom:   61    charge:    0.8203    magn:    0.0015    constr:    0.0000
atom:   62    charge:    2.6893    magn:    0.0027    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0015    constr:    0.0000

total cpu time spent up to now is    27904.7 secs

total energy              =    -770.08641910 Ry
Harris-Foulkes estimate   =    -770.08642153 Ry
estimated scf accuracy    <       0.00003321 Ry

total magnetization       =     1.01 Bohr mag/cell
absolute magnetization    =     1.11 Bohr mag/cell

iteration # 12     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.32E-08,  avg # of iterations =  3.2

negative rho (up, down):  7.053E-04 7.247E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0005    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0004    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0004    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0005    constr:    0.0000
atom:    5    charge:    1.6502    magn:    0.0004    constr:    0.0000
atom:    6    charge:    1.6511    magn:    0.0004    constr:    0.0000
atom:    7    charge:    1.6504    magn:    0.0004    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:    9    charge:    1.6491    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:    1.6497    magn:    0.0005    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0005    constr:    0.0000
```

```
atom:   14    charge:    1.6500    magn:    0.0004    constr:    0.0000
atom:   15    charge:    1.6503    magn:    0.0004    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0005    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0004    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0005    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0005    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0004    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0004    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0005    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0004    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0004    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0004    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0004    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0004    constr:    0.0000
atom:   28    charge:    1.6511    magn:    0.0004    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0004    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0004    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0004    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0005    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0016    constr:    0.0000
atom:   34    charge:    2.6883    magn:    0.0033    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0013    constr:    0.0000
atom:   36    charge:    2.6597    magn:    0.0023    constr:    0.0000
atom:   37    charge:    0.8611    magn:    0.0098    constr:    0.0000
atom:   38    charge:    2.6601    magn:    0.0023    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0376    constr:    0.0000
atom:   40    charge:    2.6604    magn:    0.0023    constr:    0.0000
atom:   41    charge:    0.7236    magn:    0.0376    constr:    0.0000
atom:   42    charge:    2.6598    magn:    0.0023    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0013    constr:    0.0000
atom:   44    charge:    0.8612    magn:    0.0098    constr:    0.0000
atom:   45    charge:    2.6601    magn:    0.0023    constr:    0.0000
atom:   46    charge:    0.7240    magn:    0.0376    constr:    0.0000
atom:   47    charge:    2.6604    magn:    0.0023    constr:    0.0000
atom:   48    charge:    0.8614    magn:    0.0098    constr:    0.0000
atom:   49    charge:    2.6944    magn:    0.0018    constr:    0.0000
atom:   50    charge:    0.8195    magn:    0.0013    constr:    0.0000
atom:   51    charge:    2.6893    magn:    0.0033    constr:    0.0000
atom:   52    charge:    0.8203    magn:    0.0013    constr:    0.0000
atom:   53    charge:    2.6711    magn:   -0.0014    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0032    constr:    0.0000
atom:   55    charge:    2.6937    magn:    0.0018    constr:    0.0000
atom:   56    charge:    0.8490    magn:    0.0032    constr:    0.0000
atom:   57    charge:    2.6704    magn:   -0.0014    constr:    0.0000
atom:   58    charge:    2.6938    magn:    0.0018    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0032    constr:    0.0000
atom:   60    charge:    2.6710    magn:   -0.0014    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0013    constr:    0.0000
atom:   62    charge:    2.6893    magn:    0.0033    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0013    constr:    0.0000

total cpu time spent up to now is    29922.8 secs

total energy              =    -770.08639235 Ry
Harris-Foulkes estimate   =    -770.08642056 Ry
estimated scf accuracy    <       0.00022593 Ry

total magnetization       =     1.01 Bohr mag/cell
absolute magnetization    =     1.10 Bohr mag/cell

iteration # 13     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
```

```
     ethr =  1.32E-08,  avg # of iterations =  1.0

     negative rho (up, down):  7.042E-04 7.243E-04

     Magnetic moment per site:
     atom:    1    charge:    1.6512    magn:    0.0005    constr:    0.0000
     atom:    2    charge:    1.6497    magn:    0.0004    constr:    0.0000
     atom:    3    charge:    1.6497    magn:    0.0004    constr:    0.0000
     atom:    4    charge:    1.6485    magn:    0.0005    constr:    0.0000
     atom:    5    charge:    1.6502    magn:    0.0004    constr:    0.0000
     atom:    6    charge:    1.6512    magn:    0.0004    constr:    0.0000
     atom:    7    charge:    1.6504    magn:    0.0004    constr:    0.0000
     atom:    8    charge:    1.6495    magn:    0.0005    constr:    0.0000
     atom:    9    charge:    1.6491    magn:    0.0005    constr:    0.0000
     atom:   10    charge:    1.6484    magn:    0.0005    constr:    0.0000
     atom:   11    charge:    1.6485    magn:    0.0005    constr:    0.0000
     atom:   12    charge:    1.6497    magn:    0.0005    constr:    0.0000
     atom:   13    charge:    1.6503    magn:    0.0005    constr:    0.0000
     atom:   14    charge:    1.6500    magn:    0.0004    constr:    0.0000
     atom:   15    charge:    1.6503    magn:    0.0004    constr:    0.0000
     atom:   16    charge:    1.6496    magn:    0.0005    constr:    0.0000
     atom:   17    charge:    1.6509    magn:    0.0004    constr:    0.0000
     atom:   18    charge:    1.6495    magn:    0.0005    constr:    0.0000
     atom:   19    charge:    1.6514    magn:    0.0005    constr:    0.0000
     atom:   20    charge:    1.6518    magn:    0.0004    constr:    0.0000
     atom:   21    charge:    1.6511    magn:    0.0004    constr:    0.0000
     atom:   22    charge:    1.6499    magn:    0.0005    constr:    0.0000
     atom:   23    charge:    1.6510    magn:    0.0004    constr:    0.0000
     atom:   24    charge:    1.6504    magn:    0.0004    constr:    0.0000
     atom:   25    charge:    1.6515    magn:    0.0004    constr:    0.0000
     atom:   26    charge:    1.6515    magn:    0.0004    constr:    0.0000
     atom:   27    charge:    1.6507    magn:    0.0004    constr:    0.0000
     atom:   28    charge:    1.6511    magn:    0.0004    constr:    0.0000
     atom:   29    charge:    1.6493    magn:    0.0004    constr:    0.0000
     atom:   30    charge:    1.6509    magn:    0.0004    constr:    0.0000
     atom:   31    charge:    1.6519    magn:    0.0004    constr:    0.0000
     atom:   32    charge:    1.6518    magn:    0.0005    constr:    0.0000
     atom:   33    charge:    0.8341    magn:    0.0016    constr:    0.0000
     atom:   34    charge:    2.6883    magn:    0.0033    constr:    0.0000
     atom:   35    charge:    0.8203    magn:    0.0013    constr:    0.0000
     atom:   36    charge:    2.6597    magn:    0.0023    constr:    0.0000
     atom:   37    charge:    0.8611    magn:    0.0098    constr:    0.0000
     atom:   38    charge:    2.6600    magn:    0.0023    constr:    0.0000
     atom:   39    charge:    0.7241    magn:    0.0376    constr:    0.0000
     atom:   40    charge:    2.6604    magn:    0.0023    constr:    0.0000
     atom:   41    charge:    0.7237    magn:    0.0375    constr:    0.0000
     atom:   42    charge:    2.6598    magn:    0.0023    constr:    0.0000
     atom:   43    charge:    0.8204    magn:    0.0013    constr:    0.0000
     atom:   44    charge:    0.8612    magn:    0.0098    constr:    0.0000
     atom:   45    charge:    2.6601    magn:    0.0023    constr:    0.0000
     atom:   46    charge:    0.7241    magn:    0.0376    constr:    0.0000
     atom:   47    charge:    2.6604    magn:    0.0023    constr:    0.0000
     atom:   48    charge:    0.8614    magn:    0.0098    constr:    0.0000
     atom:   49    charge:    2.6943    magn:    0.0018    constr:    0.0000
     atom:   50    charge:    0.8195    magn:    0.0013    constr:    0.0000
     atom:   51    charge:    2.6893    magn:    0.0033    constr:    0.0000
     atom:   52    charge:    0.8203    magn:    0.0013    constr:    0.0000
     atom:   53    charge:    2.6711    magn:   -0.0014    constr:    0.0000
     atom:   54    charge:    0.8491    magn:    0.0032    constr:    0.0000
     atom:   55    charge:    2.6937    magn:    0.0018    constr:    0.0000
     atom:   56    charge:    0.8490    magn:    0.0032    constr:    0.0000
     atom:   57    charge:    2.6704    magn:   -0.0014    constr:    0.0000
```

```
atom:   58    charge:    2.6937    magn:    0.0018    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0032    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0014    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0013    constr:    0.0000
atom:   62    charge:    2.6894    magn:    0.0033    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0013    constr:    0.0000

total cpu time spent up to now is    31539.5 secs

total energy              =    -770.08639887 Ry
Harris-Foulkes estimate   =    -770.08642862 Ry
estimated scf accuracy    <       0.00112851 Ry

total magnetization       =     0.93 Bohr mag/cell
absolute magnetization    =     1.02 Bohr mag/cell

iteration # 14     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.32E-08,  avg # of iterations =  1.0

negative rho (up, down):  7.042E-04 7.242E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0004    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0004    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0004    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0004    constr:    0.0000
atom:    5    charge:    1.6503    magn:    0.0004    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0004    constr:    0.0000
atom:    7    charge:    1.6505    magn:    0.0004    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0004    constr:    0.0000
atom:    9    charge:    1.6491    magn:    0.0004    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0004    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0004    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0004    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0004    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0004    constr:    0.0000
atom:   15    charge:    1.6504    magn:    0.0004    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0004    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0003    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0004    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0004    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0004    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0004    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0004    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0003    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0004    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0004    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0004    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0004    constr:    0.0000
atom:   28    charge:    1.6511    magn:    0.0003    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0004    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0004    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0004    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0004    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0015    constr:    0.0000
atom:   34    charge:    2.6883    magn:    0.0035    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   36    charge:    2.6597    magn:    0.0024    constr:    0.0000
atom:   37    charge:    0.8612    magn:    0.0097    constr:    0.0000
atom:   38    charge:    2.6600    magn:    0.0024    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0375    constr:    0.0000
```

```
atom:   40    charge:    2.6604    magn:    0.0024    constr:    0.0000
atom:   41    charge:    0.7237    magn:    0.0375    constr:    0.0000
atom:   42    charge:    2.6597    magn:    0.0024    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   44    charge:    0.8612    magn:    0.0097    constr:    0.0000
atom:   45    charge:    2.6601    magn:    0.0024    constr:    0.0000
atom:   46    charge:    0.7241    magn:    0.0375    constr:    0.0000
atom:   47    charge:    2.6604    magn:    0.0024    constr:    0.0000
atom:   48    charge:    0.8615    magn:    0.0097    constr:    0.0000
atom:   49    charge:    2.6943    magn:    0.0019    constr:    0.0000
atom:   50    charge:    0.8195    magn:    0.0012    constr:    0.0000
atom:   51    charge:    2.6893    magn:    0.0035    constr:    0.0000
atom:   52    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   53    charge:    2.6711    magn:   -0.0012    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   55    charge:    2.6937    magn:    0.0019    constr:    0.0000
atom:   56    charge:    0.8490    magn:    0.0031    constr:    0.0000
atom:   57    charge:    2.6704    magn:   -0.0012    constr:    0.0000
atom:   58    charge:    2.6937    magn:    0.0019    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0012    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   62    charge:    2.6893    magn:    0.0035    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0012    constr:    0.0000

total cpu time spent up to now is    33139.7 secs

total energy              =    -770.08641362 Ry
Harris-Foulkes estimate   =    -770.08641300 Ry
estimated scf accuracy    <       0.00000786 Ry

total magnetization       =     0.98 Bohr mag/cell
absolute magnetization    =     1.07 Bohr mag/cell

iteration # 15     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  3.13E-09,  avg # of iterations =  1.9

negative rho (up, down):  7.043E-04 7.242E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0003    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0003    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0003    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0003    constr:    0.0000
atom:    5    charge:    1.6503    magn:    0.0003    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0003    constr:    0.0000
atom:    7    charge:    1.6504    magn:    0.0003    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0003    constr:    0.0000
atom:    9    charge:    1.6491    magn:    0.0003    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0003    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0003    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0003    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0003    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0003    constr:    0.0000
atom:   15    charge:    1.6504    magn:    0.0003    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0003    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0003    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0004    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0003    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0003    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0003    constr:    0.0000
```

```
atom:   22    charge:    1.6499    magn:    0.0003    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0003    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0003    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0003    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0003    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0003    constr:    0.0000
atom:   28    charge:    1.6511    magn:    0.0003    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0003    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0003    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0003    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0003    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0015    constr:    0.0000
atom:   34    charge:    2.6884    magn:    0.0035    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   36    charge:    2.6597    magn:    0.0024    constr:    0.0000
atom:   37    charge:    0.8611    magn:    0.0097    constr:    0.0000
atom:   38    charge:    2.6601    magn:    0.0024    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0375    constr:    0.0000
atom:   40    charge:    2.6604    magn:    0.0024    constr:    0.0000
atom:   41    charge:    0.7237    magn:    0.0375    constr:    0.0000
atom:   42    charge:    2.6598    magn:    0.0024    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   44    charge:    0.8612    magn:    0.0097    constr:    0.0000
atom:   45    charge:    2.6601    magn:    0.0024    constr:    0.0000
atom:   46    charge:    0.7241    magn:    0.0375    constr:    0.0000
atom:   47    charge:    2.6604    magn:    0.0024    constr:    0.0000
atom:   48    charge:    0.8615    magn:    0.0097    constr:    0.0000
atom:   49    charge:    2.6944    magn:    0.0019    constr:    0.0000
atom:   50    charge:    0.8195    magn:    0.0012    constr:    0.0000
atom:   51    charge:    2.6894    magn:    0.0035    constr:    0.0000
atom:   52    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   53    charge:    2.6711    magn:   -0.0011    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   55    charge:    2.6937    magn:    0.0019    constr:    0.0000
atom:   56    charge:    0.8490    magn:    0.0031    constr:    0.0000
atom:   57    charge:    2.6704    magn:   -0.0011    constr:    0.0000
atom:   58    charge:    2.6938    magn:    0.0019    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0011    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   62    charge:    2.6894    magn:    0.0035    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0012    constr:    0.0000

total cpu time spent up to now is    34778.6 secs

total energy              =    -770.08641351 Ry
Harris-Foulkes estimate   =    -770.08641404 Ry
estimated scf accuracy    <       0.00002535 Ry

total magnetization       =     0.97 Bohr mag/cell
absolute magnetization    =     1.06 Bohr mag/cell

iteration # 16     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  3.13E-09,  avg # of iterations =  1.0

negative rho (up, down):  7.043E-04 7.241E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0003    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0003    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0003    constr:    0.0000
```

```
atom:    4    charge:    1.6485    magn:    0.0003    constr:    0.0000
atom:    5    charge:    1.6503    magn:    0.0003    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0003    constr:    0.0000
atom:    7    charge:    1.6505    magn:    0.0003    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0003    constr:    0.0000
atom:    9    charge:    1.6491    magn:    0.0003    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0003    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0003    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0003    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0003    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0003    constr:    0.0000
atom:   15    charge:    1.6504    magn:    0.0003    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0003    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0003    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0003    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0003    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0003    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0003    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0003    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0003    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0003    constr:    0.0000
atom:   25    charge:    1.6515    magn:    0.0003    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0003    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0003    constr:    0.0000
atom:   28    charge:    1.6511    magn:    0.0003    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0003    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0003    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0003    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0003    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0015    constr:    0.0000
atom:   34    charge:    2.6884    magn:    0.0035    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   36    charge:    2.6597    magn:    0.0025    constr:    0.0000
atom:   37    charge:    0.8611    magn:    0.0097    constr:    0.0000
atom:   38    charge:    2.6601    magn:    0.0025    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0375    constr:    0.0000
atom:   40    charge:    2.6604    magn:    0.0025    constr:    0.0000
atom:   41    charge:    0.7237    magn:    0.0374    constr:    0.0000
atom:   42    charge:    2.6598    magn:    0.0025    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   44    charge:    0.8612    magn:    0.0097    constr:    0.0000
atom:   45    charge:    2.6601    magn:    0.0025    constr:    0.0000
atom:   46    charge:    0.7241    magn:    0.0375    constr:    0.0000
atom:   47    charge:    2.6604    magn:    0.0025    constr:    0.0000
atom:   48    charge:    0.8614    magn:    0.0097    constr:    0.0000
atom:   49    charge:    2.6944    magn:    0.0020    constr:    0.0000
atom:   50    charge:    0.8195    magn:    0.0012    constr:    0.0000
atom:   51    charge:    2.6893    magn:    0.0035    constr:    0.0000
atom:   52    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   53    charge:    2.6711    magn:   -0.0011    constr:    0.0000
atom:   54    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   55    charge:    2.6937    magn:    0.0020    constr:    0.0000
atom:   56    charge:    0.8490    magn:    0.0031    constr:    0.0000
atom:   57    charge:    2.6704    magn:   -0.0011    constr:    0.0000
atom:   58    charge:    2.6938    magn:    0.0020    constr:    0.0000
atom:   59    charge:    0.8491    magn:    0.0031    constr:    0.0000
atom:   60    charge:    2.6711    magn:   -0.0011    constr:    0.0000
atom:   61    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   62    charge:    2.6894    magn:    0.0035    constr:    0.0000
atom:   63    charge:    0.8194    magn:    0.0012    constr:    0.0000

total cpu time spent up to now is    36414.7 secs
```

```
total energy              =    -770.08641390 Ry
Harris-Foulkes estimate   =    -770.08641382 Ry
estimated scf accuracy    <       0.00000113 Ry

total magnetization       =     0.97 Bohr mag/cell
absolute magnetization    =     1.06 Bohr mag/cell

iteration # 17     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  4.51E-10,  avg # of iterations =  2.8

negative rho (up, down):  7.044E-04 7.241E-04

Magnetic moment per site:
atom:    1    charge:    1.6512    magn:    0.0002    constr:    0.0000
atom:    2    charge:    1.6497    magn:    0.0002    constr:    0.0000
atom:    3    charge:    1.6497    magn:    0.0002    constr:    0.0000
atom:    4    charge:    1.6485    magn:    0.0002    constr:    0.0000
atom:    5    charge:    1.6503    magn:    0.0002    constr:    0.0000
atom:    6    charge:    1.6512    magn:    0.0002    constr:    0.0000
atom:    7    charge:    1.6505    magn:    0.0002    constr:    0.0000
atom:    8    charge:    1.6495    magn:    0.0002    constr:    0.0000
atom:    9    charge:    1.6492    magn:    0.0002    constr:    0.0000
atom:   10    charge:    1.6484    magn:    0.0002    constr:    0.0000
atom:   11    charge:    1.6485    magn:    0.0002    constr:    0.0000
atom:   12    charge:    1.6497    magn:    0.0002    constr:    0.0000
atom:   13    charge:    1.6503    magn:    0.0002    constr:    0.0000
atom:   14    charge:    1.6500    magn:    0.0002    constr:    0.0000
atom:   15    charge:    1.6504    magn:    0.0002    constr:    0.0000
atom:   16    charge:    1.6496    magn:    0.0002    constr:    0.0000
atom:   17    charge:    1.6509    magn:    0.0002    constr:    0.0000
atom:   18    charge:    1.6495    magn:    0.0002    constr:    0.0000
atom:   19    charge:    1.6514    magn:    0.0002    constr:    0.0000
atom:   20    charge:    1.6518    magn:    0.0002    constr:    0.0000
atom:   21    charge:    1.6511    magn:    0.0002    constr:    0.0000
atom:   22    charge:    1.6499    magn:    0.0002    constr:    0.0000
atom:   23    charge:    1.6510    magn:    0.0002    constr:    0.0000
atom:   24    charge:    1.6504    magn:    0.0002    constr:    0.0000
atom:   25    charge:    1.6516    magn:    0.0002    constr:    0.0000
atom:   26    charge:    1.6515    magn:    0.0002    constr:    0.0000
atom:   27    charge:    1.6507    magn:    0.0002    constr:    0.0000
atom:   28    charge:    1.6511    magn:    0.0002    constr:    0.0000
atom:   29    charge:    1.6493    magn:    0.0002    constr:    0.0000
atom:   30    charge:    1.6509    magn:    0.0002    constr:    0.0000
atom:   31    charge:    1.6519    magn:    0.0002    constr:    0.0000
atom:   32    charge:    1.6518    magn:    0.0002    constr:    0.0000
atom:   33    charge:    0.8341    magn:    0.0015    constr:    0.0000
atom:   34    charge:    2.6883    magn:    0.0035    constr:    0.0000
atom:   35    charge:    0.8203    magn:    0.0012    constr:    0.0000
atom:   36    charge:    2.6597    magn:    0.0025    constr:    0.0000
atom:   37    charge:    0.8611    magn:    0.0097    constr:    0.0000
atom:   38    charge:    2.6601    magn:    0.0025    constr:    0.0000
atom:   39    charge:    0.7240    magn:    0.0374    constr:    0.0000
atom:   40    charge:    2.6604    magn:    0.0025    constr:    0.0000
atom:   41    charge:    0.7236    magn:    0.0374    constr:    0.0000
atom:   42    charge:    2.6598    magn:    0.0025    constr:    0.0000
atom:   43    charge:    0.8204    magn:    0.0012    constr:    0.0000
atom:   44    charge:    0.8612    magn:    0.0097    constr:    0.0000
atom:   45    charge:    2.6601    magn:    0.0025    constr:    0.0000
atom:   46    charge:    0.7240    magn:    0.0375    constr:    0.0000
atom:   47    charge:    2.6604    magn:    0.0025    constr:    0.0000
```

```
     atom:   48    charge:    0.8614    magn:    0.0097    constr:    0.0000
     atom:   49    charge:    2.6944    magn:    0.0020    constr:    0.0000
     atom:   50    charge:    0.8195    magn:    0.0012    constr:    0.0000
     atom:   51    charge:    2.6893    magn:    0.0035    constr:    0.0000
     atom:   52    charge:    0.8203    magn:    0.0012    constr:    0.0000
     atom:   53    charge:    2.6711    magn:   -0.0011    constr:    0.0000
     atom:   54    charge:    0.8491    magn:    0.0031    constr:    0.0000
     atom:   55    charge:    2.6937    magn:    0.0020    constr:    0.0000
     atom:   56    charge:    0.8490    magn:    0.0031    constr:    0.0000
     atom:   57    charge:    2.6704    magn:   -0.0011    constr:    0.0000
     atom:   58    charge:    2.6938    magn:    0.0020    constr:    0.0000
     atom:   59    charge:    0.8491    magn:    0.0031    constr:    0.0000
     atom:   60    charge:    2.6710    magn:   -0.0011    constr:    0.0000
     atom:   61    charge:    0.8204    magn:    0.0012    constr:    0.0000
     atom:   62    charge:    2.6893    magn:    0.0035    constr:    0.0000
     atom:   63    charge:    0.8194    magn:    0.0012    constr:    0.0000

     total cpu time spent up to now is    38064.2 secs

     End of self-consistent calculation

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


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

   -21.6664 -21.3637 -20.5099 -20.5097 -20.4834 -20.3724 -20.3721 -20.0507
   -19.8149 -19.8142 -19.8131 -19.8094 -19.8086 -19.8079 -18.5217 -18.5216
   -18.3508 -18.3505 -18.2113 -18.2111 -18.1978 -18.0798 -16.8153 -16.8143
   -16.8134 -16.8133 -16.8108 -16.8092 -15.6523 -15.6469 -15.6449 -14.9412
   -14.9407 -14.9391 -12.8453 -12.5885 -12.5883 -12.5346 -11.8144 -11.8076
   -11.8007 -11.7983 -11.7926 -11.7885 -11.2618 -11.2288 -11.2285 -10.9092
   -10.9089 -10.5344 -10.5326 -10.5305 -10.5296 -10.5272 -10.5254 -10.1726
    -9.5434  -9.5432  -9.4527  -9.3787  -9.2428  -9.1503  -8.9334  -8.9333
    -8.6603  -8.6546  -8.6506  -8.6495  -8.6489  -8.6400  -8.4637  -8.3316
    -8.3315  -8.0054  -8.0052  -7.7734  -7.7710  -7.7645  -7.5084  -7.5081
    -7.4919  -7.4901  -7.4900  -7.4865  -7.4853  -7.4847  -7.4818  -7.4557
    -7.3746  -7.3743  -7.0199  -6.8861  -6.8718  -6.8717  -6.2852  -6.2847
    -6.2828  -6.2828  -6.2771  -6.2761  -6.2379  -6.2317  -6.2315  -5.7180
    -4.7054  -4.7053  -4.6622  -4.6621  -4.5255  -4.5251  -4.3738  -4.3092
    -4.2641  -4.2640  -4.0734  -4.0707  -4.0459  -4.0447  -4.0420  -4.0386
    -4.0373  -4.0339  -3.6025  -3.6009  -3.5998  -1.2736   0.6686   0.6690
     0.6710   1.2480   1.7145   1.7146   1.7476   1.9679   1.9730   1.9977
     2.0148   2.0160   2.0260   2.0349   2.0491   2.1528   2.1559   2.4535
     2.6932   2.8096   2.9858   2.9860   3.1285   3.1286   3.3663

     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   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.6309 -21.3202 -20.7906 -20.6255 -20.5393 -20.2829 -20.1916 -20.0953
 -20.0258 -20.0252 -19.8981 -19.5132 -19.5123 -19.2572 -18.7641 -18.7453
 -18.3665 -18.3186 -18.2717 -18.2244 -18.0968 -17.8536 -17.5048 -17.5024
 -16.7726 -16.7718 -16.2921 -16.0604 -16.0567 -15.8608 -15.8559 -14.6584
 -14.6576 -14.2314 -12.8801 -12.5293 -12.5249 -12.5219 -12.5051 -12.2977
 -12.1762 -12.1720 -11.6414 -11.4466 -11.2565 -11.2504 -11.2305 -11.0190
 -11.0151 -10.9763 -10.6627 -10.1523 -10.1464 -10.1200  -9.8746  -9.8158
  -9.7740  -9.7707  -9.5769  -9.3440  -9.2967  -9.2247  -9.1984  -9.1877
  -9.1007  -8.9533  -8.7598  -8.6888  -8.5562  -8.2873  -8.1013  -8.0873
  -8.0358  -7.9321  -7.9045  -7.8957  -7.7435  -7.7427  -7.7267  -7.7016
  -7.6847  -7.5900  -7.5295  -7.5152  -7.5091  -7.1362  -7.1317  -7.1090
  -6.9967  -6.9894  -6.9017  -6.8403  -6.7259  -6.7089  -6.6913  -6.6367
  -6.6328  -6.5324  -6.3238  -6.1851  -6.1769  -6.0243  -5.8128  -5.7553
  -5.1106  -5.0453  -4.8233  -4.8054  -4.7991  -4.7420  -4.5306  -4.4544
  -4.3845  -4.2848  -4.2457  -4.1707  -4.1314  -4.0160  -4.0148  -3.9552
  -3.8832  -3.6370  -3.6351  -3.2534  -3.2476  -1.2353   0.7555   0.7568
   1.0235   1.1240   1.1432   1.3015   1.7866   1.8050   1.8728   1.9093
   1.9193   2.0701   2.0806   2.1208   2.1244   2.4454   2.5075   2.6244
   2.7557   2.8209   2.8436   2.8863   3.1108   3.1763   3.2036

   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   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.5265 -21.1900 -21.0889 -20.7255 -20.6706 -20.6041 -20.1546 -20.1540
 -19.8991 -19.8409 -19.5427 -19.1596 -19.1312 -19.1300 -19.0416 -18.6228
 -18.5839 -18.3478 -18.2604 -18.2504 -18.1242 -18.1224 -17.9416 -17.6021
 -17.1285 -16.6510 -16.6496 -16.1790 -16.1758 -15.2674 -15.2627 -14.1250
 -14.1226 -13.3648 -13.3589 -13.2048 -12.8494 -12.8330 -12.8288 -12.3514
 -12.2681 -11.9475 -11.8767 -11.7171 -11.5718 -11.2667 -11.2583 -11.2549
 -10.9736 -10.7843 -10.7782 -10.2804 -10.2077 -10.0151  -9.8049  -9.7891
  -9.7778  -9.7110  -9.4855  -9.4781  -9.1842  -9.1482  -8.9535  -8.8902
  -8.8855  -8.8176  -8.7123  -8.5199  -8.4194  -8.3531  -8.2749  -8.2664
  -8.2038  -8.1613  -7.8968  -7.8947  -7.8240  -7.7077  -7.6563  -7.5994
  -7.5960  -7.5912  -7.3517  -7.2756  -7.2388  -7.2309  -7.0847  -6.9692
  -6.9519  -6.9197  -6.7059  -6.6834  -6.6792  -6.6086  -6.6014  -6.4534
```

```
  -6.2851  -6.2781  -6.2294  -6.1660  -6.1039  -6.0014  -5.7331  -5.6829
  -5.5279  -5.5251  -5.5072  -5.3009  -5.1556  -4.8418  -4.8244  -4.7427
  -4.5398  -4.4850  -4.4461  -4.3889  -4.3380  -3.9444  -3.9436  -3.9326
  -3.7269  -3.7256  -3.5691  -2.5231  -2.5171  -1.1285   0.3421   0.3600
   0.9927   0.9936   1.4506   1.6545   1.6612   1.8909   1.9034   1.9211
   1.9790   2.0000   2.0686   2.0743   2.2667   2.2960   2.3697   2.6054
   2.6595   2.6902   2.7132   2.9248   2.9481   3.0143   3.0669

   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   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.3985 -21.2829 -20.9758 -20.9707 -20.7597 -20.6293 -20.1976 -20.1970
 -19.6890 -19.5789 -19.5191 -19.3246 -19.1712 -18.8153 -18.6679 -18.6673
 -18.6659 -18.6656 -18.3306 -18.2697 -18.2586 -17.9121 -17.9107 -17.8828
 -17.5053 -16.4527 -16.4506 -16.4487 -16.4468 -14.6780 -14.6726 -13.9761
 -13.9747 -13.5046 -13.5012 -13.5002 -13.4969 -12.7993 -12.2087 -12.1129
 -12.1073 -12.0878 -12.0293 -11.9338 -11.8202 -11.6586 -11.3296 -11.3266
 -11.0600 -10.9259 -10.3042 -10.3026 -10.2970 -10.2945 -10.0935  -9.8796
  -9.7430  -9.7299  -9.5316  -8.8906  -8.8830  -8.8304  -8.8242  -8.8210
  -8.8157  -8.8149  -8.7599  -8.6397  -8.5759  -8.2033  -8.0530  -8.0317
  -8.0274  -8.0137  -8.0098  -7.9361  -7.9275  -7.9270  -7.8710  -7.7502
  -7.4794  -7.4516  -7.3933  -7.3875  -7.3712  -7.3616  -7.3605  -7.1712
  -6.9687  -6.8168  -6.7497  -6.3986  -6.3961  -6.3096  -6.2631  -6.1855
  -6.1391  -6.1380  -6.1328  -6.1316  -6.0559  -5.9526  -5.7826  -5.6803
  -5.6334  -5.5539  -5.5213  -5.5176  -5.3069  -5.3033  -5.2428  -4.8718
  -4.8517  -4.8413  -4.4361  -4.3904  -4.3850  -3.8676  -3.8434  -3.8425
  -3.8372  -3.8360  -3.4217  -2.1553  -2.1497  -1.0602  -0.0431  -0.0253
   1.3186   1.3195   1.3217   1.3231   1.5939   1.7960   1.8052   1.9168
   2.0425   2.1392   2.2138   2.2780   2.3176   2.3643   2.3836   2.5888
   2.6066   2.7482   2.8707   2.9971   3.0015   3.0222   3.2425

   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   1.0710   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5607 -21.2334 -20.9624 -20.8617 -20.4567 -20.4534 -20.3938 -20.1778
   -19.7539 -19.6927 -19.6847 -19.6829 -19.1139 -18.9191 -18.9171 -18.8273
   -18.5569 -18.4573 -18.2977 -18.1645 -18.0641 -18.0427 -17.6513 -17.4221
   -17.4209 -16.6855 -16.6838 -15.9827 -15.9807 -15.5440 -15.2945 -14.8219
   -13.7037 -13.7024 -13.1285 -13.1234 -12.9657 -12.8511 -12.5180 -12.1949
   -12.0136 -11.8681 -11.8105 -11.8054 -11.7446 -11.6926 -11.4991 -10.9249
   -10.6445 -10.4562 -10.3834 -10.3811 -10.3777 -10.3757 -10.1799  -9.8988
    -9.8517  -9.3473  -9.2405  -9.2321  -9.2131  -9.2032  -9.1875  -9.1137
    -9.0021  -8.6661  -8.6590  -8.5221  -8.4737  -8.3276  -8.3110  -8.2591
    -8.2561  -8.1679  -8.1633  -8.0511  -7.8166  -7.8140  -7.7055  -7.6190
    -7.3524  -7.3360  -7.3345  -7.1451  -7.1354  -7.0453  -7.0435  -7.0240
    -6.9992  -6.9946  -6.8498  -6.7902  -6.7862  -6.7854  -6.5532  -6.4936
    -6.4397  -6.4365  -6.4350  -6.3866  -5.9131  -5.7895  -5.7056  -5.6939
    -5.6410  -5.5368  -5.1416  -5.0296  -4.8586  -4.8215  -4.7293  -4.7282
    -4.6318  -4.5706  -4.4356  -4.3686  -4.1458  -4.1445  -4.0917  -4.0351
    -3.6523  -3.4402  -3.2497  -3.2473  -2.4670  -1.1563   0.3502   0.6395
     1.0070   1.0167   1.4038   1.4052   1.4077   1.7951   1.9113   2.0059
     2.0432   2.0464   2.2082   2.2346   2.3165   2.3933   2.5913   2.6113
     2.6350   2.6698   2.6814   2.6832   2.8819   3.0061   3.0080

     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   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4273 -21.1950 -21.0599 -20.9594 -20.8003 -20.5413 -20.3748 -19.9634
   -19.7692 -19.6118 -19.3903 -19.2781 -19.2587 -19.0599 -18.7728 -18.7507
   -18.5849 -18.4971 -18.3462 -18.2453 -18.0415 -17.9984 -17.9083 -17.4996
   -17.4980 -17.2560 -17.0080 -15.8311 -15.6368 -15.1904 -14.5389 -14.4343
   -14.0083 -13.8082 -13.5766 -13.1059 -12.7639 -12.6405 -12.4660 -12.3950
   -12.1191 -12.0430 -12.0174 -11.8552 -11.7679 -11.5274 -11.4605 -11.3890
   -11.1354 -10.9095 -10.6637 -10.4835 -10.4537 -10.3233  -9.8084  -9.8025
```

```
  -9.6284  -9.3658  -9.2435  -9.1944  -8.9860  -8.9094  -8.8389  -8.8113
  -8.6775  -8.6377  -8.5806  -8.4988  -8.4169  -8.3686  -8.3518  -8.3282
  -8.2328  -8.1864  -8.1422  -7.9841  -7.8923  -7.6399  -7.6222  -7.6096
  -7.5596  -7.5237  -7.4287  -7.3805  -7.3580  -7.3541  -7.1909  -7.0950
  -7.0181  -6.8281  -6.7996  -6.7874  -6.6284  -6.4914  -6.2726  -6.2328
  -6.1454  -6.0132  -6.0106  -5.9528  -5.8439  -5.8090  -5.7388  -5.7209
  -5.6842  -5.5162  -5.3930  -5.3877  -5.1768  -5.1718  -5.1132  -4.9288
  -4.8856  -4.8589  -4.7289  -4.5879  -4.5634  -4.3885  -4.0412  -3.8511
  -3.4320  -3.3168  -3.2601  -2.6821  -1.7783  -1.0502  -0.3342   0.3748
   0.6779   0.8283   1.5786   1.7714   1.8537   1.8574   1.9071   1.9864
   2.0011   2.1594   2.2166   2.2539   2.2996   2.4203   2.4773   2.5190
   2.5436   2.7353   2.8433   2.8750   2.8919   3.0498   3.1260

   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   1.0057   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.3096 -21.2615 -21.1089 -20.8478 -20.8433 -20.8394 -20.1155 -20.0682
 -19.7847 -19.3020 -19.3007 -19.2996 -19.1369 -19.0859 -19.0537 -18.9108
 -18.8890 -18.3850 -17.9369 -17.9145 -17.7905 -17.7900 -17.7889 -17.7879
 -17.7873 -17.7866 -17.4501 -15.2221 -15.2147 -15.2103 -14.4817 -14.4811
 -14.4793 -13.9276 -13.9202 -12.6674 -12.3929 -12.3698 -12.2549 -12.2146
 -12.0322 -12.0302 -12.0284 -12.0280 -12.0245 -12.0203 -11.8467 -11.2298
 -11.2249 -11.2161 -10.9745 -10.7160 -10.5038 -10.0564  -9.6767  -9.6739
  -9.6683  -8.9725  -8.9620  -8.9539  -8.8968  -8.8661  -8.8424  -8.7435
  -8.7255  -8.7206  -8.7133  -8.6383  -8.5711  -8.5493  -8.4278  -7.9317
  -7.9284  -7.9200  -7.9140  -7.9116  -7.9087  -7.7719  -7.7707  -7.7690
  -7.7498  -7.6434  -7.5645  -7.5051  -7.4114  -7.3929  -7.3450  -6.9775
  -6.9266  -6.8833  -6.8782  -6.8763  -6.8721  -6.6254  -6.1754  -6.1546
  -5.8252  -5.8213  -5.8144  -5.7813  -5.6961  -5.5684  -5.4874  -5.4872
  -5.4856  -5.3315  -5.3218  -5.2351  -5.2301  -5.2210  -5.1667  -5.1652
  -5.1611  -5.1428  -5.1343  -5.1318  -5.0470  -4.7117  -3.8750  -3.8414
  -3.3686  -2.9594  -2.9542  -2.9497  -1.0469  -1.0431  -0.9996   0.4683
   0.4720   0.4769   1.6876   1.7388   1.7476   1.8459   1.9069   1.9797
   2.1087   2.1896   2.3065   2.4599   2.4756   2.4989   2.7741   2.7824
   2.7898   2.9415   2.9442   2.9452   2.9543   2.9583   2.9630

   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   0.8908   0.7057   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.6309 -21.3202 -20.7906 -20.6254 -20.5395 -20.2833 -20.1915 -20.0955
 -20.0254 -20.0250 -19.8981 -19.5127 -19.5124 -19.2579 -18.7638 -18.7455
 -18.3666 -18.3184 -18.2716 -18.2244 -18.0971 -17.8534 -17.5048 -17.5036
 -16.7706 -16.7702 -16.2949 -16.0610 -16.0589 -15.8569 -15.8555 -14.6583
 -14.6581 -14.2328 -12.8801 -12.5276 -12.5248 -12.5233 -12.5052 -12.2976
 -12.1766 -12.1755 -11.6413 -11.4467 -11.2528 -11.2481 -11.2304 -11.0168
 -11.0146 -10.9764 -10.6627 -10.1497 -10.1481 -10.1201  -9.8747  -9.8223
  -9.7767  -9.7741  -9.5769  -9.3331  -9.2966  -9.2232  -9.2027  -9.1876
  -9.1007  -8.9534  -8.7597  -8.6886  -8.5563  -8.2873  -8.0971  -8.0855
  -8.0397  -7.9321  -7.9043  -7.9019  -7.7426  -7.7423  -7.7202  -7.7016
  -7.6846  -7.5902  -7.5295  -7.5206  -7.5092  -7.1352  -7.1318  -7.1089
  -6.9969  -6.9893  -6.9018  -6.8392  -6.7259  -6.7044  -6.6911  -6.6402
  -6.6383  -6.5324  -6.3238  -6.1835  -6.1806  -6.0242  -5.8074  -5.7554
  -5.1105  -5.0455  -4.8232  -4.8049  -4.8000  -4.7421  -4.5305  -4.4544
  -4.3845  -4.2847  -4.2475  -4.1689  -4.1316  -4.0151  -4.0149  -3.9551
  -3.8841  -3.6360  -3.6348  -3.2535  -3.2487  -1.2353   0.7557   0.7567
   1.0225   1.1275   1.1421   1.3015   1.7865   1.8050   1.8727   1.9097
   1.9155   2.0685   2.0808   2.1205   2.1264   2.4456   2.5075   2.6244
   2.7555   2.8212   2.8434   2.8871   2.9051   3.1109   3.1763

   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   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.6309 -21.3202 -20.7906 -20.6256 -20.5392 -20.2828 -20.1917 -20.0952
 -20.0260 -20.0253 -19.8982 -19.5131 -19.5124 -19.2569 -18.7641 -18.7452
```

```
 -18.3664 -18.3187 -18.2718 -18.2243 -18.0967 -17.8536 -17.5044 -17.5024
 -16.7732 -16.7726 -16.2912 -16.0598 -16.0563 -15.8609 -15.8573 -14.6583
 -14.6577 -14.2309 -12.8800 -12.5292 -12.5250 -12.5222 -12.5051 -12.2977
 -12.1750 -12.1720 -11.6415 -11.4465 -11.2580 -11.2510 -11.2306 -11.0194
 -11.0156 -10.9763 -10.6628 -10.1516 -10.1473 -10.1200  -9.8746  -9.8134
  -9.7732  -9.7693  -9.5769  -9.3475  -9.2967  -9.2259  -9.1967  -9.1877
  -9.1007  -8.9533  -8.7597  -8.6888  -8.5562  -8.2872  -8.1032  -8.0873
  -8.0347  -7.9320  -7.9022  -7.8958  -7.7436  -7.7431  -7.7290  -7.7016
  -7.6848  -7.5900  -7.5295  -7.5132  -7.5091  -7.1367  -7.1315  -7.1091
  -6.9966  -6.9894  -6.9017  -6.8407  -6.7260  -6.7106  -6.6912  -6.6349
  -6.6314  -6.5324  -6.3239  -6.1838  -6.1774  -6.0243  -5.8148  -5.7552
  -5.1106  -5.0453  -4.8233  -4.8058  -4.7985  -4.7420  -4.5305  -4.4545
  -4.3846  -4.2847  -4.2449  -4.1716  -4.1313  -4.0159  -4.0151  -3.9552
  -3.8829  -3.6370  -3.6355  -3.2537  -3.2469  -1.2353   0.7557   0.7565
   1.0240   1.1221   1.1443   1.3015   1.7866   1.8050   1.8729   1.9115
   1.9183   2.0702   2.0806   2.1208   2.1242   2.4454   2.5075   2.6244
   2.7556   2.8209   2.8436   2.8911   3.1108   3.1763   3.2037

   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   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.5265 -21.1900 -21.0889 -20.7253 -20.6708 -20.6043 -20.1542 -20.1538
 -19.8989 -19.8410 -19.5427 -19.1593 -19.1307 -19.1304 -19.0418 -18.6238
 -18.5837 -18.3481 -18.2603 -18.2503 -18.1240 -18.1232 -17.9420 -17.6019
 -17.1303 -16.6487 -16.6482 -16.1760 -16.1751 -15.2688 -15.2660 -14.1242
 -14.1236 -13.3631 -13.3600 -13.2073 -12.8494 -12.8324 -12.8312 -12.3513
 -12.2683 -11.9473 -11.8767 -11.7171 -11.5718 -11.2668 -11.2553 -11.2531
 -10.9779 -10.7800 -10.7754 -10.2804 -10.2077 -10.0151  -9.8052  -9.7831
  -9.7759  -9.7112  -9.4836  -9.4816  -9.1843  -9.1491  -8.9535  -8.8940
  -8.8907  -8.8174  -8.7121  -8.5199  -8.4194  -8.3531  -8.2743  -8.2720
  -8.2037  -8.1612  -7.8963  -7.8947  -7.8238  -7.7078  -7.6562  -7.5970
  -7.5952  -7.5876  -7.3521  -7.2754  -7.2404  -7.2358  -7.0778  -6.9696
  -6.9523  -6.9195  -6.7058  -6.6840  -6.6820  -6.6087  -6.6014  -6.4587
  -6.2817  -6.2791  -6.2291  -6.1661  -6.1065  -6.0008  -5.7335  -5.6828
  -5.5280  -5.5186  -5.5067  -5.3027  -5.1554  -4.8418  -4.8246  -4.7443
  -4.5396  -4.4849  -4.4439  -4.3888  -4.3379  -3.9435  -3.9435  -3.9328
  -3.7261  -3.7252  -3.5691  -2.5241  -2.5189  -1.1286   0.3465   0.3599
   0.9929   0.9932   1.4505   1.6549   1.6587   1.8877   1.9026   1.9210
   1.9789   1.9999   2.0706   2.0747   2.2665   2.2959   2.3695   2.6052
   2.6596   2.6903   2.7136   2.9253   2.9476   3.0143   3.0668

   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   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   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):

  -21.5265 -21.1900 -21.0889 -20.7255 -20.6705 -20.6041 -20.1548 -20.1541
  -19.8991 -19.8408 -19.5427 -19.1596 -19.1310 -19.1302 -19.0416 -18.6225
  -18.5840 -18.3477 -18.2606 -18.2503 -18.1239 -18.1224 -17.9416 -17.6022
  -17.1278 -16.6514 -16.6504 -16.1793 -16.1769 -15.2666 -15.2619 -14.1247
  -14.1229 -13.3646 -13.3592 -13.2039 -12.8494 -12.8321 -12.8290 -12.3515
  -12.2681 -11.9475 -11.8767 -11.7170 -11.5719 -11.2668 -11.2594 -11.2557
  -10.9720 -10.7859 -10.7790 -10.2804 -10.2077 -10.0151  -9.8048  -9.7907
   -9.7790  -9.7111  -9.4842  -9.4788  -9.1842  -9.1479  -8.9535  -8.8888
   -8.8837  -8.8176  -8.7122  -8.5199  -8.4194  -8.3531  -8.2728  -8.2666
   -8.2038  -8.1613  -7.8970  -7.8947  -7.8240  -7.7077  -7.6564  -7.5998
   -7.5968  -7.5927  -7.3518  -7.2756  -7.2375  -7.2298  -7.0872  -6.9692
   -6.9519  -6.9197  -6.7060  -6.6827  -6.6788  -6.6085  -6.6015  -6.4514
   -6.2847  -6.2791  -6.2293  -6.1660  -6.1030  -6.0014  -5.7330  -5.6829
   -5.5279  -5.5270  -5.5077  -5.3004  -5.1556  -4.8419  -4.8244  -4.7419
   -4.5399  -4.4849  -4.4470  -4.3890  -4.3380  -3.9444  -3.9438  -3.9325
   -3.7270  -3.7259  -3.5691  -2.5232  -2.5162  -1.1285   0.3400   0.3608
    0.9929   0.9935   1.4506   1.6560   1.6605   1.8922   1.9033   1.9211
    1.9789   2.0000   2.0685   2.0743   2.2666   2.2960   2.3698   2.6053
    2.6595   2.6902   2.7131   2.9249   2.9481   3.0143   3.0670

    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   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   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):

   -21.3985 -21.2828 -20.9752 -20.9716 -20.7595 -20.6295 -20.1971 -20.1967
   -19.6891 -19.5787 -19.5189 -19.3250 -19.1711 -18.8151 -18.6679 -18.6675
   -18.6660 -18.6659 -18.3309 -18.2695 -18.2584 -17.9132 -17.9122 -17.8831
   -17.5051 -16.4496 -16.4488 -16.4474 -16.4458 -14.6823 -14.6781 -13.9733
   -13.9721 -13.5031 -13.5021 -13.5001 -13.4991 -12.7993 -12.2085 -12.1155
   -12.1114 -12.0882 -12.0292 -11.9337 -11.8202 -11.6586 -11.3265 -11.3242
   -11.0598 -10.9258 -10.2991 -10.2980 -10.2944 -10.2921 -10.0936  -9.8797
    -9.7432  -9.7303  -9.5317  -8.8895  -8.8845  -8.8283  -8.8254  -8.8235
    -8.8203  -8.8155  -8.7599  -8.6397  -8.5756  -8.2034  -8.0528  -8.0466
    -8.0436  -8.0160  -8.0126  -7.9361  -7.9175  -7.9168  -7.8708  -7.7504
    -7.4790  -7.4516  -7.3930  -7.3793  -7.3669  -7.3619  -7.3608  -7.1717
    -6.9690  -6.8171  -6.7500  -6.4022  -6.4009  -6.3097  -6.2630  -6.1852
    -6.1392  -6.1383  -6.1258  -6.1242  -6.0553  -5.9530  -5.7826  -5.6806
    -5.6335  -5.5532  -5.5375  -5.5323  -5.2954  -5.2946  -5.2427  -4.8721
    -4.8483  -4.8401  -4.4360  -4.3903  -4.3849  -3.8679  -3.8428  -3.8402
    -3.8387  -3.8352  -3.4217  -2.1572  -2.1521  -1.0602  -0.0378  -0.0246
     1.3184   1.3203   1.3206   1.3216   1.5931   1.7959   1.8052   1.9171
     2.0446   2.1381   2.2137   2.2781   2.3173   2.3641   2.3836   2.5884
     2.6070   2.7478   2.8704   2.9972   3.0009   3.0090   3.0221

     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   1.0709   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.3985 -21.2829 -20.9762 -20.9702 -20.7597 -20.6292 -20.1977 -20.1970
   -19.6889 -19.5790 -19.5191 -19.3245 -19.1712 -18.8155 -18.6677 -18.6670
   -18.6663 -18.6657 -18.3304 -18.2696 -18.2587 -17.9118 -17.9100 -17.8827
   -17.5054 -16.4533 -16.4518 -16.4490 -16.4473 -14.6767 -14.6705 -13.9771
   -13.9755 -13.5044 -13.5018 -13.4993 -13.4969 -12.7993 -12.2087 -12.1121
   -12.1055 -12.0877 -12.0294 -11.9338 -11.8203 -11.6586 -11.3309 -11.3273
   -11.0599 -10.9260 -10.3056 -10.3047 -10.2973 -10.2960 -10.0935  -9.8797
    -9.7430  -9.7297  -9.5316  -8.8912  -8.8823  -8.8292  -8.8239  -8.8202
    -8.8157  -8.8144  -8.7599  -8.6397  -8.5758  -8.2034  -8.0530  -8.0264
    -8.0221  -8.0125  -8.0070  -7.9360  -7.9321  -7.9311  -7.8711  -7.7502
    -7.4795  -7.4517  -7.3934  -7.3913  -7.3717  -7.3616  -7.3609  -7.1711
    -6.9687  -6.8169  -6.7497  -6.3973  -6.3943  -6.3095  -6.2631  -6.1856
    -6.1397  -6.1385  -6.1346  -6.1334  -6.0560  -5.9526  -5.7825  -5.6802
    -5.6334  -5.5539  -5.5158  -5.5115  -5.3111  -5.3068  -5.2429  -4.8718
    -4.8535  -4.8415  -4.4360  -4.3904  -4.3851  -3.8676  -3.8444  -3.8427
    -3.8370  -3.8355  -3.4218  -2.1550  -2.1485  -1.0602  -0.0455  -0.0248
```

```
     1.3190   1.3204   1.3213   1.3227   1.5940   1.7959   1.8052   1.9168
     2.0423   2.1392   2.2137   2.2781   2.3175   2.3642   2.3837   2.5887
     2.6068   2.7482   2.8708   2.9976   3.0004   3.0110   3.0224

     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   1.0711   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5607 -21.2334 -20.9623 -20.8618 -20.4578 -20.4524 -20.3937 -20.1780
   -19.7538 -19.6927 -19.6836 -19.6828 -19.1138 -18.9205 -18.9172 -18.8274
   -18.5569 -18.4571 -18.2979 -18.1661 -18.0642 -18.0428 -17.6512 -17.4210
   -17.4188 -16.6870 -16.6846 -15.9832 -15.9792 -15.5368 -15.2985 -14.8237
   -13.7059 -13.7040 -13.1336 -13.1257 -12.9603 -12.8511 -12.5181 -12.1946
   -12.0137 -11.8679 -11.8089 -11.8004 -11.7447 -11.6940 -11.4990 -10.9252
   -10.6445 -10.4532 -10.3876 -10.3822 -10.3746 -10.3709 -10.1800  -9.8988
    -9.8517  -9.3474  -9.2484  -9.2353  -9.2073  -9.2033  -9.1906  -9.1134
    -9.0021  -8.6629  -8.6573  -8.5221  -8.4733  -8.3277  -8.3190  -8.2594
    -8.2543  -8.1682  -8.1633  -8.0511  -7.8135  -7.8074  -7.7057  -7.6188
    -7.3522  -7.3371  -7.3346  -7.1453  -7.1356  -7.0420  -7.0374  -7.0239
    -7.0048  -6.9967  -6.8501  -6.7931  -6.7921  -6.7899  -6.5531  -6.4936
    -6.4393  -6.4390  -6.4347  -6.3867  -5.9133  -5.7897  -5.7079  -5.6878
    -5.6410  -5.5294  -5.1415  -5.0295  -4.8585  -4.8216  -4.7312  -4.7283
    -4.6318  -4.5719  -4.4356  -4.3671  -4.1460  -4.1449  -4.0917  -4.0352
    -3.6523  -3.4382  -3.2507  -3.2466  -2.4687  -1.1563   0.3534   0.6391
     1.0038   1.0188   1.4035   1.4044   1.4058   1.7949   1.9111   2.0045
     2.0444   2.0470   2.2082   2.2346   2.3167   2.3933   2.5923   2.6112
     2.6351   2.6669   2.6814   2.6884   2.8820   3.0064   3.0079

     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   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5607 -21.2334 -20.9623 -20.8618 -20.4574 -20.4528 -20.3938 -20.1779
   -19.7538 -19.6927 -19.6840 -19.6827 -19.1139 -18.9201 -18.9172 -18.8274
   -18.5569 -18.4572 -18.2978 -18.1657 -18.0642 -18.0428 -17.6512 -17.4214
   -17.4192 -16.6872 -16.6838 -15.9836 -15.9791 -15.5387 -15.2975 -14.8233
   -13.7057 -13.7032 -13.1321 -13.1252 -12.9616 -12.8511 -12.5181 -12.1947
   -12.0136 -11.8680 -11.8095 -11.8016 -11.7447 -11.6937 -11.4990 -10.9252
   -10.6445 -10.4539 -10.3877 -10.3807 -10.3758 -10.3717 -10.1800  -9.8987
    -9.8517  -9.3473  -9.2463  -9.2345  -9.2087  -9.2033  -9.1899  -9.1134
    -9.0021  -8.6649  -8.6568  -8.5220  -8.4733  -8.3277  -8.3169  -8.2593
    -8.2548  -8.1682  -8.1633  -8.0511  -7.8159  -7.8076  -7.7058  -7.6189
    -7.3523  -7.3376  -7.3338  -7.1452  -7.1355  -7.0439  -7.0379  -7.0240
    -7.0040  -6.9955  -6.8501  -6.7914  -6.7901  -6.7898  -6.5532  -6.4936
    -6.4393  -6.4390  -6.4342  -6.3867  -5.9133  -5.7897  -5.7081  -5.6886
    -5.6411  -5.5313  -5.1416  -5.0295  -4.8585  -4.8216  -4.7307  -4.7283
    -4.6318  -4.5715  -4.4355  -4.3676  -4.1461  -4.1446  -4.0917  -4.0352
    -3.6523  -3.4387  -3.2504  -3.2468  -2.4682  -1.1562   0.3526   0.6391
     1.0049   1.0180   1.4036   1.4045   1.4065   1.7949   1.9111   2.0046
     2.0444   2.0469   2.2082   2.2346   2.3167   2.3933   2.5923   2.6112
     2.6349   2.6682   2.6813   2.6864   2.8821   3.0060   3.0082

     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   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4273 -21.1950 -21.0600 -20.9595 -20.8002 -20.5414 -20.3748 -19.9636
   -19.7690 -19.6117 -19.3902 -19.2783 -19.2576 -19.0599 -18.7728 -18.7519
   -18.5849 -18.4986 -18.3463 -18.2456 -18.0416 -17.9965 -17.9083 -17.4996
   -17.4976 -17.2546 -17.0100 -15.8337 -15.6324 -15.1881 -14.5429 -14.4335
   -14.0112 -13.8107 -13.5717 -13.1100 -12.7639 -12.6413 -12.4612 -12.3952
   -12.1190 -12.0430 -12.0183 -11.8550 -11.7678 -11.5264 -11.4605 -11.3860
   -11.1357 -10.9140 -10.6636 -10.4828 -10.4538 -10.3233  -9.8093  -9.8026
    -9.6215  -9.3658  -9.2354  -9.1941  -8.9897  -8.9170  -8.8393  -8.8113
    -8.6786  -8.6463  -8.5804  -8.4988  -8.4168  -8.3733  -8.3518  -8.3283
    -8.2290  -8.1865  -8.1332  -7.9841  -7.8925  -7.6387  -7.6164  -7.6093
    -7.5621  -7.5238  -7.4285  -7.3827  -7.3583  -7.3541  -7.1909  -7.0949
```

```
 -7.0221  -6.8251  -6.7995  -6.7874  -6.6324  -6.4912  -6.2725  -6.2365
 -6.1453  -6.0114  -6.0105  -5.9570  -5.8441  -5.8091  -5.7344  -5.7210
 -5.6843  -5.5161  -5.3876  -5.3850  -5.1817  -5.1707  -5.1131  -4.9288
 -4.8855  -4.8590  -4.7291  -4.5887  -4.5634  -4.3883  -4.0412  -3.8511
 -3.4321  -3.3149  -3.2616  -2.6817  -1.7796  -1.0502  -0.3322   0.3739
  0.6770   0.8294   1.5783   1.7715   1.8505   1.8583   1.9070   1.9853
  2.0009   2.1596   2.2168   2.2543   2.3031   2.4197   2.4769   2.5193
  2.5435   2.7355   2.8432   2.8750   2.8922   3.0498   3.1259

  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   1.0058   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   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):

-21.4273 -21.1950 -21.0600 -20.9594 -20.8003 -20.5411 -20.3748 -19.9635
-19.7686 -19.6116 -19.3904 -19.2781 -19.2582 -19.0600 -18.7727 -18.7518
-18.5849 -18.4980 -18.3463 -18.2466 -18.0415 -17.9972 -17.9085 -17.4995
-17.4993 -17.2537 -17.0079 -15.8303 -15.6315 -15.1925 -14.5444 -14.4347
-14.0095 -13.8109 -13.5714 -13.1082 -12.7639 -12.6439 -12.4631 -12.3952
-12.1190 -12.0430 -12.0170 -11.8550 -11.7679 -11.5306 -11.4604 -11.3839
-11.1357 -10.9092 -10.6635 -10.4793 -10.4538 -10.3234  -9.8062  -9.8027
 -9.6256  -9.3660  -9.2334  -9.1943  -8.9897  -8.9166  -8.8389  -8.8113
 -8.6779  -8.6442  -8.5804  -8.4988  -8.4256  -8.3763  -8.3459  -8.3282
 -8.2320  -8.1864  -8.1386  -7.9841  -7.8923  -7.6328  -7.6255  -7.6096
 -7.5646  -7.5240  -7.4244  -7.3756  -7.3579  -7.3541  -7.1910  -7.0951
 -7.0200  -6.8274  -6.7995  -6.7874  -6.6300  -6.4917  -6.2725  -6.2364
 -6.1449  -6.0176  -6.0107  -5.9538  -5.8437  -5.8091  -5.7323  -5.7213
 -5.6896  -5.5162  -5.3873  -5.3852  -5.1808  -5.1700  -5.1131  -4.9291
 -4.8840  -4.8588  -4.7276  -4.5885  -4.5634  -4.3883  -4.0411  -3.8513
 -3.4320  -3.3147  -3.2602  -2.6837  -1.7809  -1.0502  -0.3307   0.3766
  0.6767   0.8278   1.5780   1.7715   1.8521   1.8574   1.9071   1.9871
  2.0011   2.1596   2.2165   2.2531   2.3018   2.4159   2.4775   2.5201
  2.5437   2.7353   2.8431   2.8752   2.8916   3.0498   3.1263

  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   1.0061   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4273 -21.1950 -21.0599 -20.9595 -20.8001 -20.5414 -20.3748 -19.9635
   -19.7692 -19.6117 -19.3902 -19.2783 -19.2577 -19.0599 -18.7729 -18.7516
   -18.5849 -18.4985 -18.3462 -18.2452 -18.0416 -17.9967 -17.9083 -17.4996
   -17.4971 -17.2553 -17.0102 -15.8342 -15.6339 -15.1871 -14.5413 -14.4334
   -14.0110 -13.8100 -13.5731 -13.1096 -12.7639 -12.6401 -12.4618 -12.3952
   -12.1190 -12.0430 -12.0185 -11.8550 -11.7678 -11.5252 -11.4605 -11.3876
   -11.1357 -10.9145 -10.6637 -10.4843 -10.4538 -10.3233  -9.8101  -9.8025
    -9.6219  -9.3658  -9.2382  -9.1941  -8.9888  -8.9151  -8.8393  -8.8113
    -8.6785  -8.6447  -8.5804  -8.4988  -8.4135  -8.3709  -8.3542  -8.3283
    -8.2290  -8.1865  -8.1337  -7.9840  -7.8925  -7.6412  -7.6147  -7.6094
    -7.5605  -7.5239  -7.4301  -7.3847  -7.3583  -7.3541  -7.1909  -7.0949
    -7.0217  -6.8251  -6.7995  -6.7874  -6.6323  -6.4912  -6.2726  -6.2356
    -6.1453  -6.0105  -6.0096  -5.9570  -5.8441  -5.8091  -5.7361  -5.7210
    -5.6825  -5.5161  -5.3875  -5.3871  -5.1809  -5.1711  -5.1132  -4.9288
    -4.8860  -4.8590  -4.7297  -4.5886  -4.5634  -4.3884  -4.0412  -3.8511
    -3.4321  -3.3154  -3.2616  -2.6812  -1.7789  -1.0502  -0.3332   0.3733
     0.6772   0.8297   1.5784   1.7715   1.8508   1.8583   1.9070   1.9852
     2.0009   2.1596   2.2168   2.2545   2.3026   2.4214   2.4769   2.5191
     2.5431   2.7355   2.8431   2.8750   2.8923   3.0498   3.1260

     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   1.0056   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4273 -21.1950 -21.0599 -20.9595 -20.8002 -20.5414 -20.3748 -19.9634
   -19.7693 -19.6119 -19.3902 -19.2782 -19.2585 -19.0599 -18.7729 -18.7507
   -18.5849 -18.4973 -18.3462 -18.2449 -18.0415 -17.9981 -17.9083 -17.4996
   -17.4974 -17.2563 -17.0088 -15.8323 -15.6372 -15.1888 -14.5384 -14.4339
   -14.0089 -13.8082 -13.5767 -13.1066 -12.7639 -12.6395 -12.4653 -12.3951
   -12.1191 -12.0430 -12.0179 -11.8552 -11.7679 -11.5259 -11.4605 -11.3898
```

```
 -11.1355 -10.9112 -10.6637 -10.4848 -10.4537 -10.3233  -9.8095  -9.8025
  -9.6269  -9.3658  -9.2441  -9.1943  -8.9860  -8.9096  -8.8389  -8.8113
  -8.6777  -8.6384  -8.5806  -8.4988  -8.4135  -8.3675  -8.3541  -8.3282
  -8.2318  -8.1865  -8.1403  -7.9841  -7.8923  -7.6421  -7.6189  -7.6096
  -7.5587  -7.5238  -7.4302  -7.3830  -7.3581  -7.3541  -7.1909  -7.0949
  -7.0187  -6.8273  -6.7996  -6.7873  -6.6294  -6.4914  -6.2726  -6.2328
  -6.1454  -6.0110  -6.0105  -5.9539  -5.8438  -5.8090  -5.7394  -5.7209
  -5.6824  -5.5162  -5.3930  -5.3877  -5.1774  -5.1719  -5.1132  -4.9288
  -4.8861  -4.8589  -4.7295  -4.5879  -4.5634  -4.3885  -4.0412  -3.8511
  -3.4321  -3.3168  -3.2605  -2.6815  -1.7778  -1.0502  -0.3347   0.3739
   0.6780   0.8288   1.5786   1.7714   1.8531   1.8574   1.9071   1.9863
   2.0011   2.1594   2.2166   2.2540   2.3001   2.4218   2.4774   2.5186
   2.5432   2.7353   2.8432   2.8751   2.8921   3.0498   3.1261

   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   1.0056   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.4273 -21.1950 -21.0600 -20.9594 -20.8004 -20.5411 -20.3749 -19.9635
 -19.7686 -19.6116 -19.3904 -19.2781 -19.2584 -19.0599 -18.7727 -18.7515
 -18.5849 -18.4976 -18.3463 -18.2465 -18.0415 -17.9977 -17.9085 -17.4995
 -17.4994 -17.2541 -17.0074 -15.8297 -15.6326 -15.1931 -14.5433 -14.4349
 -14.0088 -13.8102 -13.5726 -13.1071 -12.7639 -12.6437 -12.4644 -12.3951
 -12.1190 -12.0431 -12.0167 -11.8550 -11.7679 -11.5308 -11.4604 -11.3847
 -11.1356 -10.9080 -10.6636 -10.4794 -10.4538 -10.3234  -9.8059  -9.8026
  -9.6274  -9.3660  -9.2356  -9.1942  -8.9887  -8.9146  -8.8389  -8.8113
  -8.6776  -8.6419  -8.5804  -8.4988  -8.4257  -8.3751  -8.3460  -8.3282
  -8.2330  -8.1864  -8.1410  -7.9841  -7.8923  -7.6331  -7.6270  -7.6096
  -7.5639  -7.5240  -7.4245  -7.3750  -7.3578  -7.3541  -7.1910  -7.0952
  -7.0189  -6.8282  -6.7996  -6.7874  -6.6289  -6.4917  -6.2725  -6.2355
  -6.1449  -6.0180  -6.0107  -5.9528  -5.8438  -5.8091  -5.7335  -5.7213
  -5.6896  -5.5162  -5.3873  -5.3872  -5.1795  -5.1703  -5.1131  -4.9291
  -4.8841  -4.8589  -4.7276  -4.5883  -4.5634  -4.3883  -4.0411  -3.8513
  -3.4320  -3.3152  -3.2599  -2.6838  -1.7805  -1.0502  -0.3311   0.3768
   0.6768   0.8275   1.5781   1.7714   1.8530   1.8574   1.9071   1.9871
   2.0011   2.1596   2.2165   2.2531   2.3008   2.4160   2.4773   2.5203
   2.5436   2.7353   2.8431   2.8751   2.8916   3.0498   3.1263

   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   1.0060   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.6492 -21.3627 -20.4864 -20.4862 -20.4728 -20.3640 -20.3637 -20.0205
   -19.8139 -19.8132 -19.8121 -19.8084 -19.8076 -19.8069 -18.5088 -18.5087
   -18.3442 -18.3439 -18.1961 -18.1958 -18.1947 -18.0611 -16.8143 -16.8133
   -16.8125 -16.8123 -16.8098 -16.8082 -15.6511 -15.6458 -15.6438 -14.9406
   -14.9401 -14.9385 -12.7741 -12.5685 -12.5684 -12.4628 -11.8135 -11.8067
   -11.7998 -11.7974 -11.7917 -11.7876 -11.2585 -11.2104 -11.2101 -10.8910
   -10.8908 -10.5340 -10.5322 -10.5301 -10.5292 -10.5267 -10.5249 -10.0612
    -9.5193  -9.5191  -9.4397  -9.3761  -9.2368  -9.0885  -8.9139  -8.9138
    -8.6596  -8.6539  -8.6499  -8.6489  -8.6483  -8.6393  -8.4573  -8.3182
    -8.3181  -7.9887  -7.9885  -7.7730  -7.7706  -7.7641  -7.4892  -7.4873
    -7.4838  -7.4826  -7.4820  -7.4790  -7.4622  -7.4478  -7.4365  -7.4363
    -7.3399  -7.3396  -6.8589  -6.8588  -6.8444  -6.7066  -6.2848  -6.2843
    -6.2824  -6.2824  -6.2767  -6.2757  -6.2346  -6.2228  -6.2227  -5.7065
    -4.6918  -4.6917  -4.6181  -4.6181  -4.4775  -4.4772  -4.3317  -4.2968
    -4.2109  -4.2107  -4.0730  -4.0702  -4.0430  -4.0417  -4.0390  -4.0357
    -4.0343  -4.0309  -3.5994  -3.5978  -3.5967  -0.6122   0.6715   0.6718
     0.6738   1.2881   1.7655   1.8718   1.8720   1.9764   2.0011   2.0183
     2.0194   2.0281   2.0294   2.0383   2.0565   2.4613   2.4644   2.4676
     2.6993   2.8364   3.1579   3.1580   3.3634   3.3638   3.3961

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.6139 -21.3192 -20.7753 -20.6070 -20.5200 -20.2819 -20.1784 -20.0823
   -20.0248 -20.0242 -19.8733 -19.5122 -19.5113 -19.2562 -18.7522 -18.7335
   -18.3539 -18.3056 -18.2658 -18.2100 -18.0886 -17.8390 -17.5038 -17.5015
   -16.7717 -16.7709 -16.2912 -16.0595 -16.0557 -15.8598 -15.8548 -14.6577
   -14.6568 -14.2307 -12.8000 -12.5285 -12.5210 -12.5054 -12.4758 -12.2473
   -12.1753 -12.1712 -11.6301 -11.4292 -11.2557 -11.2496 -11.2160 -11.0186
   -11.0146 -10.9340 -10.6471 -10.1518 -10.1460 -10.0434  -9.8520  -9.8151
    -9.7736  -9.7702  -9.5579  -9.3418  -9.2809  -9.2240  -9.1973  -9.1717
    -9.0397  -8.9406  -8.7468  -8.6660  -8.5402  -8.2492  -8.1003  -8.0866
    -8.0335  -7.9041  -7.8953  -7.8828  -7.7408  -7.7401  -7.7262  -7.6882
    -7.6273  -7.5145  -7.5117  -7.5019  -7.5006  -7.1334  -7.1290  -7.0604
    -6.9680  -6.9443  -6.8899  -6.8377  -6.7085  -6.6362  -6.6324  -6.5997
    -6.5582  -6.5268  -6.3104  -6.1847  -6.1765  -6.0165  -5.8124  -5.7421
    -5.0661  -4.9915  -4.8097  -4.8024  -4.7962  -4.7297  -4.4768  -4.4171
    -4.3489  -4.2453  -4.2346  -4.1703  -4.0885  -4.0130  -4.0118  -3.9171
    -3.8801  -3.6340  -3.6320  -3.2504  -3.2445  -0.5842   0.7585   0.7597
     1.0264   1.1273   1.1466   1.3436   1.8237   1.9127   1.9227   1.9383
     2.0170   2.1152   2.1702   2.3691   2.4252   2.5265   2.5395   2.7635
     2.8194   2.8748   2.8865   2.9098   3.0325   3.1853   3.2388

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5102 -21.1890 -21.0722 -20.7078 -20.6696 -20.5834 -20.1536 -20.1530
   -19.8853 -19.8227 -19.5270 -19.1467 -19.1302 -19.1290 -19.0297 -18.6219
   -18.5684 -18.3348 -18.2560 -18.2355 -18.1233 -18.1214 -17.9322 -17.5893
   -17.1275 -16.6500 -16.6486 -16.1781 -16.1748 -15.2664 -15.2617 -14.1242
   -14.1218 -13.3639 -13.3581 -13.2040 -12.8322 -12.8280 -12.7601 -12.3334
   -12.2338 -11.9357 -11.8578 -11.6953 -11.5537 -11.2579 -11.2545 -11.1970
   -10.9729 -10.7835 -10.7774 -10.2595 -10.1940  -9.9938  -9.7884  -9.7771
    -9.7612  -9.6916  -9.4850  -9.4776  -9.1674  -9.1456  -8.8961  -8.8897
    -8.8851  -8.7995  -8.6799  -8.5173  -8.3788  -8.2937  -8.2745  -8.2659
    -8.1669  -8.1531  -7.8941  -7.8920  -7.7678  -7.6462  -7.6195  -7.5988
    -7.5955  -7.5907  -7.3406  -7.2597  -7.2384  -7.2305  -7.0843  -6.9423
    -6.9143  -6.8962  -6.6807  -6.6764  -6.6567  -6.5842  -6.5370  -6.4528
    -6.2846  -6.2777  -6.1675  -6.1011  -6.0907  -5.9904  -5.7160  -5.6355
    -5.5225  -5.5044  -5.4637  -5.3003  -5.1395  -4.8156  -4.7786  -4.7422
    -4.5368  -4.4456  -4.4330  -4.3714  -4.2850  -3.9414  -3.9406  -3.8741
    -3.7239  -3.7225  -3.5365  -2.5200  -2.5140  -0.4970   0.3454   0.3633
     0.9957   0.9966   1.5043   1.6578   1.6645   1.8948   1.9920   2.0630
```

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   2.1105   2.1207   2.2535   2.2997   2.3576   2.3814   2.5071   2.7074
   2.7294   2.7962   2.8230   2.9478   2.9993   3.0388   3.1168

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.3851 -21.2631 -20.9748 -20.9697 -20.7421 -20.6082 -20.1966 -20.1960
 -19.6688 -19.5655 -19.5055 -19.3141 -19.1605 -18.7958 -18.6669 -18.6663
 -18.6649 -18.6647 -18.3182 -18.2542 -18.2540 -17.9111 -17.9097 -17.8730
 -17.4929 -16.4517 -16.4497 -16.4478 -16.4458 -14.6769 -14.6715 -13.9754
 -13.9740 -13.5037 -13.5004 -13.4995 -13.4961 -12.7031 -12.1931 -12.1121
 -12.1065 -12.0656 -12.0187 -11.9194 -11.7978 -11.6048 -11.3291 -11.3261
 -11.0384 -10.8758 -10.3035 -10.3019 -10.2963 -10.2938 -10.0710  -9.8708
  -9.7237  -9.7026  -9.5081  -8.8880  -8.8803  -8.8299  -8.8237  -8.8205
  -8.8144  -8.7510  -8.7205  -8.5604  -8.5594  -8.1530  -8.0447  -8.0308
  -8.0265  -8.0132  -8.0093  -7.9271  -7.9252  -7.9247  -7.8151  -7.6598
  -7.4609  -7.4428  -7.3872  -7.3860  -7.3708  -7.3610  -7.3599  -7.1614
  -6.9612  -6.7666  -6.6836  -6.3981  -6.3956  -6.2367  -6.2193  -6.1363
  -6.1352  -6.1317  -6.1301  -6.1288  -6.0437  -5.8927  -5.7722  -5.6601
  -5.5863  -5.5206  -5.5185  -5.5169  -5.3042  -5.3006  -5.1490  -4.8656
  -4.8513  -4.8409  -4.3897  -4.3691  -4.3317  -3.8404  -3.8394  -3.8341
  -3.8329  -3.8012  -3.3914  -2.1521  -2.1465  -0.4375  -0.0399  -0.0221
   1.3218   1.3226   1.3248   1.3262   1.6925   1.8642   1.9979   2.0287
   2.2581   2.3115   2.3264   2.3779   2.4207   2.4400   2.5784   2.6057
   2.6201   2.9142   2.9395   3.0018   3.0116   3.0298   3.0771

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.5441 -21.2323 -20.9495 -20.8389 -20.4557 -20.4524 -20.3748 -20.1624
 -19.7421 -19.6837 -19.6819 -19.6717 -19.1010 -18.9181 -18.9162 -18.8155
 -18.5459 -18.4431 -18.2847 -18.1636 -18.0560 -18.0327 -17.6382 -17.4211
 -17.4199 -16.6845 -16.6828 -15.9817 -15.9798 -15.5429 -15.2936 -14.8212
 -13.7029 -13.7017 -13.1277 -13.1225 -12.9647 -12.7628 -12.4920 -12.1752
 -11.9789 -11.8536 -11.8097 -11.8046 -11.7287 -11.6922 -11.4617 -10.8985
 -10.6002 -10.4554 -10.3827 -10.3804 -10.3772 -10.3752 -10.1556  -9.8844
  -9.8235  -9.3314  -9.2401  -9.2317  -9.2105  -9.1871  -9.1819  -9.0623
  -8.9432  -8.6654  -8.6582  -8.5099  -8.4590  -8.3135  -8.3106  -8.2564
  -8.2535  -8.1556  -8.1256  -7.9592  -7.8162  -7.8136  -7.6259  -7.6090
  -7.3333  -7.3318  -7.2889  -7.1302  -7.0661  -7.0448  -7.0431  -7.0143
  -6.9986  -6.9940  -6.8402  -6.7858  -6.7850  -6.7847  -6.5338  -6.4595
  -6.4337  -6.4322  -6.3461  -6.2794  -5.8985  -5.7747  -5.7050  -5.6935
  -5.5845  -5.5342  -5.0925  -5.0157  -4.8131  -4.8110  -4.7264  -4.7253
  -4.5804  -4.5701  -4.3773  -4.3682  -4.1428  -4.1415  -4.0547  -3.9937
  -3.6127  -3.4371  -3.2467  -3.2442  -2.4638  -0.5197   0.3535   0.6425
   1.0102   1.0200   1.4079   1.4107   1.4524   1.9253   1.9396   2.1897
   2.2181   2.2884   2.2889   2.3573   2.4374   2.6011   2.6459   2.6705
   2.6744   2.6870   2.7436   2.7764   2.8914   3.0158   3.0433

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.4121 -21.1790 -21.0589 -20.9377 -20.7992 -20.5403 -20.3560 -19.9464
 -19.7682 -19.5969 -19.3780 -19.2636 -19.2577 -19.0486 -18.7566 -18.7497
 -18.5741 -18.4961 -18.3315 -18.2443 -18.0328 -17.9974 -17.8990 -17.4971
 -17.4870 -17.2550 -17.0070 -15.8301 -15.6358 -15.1894 -14.5379 -14.4336
 -14.0076 -13.8075 -13.5757 -13.1052 -12.6690 -12.6397 -12.4652 -12.3706
 -12.0959 -12.0216 -12.0170 -11.8371 -11.7471 -11.5266 -11.4405 -11.3883
 -11.0915 -10.9088 -10.6393 -10.4830 -10.4298 -10.2956  -9.8077  -9.7593
  -9.6279  -9.3486  -9.2427  -9.1626  -8.9834  -8.9090  -8.8227  -8.7599
  -8.6749  -8.6372  -8.5587  -8.4413  -8.4161  -8.3681  -8.3495  -8.2943
  -8.2321  -8.1418  -8.1020  -7.9748  -7.8831  -7.6395  -7.6217  -7.5973
  -7.5592  -7.4456  -7.4261  -7.3801  -7.3346  -7.2853  -7.1846  -7.0840
  -7.0176  -6.8253  -6.7865  -6.7232  -6.6278  -6.4535  -6.2300  -6.2118
```

```
   -6.1161  -6.0126  -5.9622  -5.9500  -5.8152  -5.7424  -5.7384  -5.7021
   -5.6814  -5.4645  -5.3903  -5.3701  -5.1763  -5.1713  -5.0454  -4.9211
   -4.8827  -4.8211  -4.7285  -4.5849  -4.4866  -4.3855  -4.0062  -3.8058
   -3.3941  -3.3137  -3.2570  -2.6790  -1.7750  -0.4264  -0.3309   0.3779
    0.6810   0.8314   1.6547   1.8569   1.9261   1.9857   2.0074   2.1648
    2.2211   2.2381   2.3032   2.3750   2.4103   2.4297   2.4937   2.5640
    2.6549   2.8300   2.8552   2.8879   2.9215   3.1347   3.1922

    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   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   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):

  -21.2950 -21.2506 -21.0810 -20.8468 -20.8423 -20.8383 -20.0951 -20.0514
  -19.7725 -19.3010 -19.2997 -19.2987 -19.1216 -19.0735 -19.0441 -18.8991
  -18.8729 -18.3688 -17.9296 -17.9043 -17.7896 -17.7890 -17.7879 -17.7869
  -17.7864 -17.7856 -17.4376 -15.2210 -15.2135 -15.2092 -14.4811 -14.4804
  -14.4786 -13.9266 -13.9192 -12.5687 -12.3695 -12.3661 -12.2103 -12.2014
  -12.0314 -12.0295 -12.0276 -12.0273 -12.0238 -12.0196 -11.8387 -11.2206
  -11.2074 -11.2063 -10.9378 -10.6904 -10.4706  -9.9743  -9.6762  -9.6734
   -9.6679  -8.9717  -8.9612  -8.9532  -8.8860  -8.8569  -8.8151  -8.7287
   -8.7229  -8.7180  -8.7108  -8.5962  -8.5390  -8.5376  -8.3057  -7.9313
   -7.9280  -7.9196  -7.9136  -7.9112  -7.9083  -7.7715  -7.7703  -7.7685
   -7.6745  -7.6327  -7.5593  -7.5003  -7.3792  -7.3384  -7.3318  -6.9166
   -6.9141  -6.8755  -6.8735  -6.8694  -6.8225  -6.5549  -6.1573  -6.1359
   -5.8246  -5.8207  -5.8139  -5.7223  -5.6832  -5.5088  -5.4805  -5.4570
   -5.4366  -5.2829  -5.2564  -5.2338  -5.2287  -5.2196  -5.1638  -5.1623
   -5.1582  -5.1407  -5.1324  -5.1300  -5.0388  -4.6088  -3.8276  -3.8177
   -3.3271  -2.9562  -2.9511  -2.9465  -1.0437  -1.0398  -0.3781   0.4714
    0.4751   0.4800   1.8359   1.8620   1.8675   1.9464   2.0792   2.1704
    2.2287   2.3648   2.4297   2.5007   2.5043   2.5895   2.7874   2.7938
    2.8025   2.9449   2.9475   2.9491   2.9584   2.9618   3.1805

    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   0.7370   0.5251   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.6139 -21.3192 -20.7753 -20.6068 -20.5203 -20.2823 -20.1782 -20.0825
   -20.0244 -20.0240 -19.8733 -19.5117 -19.5115 -19.2569 -18.7519 -18.7337
   -18.3541 -18.3055 -18.2658 -18.2099 -18.0889 -17.8389 -17.5038 -17.5027
   -16.7697 -16.7692 -16.2939 -16.0600 -16.0580 -15.8559 -15.8545 -14.6576
   -14.6573 -14.2320 -12.8000 -12.5266 -12.5224 -12.5053 -12.4759 -12.2472
   -12.1758 -12.1747 -11.6299 -11.4293 -11.2519 -11.2473 -11.2160 -11.0164
   -11.0142 -10.9341 -10.6470 -10.1492 -10.1476 -10.0434  -9.8521  -9.8216
    -9.7763  -9.7737  -9.5580  -9.3309  -9.2808  -9.2225  -9.2017  -9.1716
    -9.0397  -8.9407  -8.7467  -8.6659  -8.5403  -8.2493  -8.0961  -8.0849
    -8.0375  -7.9039  -7.9015  -7.8829  -7.7399  -7.7396  -7.7199  -7.6882
    -7.6271  -7.5199  -7.5118  -7.5018  -7.5008  -7.1324  -7.1291  -7.0602
    -6.9680  -6.9444  -6.8901  -6.8365  -6.7040  -6.6398  -6.6378  -6.5997
    -6.5580  -6.5267  -6.3104  -6.1831  -6.1802  -6.0163  -5.8070  -5.7422
    -5.0660  -4.9916  -4.8095  -4.8020  -4.7971  -4.7298  -4.4768  -4.4170
    -4.3489  -4.2471  -4.2345  -4.1685  -4.0888  -4.0121  -4.0119  -3.9170
    -3.8811  -3.6329  -3.6316  -3.2504  -3.2456  -0.5842   0.7586   0.7596
     1.0255   1.1309   1.1455   1.3436   1.8238   1.9131   1.9189   1.9382
     2.0169   2.1152   2.1703   2.3672   2.4273   2.5265   2.5397   2.7634
     2.8194   2.8748   2.8906   2.9086   3.0325   3.1859   3.2388

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.6139 -21.3192 -20.7753 -20.6071 -20.5200 -20.2818 -20.1784 -20.0822
   -20.0250 -20.0243 -19.8734 -19.5121 -19.5114 -19.2560 -18.7522 -18.7335
   -18.3538 -18.3057 -18.2659 -18.2098 -18.0886 -17.8390 -17.5035 -17.5014
   -16.7722 -16.7716 -16.2902 -16.0588 -16.0553 -15.8599 -15.8562 -14.6575
   -14.6569 -14.2301 -12.7999 -12.5283 -12.5213 -12.5055 -12.4758 -12.2473
   -12.1741 -12.1711 -11.6301 -11.4291 -11.2572 -11.2502 -11.2161 -11.0190
   -11.0152 -10.9340 -10.6471 -10.1512 -10.1469 -10.0433  -9.8520  -9.8127
```

```
  -9.7728  -9.7689  -9.5580  -9.3453  -9.2809  -9.2252  -9.1956  -9.1717
  -9.0397  -8.9406  -8.7467  -8.6661  -8.5402  -8.2492  -8.1021  -8.0866
  -8.0325  -7.9018  -7.8954  -7.8828  -7.7410  -7.7404  -7.7286  -7.6882
  -7.6273  -7.5125  -7.5117  -7.5019  -7.5006  -7.1340  -7.1288  -7.0604
  -6.9680  -6.9442  -6.8900  -6.8380  -6.7102  -6.6345  -6.6310  -6.5997
  -6.5582  -6.5267  -6.3105  -6.1834  -6.1770  -6.0165  -5.8144  -5.7421
  -5.0661  -4.9914  -4.8096  -4.8029  -4.7956  -4.7297  -4.4768  -4.4171
  -4.3490  -4.2444  -4.2346  -4.1711  -4.0884  -4.0130  -4.0122  -3.9171
  -3.8798  -3.6339  -3.6324  -3.2506  -3.2439  -0.5842   0.7586   0.7594
   1.0268   1.1255   1.1476   1.3436   1.8237   1.9149   1.9217   1.9383
   2.0170   2.1152   2.1702   2.3692   2.4251   2.5265   2.5394   2.7635
   2.8195   2.8747   2.8840   2.9113   3.0324   3.1854   3.2389

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.5102 -21.1890 -21.0722 -20.7076 -20.6698 -20.5837 -20.1532 -20.1528
 -19.8851 -19.8229 -19.5270 -19.1465 -19.1297 -19.1294 -19.0299 -18.6228
 -18.5682 -18.3351 -18.2559 -18.2354 -18.1230 -18.1222 -17.9326 -17.5891
 -17.1293 -16.6478 -16.6472 -16.1750 -16.1741 -15.2678 -15.2650 -14.1235
 -14.1228 -13.3623 -13.3592 -13.2065 -12.8316 -12.8305 -12.7601 -12.3333
 -12.2340 -11.9356 -11.8577 -11.6954 -11.5537 -11.2549 -11.2526 -11.1971
 -10.9772 -10.7792 -10.7746 -10.2594 -10.1940  -9.9938  -9.7824  -9.7752
  -9.7615  -9.6918  -9.4831  -9.4811  -9.1675  -9.1464  -8.8962  -8.8936
  -8.8903  -8.7992  -8.6797  -8.5173  -8.3788  -8.2937  -8.2739  -8.2716
  -8.1668  -8.1530  -7.8936  -7.8920  -7.7676  -7.6460  -7.6197  -7.5964
  -7.5945  -7.5872  -7.3409  -7.2595  -7.2399  -7.2354  -7.0774  -6.9427
  -6.9141  -6.8966  -6.6813  -6.6793  -6.6565  -6.5842  -6.5372  -6.4581
  -6.2812  -6.2786  -6.1673  -6.1037  -6.0908  -5.9899  -5.7164  -5.6353
  -5.5160  -5.5038  -5.4638  -5.3022  -5.1392  -4.8158  -4.7785  -4.7439
  -4.5366  -4.4435  -4.4330  -4.3713  -4.2849  -3.9405  -3.9404  -3.8744
  -3.7230  -3.7221  -3.5364  -2.5210  -2.5158  -0.4970   0.3498   0.3632
   0.9959   0.9961   1.5042   1.6581   1.6619   1.8919   1.9920   2.0630
   2.1102   2.1204   2.2537   2.2996   2.3596   2.3813   2.5062   2.7073
   2.7300   2.7962   2.8230   2.9477   3.0000   3.0380   3.1170

   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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5102 -21.1889 -21.0722 -20.7078 -20.6695 -20.5834 -20.1538 -20.1531
   -19.8854 -19.8226 -19.5270 -19.1468 -19.1300 -19.1292 -19.0297 -18.6215
   -18.5685 -18.3347 -18.2561 -18.2354 -18.1230 -18.1214 -17.9322 -17.5893
   -17.1269 -16.6505 -16.6494 -16.1783 -16.1759 -15.2656 -15.2610 -14.1239
   -14.1222 -13.3637 -13.3584 -13.2031 -12.8313 -12.8282 -12.7600 -12.3335
   -12.2338 -11.9358 -11.8577 -11.6953 -11.5538 -11.2589 -11.2552 -11.1971
   -10.9713 -10.7852 -10.7782 -10.2595 -10.1940  -9.9938  -9.7900  -9.7783
    -9.7610  -9.6916  -9.4837  -9.4783  -9.1674  -9.1453  -8.8961  -8.8884
    -8.8833  -8.7995  -8.6798  -8.5172  -8.3788  -8.2937  -8.2724  -8.2662
    -8.1669  -8.1531  -7.8943  -7.8920  -7.7678  -7.6462  -7.6195  -7.5993
    -7.5962  -7.5921  -7.3406  -7.2597  -7.2371  -7.2294  -7.0868  -6.9423
    -6.9143  -6.8962  -6.6799  -6.6760  -6.6567  -6.5843  -6.5370  -6.4508
    -6.2843  -6.2787  -6.1674  -6.1002  -6.0907  -5.9905  -5.7159  -5.6355
    -5.5245  -5.5048  -5.4636  -5.2998  -5.1395  -4.8156  -4.7786  -4.7415
    -4.5369  -4.4465  -4.4329  -4.3715  -4.2850  -3.9415  -3.9408  -3.8740
    -3.7239  -3.7228  -3.5365  -2.5200  -2.5131  -0.4970   0.3433   0.3640
     0.9959   0.9965   1.5043   1.6592   1.6637   1.8959   1.9920   2.0630
     2.1105   2.1207   2.2535   2.2996   2.3574   2.3814   2.5072   2.7074
     2.7292   2.7962   2.8230   2.9478   2.9994   3.0387   3.1169

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.3851 -21.2630 -20.9742 -20.9705 -20.7420 -20.6084 -20.1961 -20.1957
   -19.6690 -19.5653 -19.5053 -19.3145 -19.1604 -18.7955 -18.6669 -18.6665
```

```
 -18.6650 -18.6649 -18.3186 -18.2541 -18.2538 -17.9122 -17.9112 -17.8734
 -17.4927 -16.4487 -16.4478 -16.4464 -16.4448 -14.6813 -14.6771 -13.9726
 -13.9714 -13.5023 -13.5013 -13.4993 -13.4983 -12.7031 -12.1929 -12.1147
 -12.1106 -12.0659 -12.0186 -11.9193 -11.7979 -11.6048 -11.3261 -11.3238
 -11.0383 -10.8757 -10.2983 -10.2972 -10.2937 -10.2914 -10.0710  -9.8708
  -9.7238  -9.7030  -9.5082  -8.8868  -8.8819  -8.8278  -8.8250  -8.8230
  -8.8198  -8.7508  -8.7205  -8.5604  -8.5591  -8.1531  -8.0457  -8.0445
  -8.0426  -8.0156  -8.0122  -7.9271  -7.9153  -7.9146  -7.8149  -7.6599
  -7.4604  -7.4427  -7.3857  -7.3789  -7.3665  -7.3612  -7.3602  -7.1619
  -6.9615  -6.7668  -6.6842  -6.4017  -6.4003  -6.2368  -6.2192  -6.1363
  -6.1356  -6.1314  -6.1231  -6.1215  -6.0430  -5.8931  -5.7721  -5.6604
  -5.5864  -5.5367  -5.5315  -5.5178  -5.2927  -5.2920  -5.1489  -4.8659
  -4.8479  -4.8397  -4.3898  -4.3690  -4.3313  -3.8398  -3.8371  -3.8356
  -3.8321  -3.8015  -3.3914  -2.1540  -2.1489  -0.4375  -0.0346  -0.0214
   1.3215   1.3234   1.3237   1.3247   1.6922   1.8641   1.9981   2.0287
   2.2579   2.3115   2.3283   2.3777   2.4193   2.4399   2.5785   2.6052
   2.6205   2.9135   2.9393   3.0035   3.0118   3.0296   3.0772

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.3851 -21.2630 -20.9752 -20.9692 -20.7422 -20.6082 -20.1967 -20.1960
 -19.6687 -19.5655 -19.5055 -19.3140 -19.1605 -18.7959 -18.6667 -18.6660
 -18.6653 -18.6647 -18.3181 -18.2544 -18.2539 -17.9108 -17.9091 -17.8730
 -17.4930 -16.4524 -16.4508 -16.4480 -16.4463 -14.6756 -14.6694 -13.9764
 -13.9748 -13.5036 -13.5010 -13.4985 -13.4961 -12.7030 -12.1932 -12.1113
 -12.1048 -12.0655 -12.0187 -11.9194 -11.7979 -11.6048 -11.3304 -11.3268
 -11.0384 -10.8759 -10.3049 -10.3039 -10.2966 -10.2952 -10.0710  -9.8708
  -9.7237  -9.7024  -9.5081  -8.8885  -8.8796  -8.8287  -8.8235  -8.8197
  -8.8140  -8.7510  -8.7205  -8.5604  -8.5593  -8.1531  -8.0447  -8.0256
  -8.0213  -8.0120  -8.0066  -7.9298  -7.9287  -7.9270  -7.8151  -7.6597
  -7.4610  -7.4429  -7.3909  -7.3861  -7.3713  -7.3609  -7.3602  -7.1613
  -6.9612  -6.7667  -6.6836  -6.3968  -6.3939  -6.2366  -6.2193  -6.1369
  -6.1357  -6.1320  -6.1317  -6.1306  -6.0437  -5.8927  -5.7721  -5.6600
  -5.5863  -5.5185  -5.5151  -5.5108  -5.3083  -5.3041  -5.1491  -4.8656
  -4.8531  -4.8410  -4.3896  -4.3692  -4.3316  -3.8414  -3.8397  -3.8340
  -3.8325  -3.8012  -3.3914  -2.1518  -2.1453  -0.4375  -0.0423  -0.0216
   1.3221   1.3236   1.3244   1.3259   1.6926   1.8641   1.9979   2.0287
   2.2580   2.3116   2.3262   2.3778   2.4208   2.4400   2.5783   2.6054
   2.6203   2.9142   2.9396   3.0025   3.0116   3.0245   3.0316

   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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5441 -21.2324 -20.9494 -20.8389 -20.4568 -20.4514 -20.3746 -20.1626
   -19.7420 -19.6826 -19.6818 -19.6718 -19.1009 -18.9196 -18.9162 -18.8156
   -18.5459 -18.4429 -18.2849 -18.1651 -18.0561 -18.0328 -17.6380 -17.4201
   -17.4178 -16.6860 -16.6836 -15.9822 -15.9782 -15.5357 -15.2975 -14.8231
   -13.7051 -13.7033 -13.1328 -13.1248 -12.9593 -12.7628 -12.4921 -12.1749
   -11.9790 -11.8534 -11.8082 -11.7996 -11.7288 -11.6937 -11.4616 -10.8988
   -10.6001 -10.4523 -10.3869 -10.3815 -10.3741 -10.3704 -10.1556  -9.8843
    -9.8236  -9.3315  -9.2480  -9.2348  -9.2047  -9.1902  -9.1820  -9.0620
    -8.9432  -8.6622  -8.6566  -8.5099  -8.4586  -8.3186  -8.3137  -8.2568
    -8.2516  -8.1558  -8.1256  -7.9592  -7.8131  -7.8070  -7.6261  -7.6088
    -7.3345  -7.3319  -7.2887  -7.1304  -7.0663  -7.0416  -7.0370  -7.0143
    -7.0042  -6.9961  -6.8405  -6.7927  -6.7917  -6.7844  -6.5335  -6.4595
    -6.4363  -6.4319  -6.3458  -6.2794  -5.8986  -5.7749  -5.7072  -5.6873
    -5.5845  -5.5268  -5.0925  -5.0156  -4.8130  -4.8111  -4.7283  -4.7253
    -4.5804  -4.5715  -4.3773  -4.3667  -4.1430  -4.1418  -4.0546  -3.9938
    -3.6127  -3.4350  -3.2476  -3.2435  -2.4656  -0.5197   0.3567   0.6420
     1.0070   1.0220   1.4071   1.4088   1.4523   1.9252   1.9397   2.1897
     2.2176   2.2870   2.2906   2.3572   2.4376   2.6010   2.6460   2.6693
     2.6748   2.6918   2.7430   2.7764   2.8915   3.0151   3.0440

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.5441 -21.2324 -20.9494 -20.8389 -20.4564 -20.4518 -20.3747 -20.1625
   -19.7420 -19.6830 -19.6817 -19.6717 -19.1010 -18.9192 -18.9162 -18.8156
   -18.5459 -18.4430 -18.2848 -18.1647 -18.0561 -18.0328 -17.6381 -17.4205
   -17.4182 -16.6862 -16.6828 -15.9826 -15.9781 -15.5375 -15.2965 -14.8227
   -13.7049 -13.7024 -13.1312 -13.1244 -12.9607 -12.7628 -12.4921 -12.1750
   -11.9790 -11.8534 -11.8087 -11.8009 -11.7287 -11.6933 -11.4616 -10.8988
   -10.6001 -10.4531 -10.3870 -10.3800 -10.3753 -10.3712 -10.1557  -9.8843
    -9.8235  -9.3314  -9.2458  -9.2340  -9.2062  -9.1894  -9.1820  -9.0620
    -8.9432  -8.6642  -8.6561  -8.5099  -8.4585  -8.3164  -8.3137  -8.2567
    -8.2521  -8.1558  -8.1256  -7.9592  -7.8155  -7.8072  -7.6261  -7.6089
    -7.3349  -7.3311  -7.2888  -7.1304  -7.0662  -7.0435  -7.0375  -7.0143
    -7.0034  -6.9949  -6.8405  -6.7910  -6.7897  -6.7844  -6.5336  -6.4595
    -6.4362  -6.4314  -6.3458  -6.2794  -5.8986  -5.7748  -5.7074  -5.6881
    -5.5845  -5.5288  -5.0925  -5.0155  -4.8130  -4.8112  -4.7277  -4.7253
    -4.5805  -4.5710  -4.3772  -4.3672  -4.1431  -4.1416  -4.0547  -3.9938
    -3.6127  -3.4356  -3.2474  -3.2437  -2.4651  -0.5197   0.3559   0.6420
     1.0082   1.0212   1.4073   1.4094   1.4523   1.9252   1.9397   2.1897
     2.2177   2.2869   2.2906   2.3572   2.4376   2.6010   2.6460   2.6708
     2.6739   2.6902   2.7431   2.7763   2.8915   3.0152   3.0438

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4121 -21.1790 -21.0589 -20.9377 -20.7991 -20.5403 -20.3559 -19.9465
   -19.7680 -19.5968 -19.3779 -19.2638 -19.2567 -19.0487 -18.7565 -18.7509
   -18.5740 -18.4977 -18.3316 -18.2446 -18.0328 -17.9955 -17.8990 -17.4967
   -17.4870 -17.2536 -17.0090 -15.8327 -15.6314 -15.1871 -14.5419 -14.4328
   -14.0104 -13.8100 -13.5708 -13.1092 -12.6689 -12.6405 -12.4604 -12.3707
   -12.0959 -12.0215 -12.0179 -11.8369 -11.7470 -11.5257 -11.4405 -11.3853
   -11.0918 -10.9132 -10.6392 -10.4823 -10.4298 -10.2956  -9.8085  -9.7593
    -9.6210  -9.3486  -9.2347  -9.1623  -8.9871  -8.9165  -8.8230  -8.7599
    -8.6759  -8.6458  -8.5585  -8.4413  -8.4160  -8.3728  -8.3495  -8.2944
    -8.2283  -8.1328  -8.1020  -7.9748  -7.8833  -7.6383  -7.6159  -7.5970
    -7.5617  -7.4458  -7.4259  -7.3823  -7.3348  -7.2853  -7.1846  -7.0840
    -7.0217  -6.8224  -6.7864  -6.7232  -6.6318  -6.4533  -6.2338  -6.2117
    -6.1159  -6.0108  -5.9622  -5.9542  -5.8155  -5.7425  -5.7339  -5.7022
    -5.6814  -5.4644  -5.3822  -5.3699  -5.1812  -5.1702  -5.0453  -4.9212
    -4.8826  -4.8211  -4.7287  -4.5858  -4.4867  -4.3854  -4.0062  -3.8058
    -3.3942  -3.3117  -3.2585  -2.6786  -1.7765  -0.4264  -0.3290   0.3771
```

```
    0.6799   0.8326   1.6546   1.8537   1.9261   1.9860   2.0074   2.1646
    2.2208   2.2379   2.3065   2.3752   2.4103   2.4296   2.4934   2.5640
    2.6549   2.8302   2.8551   2.8878   2.9218   3.1346   3.1922

    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   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
    0.0000   0.0000   0.0000   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):

  -21.4121 -21.1790 -21.0590 -20.9377 -20.7993 -20.5401 -20.3560 -19.9465
  -19.7676 -19.5967 -19.3781 -19.2636 -19.2572 -19.0487 -18.7564 -18.7508
  -18.5741 -18.4970 -18.3316 -18.2456 -18.0328 -17.9963 -17.8992 -17.4983
  -17.4869 -17.2527 -17.0069 -15.8293 -15.6304 -15.1915 -14.5434 -14.4340
  -14.0087 -13.8102 -13.5704 -13.1074 -12.6689 -12.6431 -12.4624 -12.3707
  -12.0958 -12.0216 -12.0166 -11.8369 -11.7471 -11.5298 -11.4404 -11.3831
  -11.0917 -10.9085 -10.6391 -10.4788 -10.4298 -10.2957  -9.8054  -9.7594
   -9.6251  -9.3488  -9.2327  -9.1624  -8.9871  -8.9161  -8.8226  -8.7599
   -8.6753  -8.6438  -8.5584  -8.4413  -8.4248  -8.3759  -8.3437  -8.2943
   -8.2313  -8.1382  -8.1019  -7.9747  -7.8831  -7.6324  -7.6250  -7.5972
   -7.5642  -7.4460  -7.4217  -7.3752  -7.3344  -7.2853  -7.1846  -7.0842
   -7.0196  -6.8247  -6.7864  -6.7233  -6.6294  -6.4538  -6.2336  -6.2116
   -6.1156  -6.0170  -5.9623  -5.9510  -5.8151  -5.7425  -5.7318  -5.7025
   -5.6868  -5.4644  -5.3824  -5.3697  -5.1803  -5.1695  -5.0453  -4.9214
   -4.8811  -4.8210  -4.7272  -4.5855  -4.4866  -4.3853  -4.0061  -3.8060
   -3.3941  -3.3115  -3.2571  -2.6806  -1.7777  -0.4264  -0.3273   0.3798
    0.6796   0.8309   1.6545   1.8553   1.9261   1.9855   2.0075   2.1650
    2.2211   2.2387   2.3051   2.3749   2.4056   2.4291   2.4941   2.5647
    2.6552   2.8300   2.8552   2.8878   2.9214   3.1349   3.1923

    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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4121 -21.1790 -21.0589 -20.9377 -20.7991 -20.5404 -20.3560 -19.9464
   -19.7682 -19.5968 -19.3779 -19.2638 -19.2567 -19.0487 -18.7566 -18.7507
   -18.5740 -18.4975 -18.3315 -18.2442 -18.0328 -17.9958 -17.8990 -17.4962
   -17.4870 -17.2543 -17.0093 -15.8332 -15.6329 -15.1861 -14.5403 -14.4326
   -14.0102 -13.8092 -13.5721 -13.1088 -12.6689 -12.6394 -12.4610 -12.3707
   -12.0959 -12.0215 -12.0182 -11.8370 -11.7470 -11.5244 -11.4405 -11.3869
   -11.0918 -10.9138 -10.6392 -10.4837 -10.4298 -10.2956  -9.8093  -9.7593
    -9.6214  -9.3486  -9.2375  -9.1622  -8.9862  -8.9147  -8.8230  -8.7599
    -8.6759  -8.6442  -8.5584  -8.4413  -8.4127  -8.3705  -8.3518  -8.2944
    -8.2283  -8.1333  -8.1020  -7.9747  -7.8833  -7.6408  -7.6142  -7.5971
    -7.5600  -7.4459  -7.4274  -7.3843  -7.3348  -7.2853  -7.1846  -7.0840
    -7.0213  -6.8223  -6.7864  -6.7232  -6.6317  -6.4533  -6.2329  -6.2118
    -6.1159  -6.0091  -5.9621  -5.9542  -5.8155  -5.7425  -5.7357  -5.7022
    -5.6796  -5.4644  -5.3843  -5.3699  -5.1804  -5.1706  -5.0454  -4.9212
    -4.8831  -4.8211  -4.7293  -4.5856  -4.4866  -4.3854  -4.0062  -3.8058
    -3.3942  -3.3123  -3.2586  -2.6780  -1.7757  -0.4264  -0.3300   0.3765
     0.6802   0.8329   1.6546   1.8540   1.9261   1.9860   2.0074   2.1645
     2.2208   2.2379   2.3061   2.3752   2.4122   2.4292   2.4935   2.5638
     2.6549   2.8302   2.8551   2.8878   2.9219   3.1346   3.1922

     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   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
     0.0000   0.0000   0.0000   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):

   -21.4121 -21.1790 -21.0589 -20.9377 -20.7992 -20.5404 -20.3560 -19.9463
   -19.7683 -19.5970 -19.3779 -19.2636 -19.2575 -19.0487 -18.7567 -18.7497
   -18.5741 -18.4964 -18.3315 -18.2439 -18.0328 -17.9972 -17.8990 -17.4965
   -17.4870 -17.2553 -17.0078 -15.8313 -15.6362 -15.1878 -14.5373 -14.4332
   -14.0081 -13.8074 -13.5758 -13.1058 -12.6689 -12.6387 -12.4646 -12.3706
   -12.0959 -12.0216 -12.0175 -11.8371 -11.7471 -11.5251 -11.4405 -11.3890
   -11.0916 -10.9105 -10.6393 -10.4843 -10.4297 -10.2956  -9.8088  -9.7593
    -9.6264  -9.3486  -9.2433  -9.1625  -8.9835  -8.9091  -8.8226  -8.7599
    -8.6751  -8.6380  -8.5587  -8.4413  -8.4127  -8.3671  -8.3518  -8.2943
    -8.2311  -8.1398  -8.1020  -7.9748  -7.8831  -7.6417  -7.6185  -7.5973
    -7.5583  -7.4457  -7.4275  -7.3826  -7.3346  -7.2853  -7.1846  -7.0840
```

```
  -7.0183  -6.8245  -6.7865  -6.7232  -6.6288  -6.4535  -6.2301  -6.2118
  -6.1161  -6.0104  -5.9621  -5.9511  -5.8151  -5.7424  -5.7390  -5.7021
  -5.6796  -5.4645  -5.3903  -5.3701  -5.1768  -5.1714  -5.0455  -4.9211
  -4.8832  -4.8211  -4.7291  -4.5850  -4.4866  -4.3855  -4.0062  -3.8058
  -3.3942  -3.3138  -3.2574  -2.6783  -1.7746  -0.4264  -0.3315   0.3771
   0.6811   0.8320   1.6547   1.8562   1.9261   1.9857   2.0074   2.1648
   2.2211   2.2380   2.3037   2.3751   2.4120   2.4294   2.4938   2.5636
   2.6548   2.8300   2.8553   2.8879   2.9217   3.1348   3.1922

   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   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   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):

 -21.4121 -21.1790 -21.0589 -20.9377 -20.7994 -20.5401 -20.3560 -19.9464
 -19.7676 -19.5967 -19.3781 -19.2636 -19.2574 -19.0487 -18.7564 -18.7505
 -18.5741 -18.4966 -18.3316 -18.2455 -18.0328 -17.9968 -17.8992 -17.4984
 -17.4869 -17.2531 -17.0064 -15.8287 -15.6316 -15.1921 -14.5424 -14.4342
 -14.0080 -13.8095 -13.5717 -13.1063 -12.6689 -12.6429 -12.4636 -12.3707
 -12.0958 -12.0216 -12.0164 -11.8369 -11.7471 -11.5300 -11.4404 -11.3839
 -11.0917 -10.9073 -10.6392 -10.4790 -10.4298 -10.2957  -9.8052  -9.7594
  -9.6269  -9.3488  -9.2348  -9.1624  -8.9862  -8.9141  -8.8226  -8.7599
  -8.6750  -8.6415  -8.5584  -8.4413  -8.4248  -8.3746  -8.3437  -8.2943
  -8.2324  -8.1406  -8.1019  -7.9747  -7.8831  -7.6327  -7.6265  -7.5973
  -7.5635  -7.4460  -7.4218  -7.3746  -7.3344  -7.2853  -7.1846  -7.0842
  -7.0185  -6.8254  -6.7865  -6.7232  -6.6283  -6.4538  -6.2327  -6.2117
  -6.1156  -6.0174  -5.9623  -5.9500  -5.8151  -5.7425  -5.7330  -5.7025
  -5.6868  -5.4645  -5.3845  -5.3696  -5.1790  -5.1697  -5.0453  -4.9214
  -4.8812  -4.8210  -4.7272  -4.5853  -4.4866  -4.3853  -4.0061  -3.8060
  -3.3941  -3.3120  -3.2567  -2.6806  -1.7773  -0.4264  -0.3278   0.3800
   0.6798   0.8306   1.6545   1.8561   1.9261   1.9855   2.0075   2.1650
   2.2211   2.2387   2.3042   2.3749   2.4057   2.4292   2.4941   2.5648
   2.6552   2.8300   2.8551   2.8878   2.9213   3.1349   3.1922

   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
```

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     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
     1.0000   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    -1.0375 ev

!    total energy              =    -770.08641375 Ry
     Harris-Foulkes estimate   =    -770.08641397 Ry
     estimated scf accuracy    <       0.00000034 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =   -8860.21560018 Ry
     hartree contribution      =    4482.88599936 Ry
     xc contribution           =    -246.06436670 Ry
     ewald contribution        =    3853.30753252 Ry
     smearing contrib. (-TS)   =       0.00002126 Ry

     total magnetization       =     0.97 Bohr mag/cell
     absolute magnetization    =     1.06 Bohr mag/cell

     convergence has been achieved in  17 iterations

     Forces acting on atoms (Ry/au):


     negative rho (up, down):  7.044E-04 7.241E-04
     atom    1 type  1   force =     0.00005536   -0.00006922    0.00034332
     atom    2 type  1   force =    -0.00004907    0.00005506    0.00008062
     atom    3 type  1   force =     0.00009507   -0.00005391   -0.00018943
     atom    4 type  1   force =     0.00000010   -0.00004233   -0.00025494
     atom    5 type  1   force =    -0.00003489    0.00007292   -0.00034339
     atom    6 type  1   force =     0.00002002   -0.00006244   -0.00025601
     atom    7 type  1   force =    -0.00006524    0.00010472    0.00049960
     atom    8 type  1   force =     0.00004578   -0.00002867   -0.00019197
     atom    9 type  1   force =     0.00009703   -0.00008167    0.00005978
     atom   10 type  1   force =    -0.00012929    0.00007414    0.00045310
     atom   11 type  1   force =     0.00001210    0.00004207   -0.00027372
     atom   12 type  1   force =     0.00009181   -0.00009875   -0.00020551
     atom   13 type  1   force =    -0.00004891   -0.00003484   -0.00035739
     atom   14 type  1   force =     0.00005164    0.00003345   -0.00026575
     atom   15 type  1   force =    -0.00007919    0.00003373    0.00049126
     atom   16 type  1   force =     0.00003254   -0.00005440   -0.00019208
     atom   17 type  1   force =     0.00010105   -0.00002292   -0.00030264
     atom   18 type  1   force =    -0.00009169    0.00003169    0.00011121
     atom   19 type  1   force =     0.00000705    0.00000592   -0.00017945
     atom   20 type  1   force =    -0.00002498   -0.00000511    0.00010998
     atom   21 type  1   force =     0.00007944    0.00000532   -0.00013289
     atom   22 type  1   force =    -0.00006705    0.00000807    0.00013923
     atom   23 type  1   force =     0.00005207    0.00002041    0.00018977
     atom   24 type  1   force =     0.00000319   -0.00002563    0.00010116
     atom   25 type  1   force =    -0.00003531    0.00000943    0.00020572
     atom   26 type  1   force =     0.00005715    0.00000732    0.00011838
     atom   27 type  1   force =     0.00000755    0.00003274    0.00010021
     atom   28 type  1   force =     0.00003319   -0.00004636    0.00019658
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atom   29 type  1   force =    -0.00005903    0.00008021    0.00013919
atom   30 type  1   force =     0.00002835   -0.00009463   -0.00012997
atom   31 type  1   force =     0.00001827    0.00007425    0.00012156
atom   32 type  1   force =    -0.00003985   -0.00005207   -0.00016641
atom   33 type  2   force =    -0.00002568    0.00003688   -0.00007188
atom   34 type  3   force =    -0.00009743    0.00002150    0.00005837
atom   35 type  2   force =    -0.00033333    0.00032418   -0.00007153
atom   36 type  3   force =     0.00005745   -0.00006677    0.00003757
atom   37 type  2   force =     0.00090681    0.00035647   -0.00010089
atom   38 type  3   force =    -0.00000749    0.00023054    0.00003816
atom   39 type  2   force =     0.00007927    0.00003133    0.00002411
atom   40 type  3   force =    -0.00012992    0.00030587    0.00003874
atom   41 type  2   force =     0.00010043   -0.00011688    0.00002465
atom   42 type  3   force =     0.00014159   -0.00000263    0.00003767
atom   43 type  2   force =    -0.00048324    0.00018864   -0.00007123
atom   44 type  2   force =     0.00017473   -0.00093793   -0.00010178
atom   45 type  3   force =    -0.00023459   -0.00012053    0.00003821
atom   46 type  2   force =     0.00004253   -0.00013064    0.00002437
atom   47 type  3   force =    -0.00036975   -0.00001528    0.00003856
atom   48 type  2   force =    -0.00079769    0.00049496   -0.00009908
atom   49 type  3   force =     0.00020404   -0.00012613    0.00007954
atom   50 type  2   force =     0.00025085    0.00013505   -0.00007055
atom   51 type  3   force =     0.00019163    0.00014935    0.00005841
atom   52 type  2   force =     0.00036446    0.00019370   -0.00007057
atom   53 type  3   force =    -0.00003509    0.00035017    0.00008114
atom   54 type  2   force =     0.00001486   -0.00015353   -0.00006200
atom   55 type  3   force =    -0.00013373   -0.00007988    0.00008023
atom   56 type  2   force =    -0.00021482    0.00011156   -0.00005994
atom   57 type  3   force =     0.00032315   -0.00020522    0.00008231
atom   58 type  3   force =    -0.00003458    0.00019787    0.00008043
atom   59 type  2   force =     0.00015360    0.00003356   -0.00006143
atom   60 type  3   force =    -0.00025461   -0.00013642    0.00008132
atom   61 type  2   force =    -0.00000025   -0.00045934   -0.00006981
atom   62 type  3   force =    -0.00002742   -0.00024184    0.00005838
atom   63 type  2   force =     0.00000996   -0.00028711   -0.00007058
The non-local contrib.  to forces
atom    1 type  1   force =    -0.00079690    0.00038390   -0.00615633
atom    2 type  1   force =    -0.00052249    0.00017356    0.00218736
atom    3 type  1   force =     0.00022719    0.00056652    0.00649474
atom    4 type  1   force =    -0.00055345   -0.00069857    0.00315221
atom    5 type  1   force =    -0.00004350   -0.00080660    0.00180930
atom    6 type  1   force =    -0.00020249   -0.00006019    0.00449229
atom    7 type  1   force =    -0.00054303   -0.00065802    0.00008936
atom    8 type  1   force =     0.00031582   -0.00059611   -0.00714340
atom    9 type  1   force =     0.00072545   -0.00042740    0.00349026
atom   10 type  1   force =    -0.00029066    0.00009088    0.01150263
atom   11 type  1   force =     0.00024541    0.00057063    0.00472317
atom   12 type  1   force =    -0.00052272   -0.00031260    0.00637016
atom   13 type  1   force =     0.00062486    0.00036051    0.00366548
atom   14 type  1   force =     0.00017033    0.00018230    0.00517672
atom   15 type  1   force =     0.00001016    0.00070041    0.00206469
atom   16 type  1   force =     0.00093238   -0.00010548   -0.00823169
atom   17 type  1   force =    -0.00031516    0.00009674   -0.00183976
atom   18 type  1   force =    -0.00013296    0.00026456   -0.01413050
atom   19 type  1   force =     0.00081757    0.00035066   -0.01000910
atom   20 type  1   force =     0.00000117    0.00012054    0.00235612
atom   21 type  1   force =     0.00004704    0.00065291   -0.00334310
atom   22 type  1   force =    -0.00120116   -0.00038255   -0.00742802
atom   23 type  1   force =     0.00093919    0.00005547    0.00207589
atom   24 type  1   force =    -0.00011054   -0.00069606   -0.00223325
atom   25 type  1   force =     0.00025022    0.00007052   -0.00424800
atom   26 type  1   force =    -0.00044100    0.00013997    0.00727525
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atom   27 type  1   force =     0.00060592    0.00068527   -0.00045539
atom   28 type  1   force =     0.00027787   -0.00082271    0.00206357
atom   29 type  1   force =    -0.00025501    0.00114238   -0.00456272
atom   30 type  1   force =    -0.00055781   -0.00017444   -0.00541634
atom   31 type  1   force =    -0.00009136   -0.00011665    0.00338761
atom   32 type  1   force =     0.00009144   -0.00056433   -0.01215261
atom   33 type  2   force =    -0.00021269    0.00012248    0.00036574
atom   34 type  3   force =     0.01431292   -0.00832959    0.00039062
atom   35 type  2   force =     0.01889248   -0.07092244    0.00038784
atom   36 type  3   force =     0.03214121   -0.02438228    0.00005690
atom   37 type  2   force =    -0.03132294   -0.01808319    0.00057730
atom   38 type  3   force =    -0.00520328    0.04020089    0.00005583
atom   39 type  2   force =     0.00006712    0.36583599   -0.00018083
atom   40 type  3   force =     0.00494841    0.04011977    0.00006063
atom   41 type  2   force =     0.31726258   -0.18321046   -0.00017777
atom   42 type  3   force =     0.03726615   -0.01561808    0.00005924
atom   43 type  2   force =     0.07083869    0.01918454    0.00038877
atom   44 type  2   force =    -0.00000778    0.03614627    0.00058031
atom   45 type  3   force =    -0.03747211   -0.01561794    0.00005693
atom   46 type  2   force =    -0.31673208   -0.18298856   -0.00018037
atom   47 type  3   force =    -0.03233420   -0.02430151    0.00005893
atom   48 type  2   force =     0.03131350   -0.01808066    0.00056604
atom   49 type  3   force =    -0.02229170    0.01284269    0.00061256
atom   50 type  2   force =    -0.07093138    0.01929056    0.00038088
atom   51 type  3   force =    -0.01443939   -0.00825097    0.00038759
atom   52 type  2   force =    -0.01841210   -0.07102925    0.00037918
atom   53 type  3   force =     0.00014145   -0.03138198    0.00034207
atom   54 type  2   force =    -0.00000845   -0.01299891    0.00037242
atom   55 type  3   force =     0.02232107    0.01298196    0.00061465
atom   56 type  2   force =    -0.01149571    0.00661684    0.00038258
atom   57 type  3   force =    -0.02729103    0.01573659    0.00035244
atom   58 type  3   force =    -0.00014369   -0.02575514    0.00061603
atom   59 type  2   force =     0.01126271    0.00645558    0.00037491
atom   60 type  3   force =     0.02734930    0.01561944    0.00034311
atom   61 type  2   force =     0.05228968    0.05144633    0.00037957
atom   62 type  3   force =    -0.00008641    0.01662094    0.00038695
atom   63 type  2   force =    -0.05215929    0.05180491    0.00037940
The ionic contribution  to forces
atom    1 type  1   force =     0.02199095   -0.01211613   10.34852306
atom    2 type  1   force =    -0.00108949    0.00132069    9.31507494
atom    3 type  1   force =    -0.01438163   -0.01400226    9.15105883
atom    4 type  1   force =    -0.01301535   -0.00508478    8.50232778
atom    5 type  1   force =     0.00128180    0.00427334    9.33871263
atom    6 type  1   force =     0.00360984    0.01242818    9.77987046
atom    7 type  1   force =     0.01552505    0.01641100    9.89224879
atom    8 type  1   force =    -0.03310471    0.01833398   11.07680833
atom    9 type  1   force =     0.01050590   -0.01053579    8.90173580
atom   10 type  1   force =     0.02202740   -0.01891524    7.93748942
atom   11 type  1   force =    -0.00672034    0.01442213    8.21020549
atom   12 type  1   force =     0.00211467    0.02333081    8.94874152
atom   13 type  1   force =     0.00601197    0.00656798    8.90815509
atom   14 type  1   force =    -0.00527417   -0.00956534    9.41076395
atom   15 type  1   force =     0.00467386   -0.01932153    9.66348889
atom   16 type  1   force =    -0.03897516    0.01985398   11.01185147
atom   17 type  1   force =    -0.00658148    0.00843989   11.43698232
atom   18 type  1   force =     0.00595849   -0.01261239   11.50239085
atom   19 type  1   force =    -0.01583312   -0.01330986   10.35609860
atom   20 type  1   force =    -0.00244810    0.00284491   10.53741584
atom   21 type  1   force =     0.00514474   -0.01309721   10.89981967
atom   22 type  1   force =     0.02799935    0.01429587   10.53675004
atom   23 type  1   force =     0.00665699    0.00630039   10.78954382
atom   24 type  1   force =     0.00743773    0.01687212   10.19256835
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atom   25 type  1   force =    -0.00847293    0.00027024   10.23294570
atom   26 type  1   force =    -0.00011916   -0.00210821   10.22512398
atom   27 type  1   force =    -0.01560505   -0.01449832    9.88953688
atom   28 type  1   force =     0.00066842   -0.00811772   10.57935972
atom   29 type  1   force =     0.00167740   -0.02741437   10.29864333
atom   30 type  1   force =     0.02029917   -0.00229087   10.92211725
atom   31 type  1   force =    -0.00106128   -0.00186164   10.60640392
atom   32 type  1   force =     0.00234980    0.01640520   10.59138916
atom   33 type  2   force =    -0.00231259    0.00135095   -7.79620999
atom   34 type  3   force =     0.11905458   -0.06941052  -13.02072238
atom   35 type  2   force =     0.31630932   -0.29762672   -7.79932260
atom   36 type  3   force =     1.30432197    0.65916225  -13.02241020
atom   37 type  2   force =     0.22603800    0.12810923   -7.79618143
atom   38 type  3   force =     1.23048395    0.79664339  -13.01503303
atom   39 type  2   force =     0.00306819    3.31444055   -7.80530975
atom   40 type  3   force =    -1.22553267    0.80061315  -13.00865168
atom   41 type  2   force =     2.87517382   -1.66083359   -7.81056974
atom   42 type  3   force =     0.08068162   -1.46016426  -13.02401725
atom   43 type  2   force =     0.41530814   -0.12519608   -7.80000085
atom   44 type  2   force =     0.00205113   -0.25987897   -7.79751443
atom   45 type  3   force =    -0.07418399   -1.46432040  -13.01707474
atom   46 type  2   force =    -2.86871925   -1.66067685   -7.80592445
atom   47 type  3   force =    -1.30577336    0.66047774  -13.00911210
atom   48 type  2   force =    -0.22562813    0.13026737   -7.78973652
atom   49 type  3   force =    -0.26677507    0.15452003  -13.01012355
atom   50 type  2   force =    -0.41580046   -0.12867665   -7.79591691
atom   51 type  3   force =    -0.12375587   -0.07185655  -13.01372826
atom   52 type  2   force =    -0.32023437   -0.29837942   -7.79392953
atom   53 type  3   force =    -0.00625421    0.35163967  -13.01260543
atom   54 type  2   force =    -0.00255517    0.10713009   -7.79453678
atom   55 type  3   force =     0.26152098    0.15117017  -13.01647981
atom   56 type  2   force =     0.09268180   -0.05291128   -7.79624448
atom   57 type  3   force =     0.30850339   -0.17724619  -13.01334350
atom   58 type  3   force =     0.00017752   -0.30073122  -13.01808518
atom   59 type  2   force =    -0.09402612   -0.05087337   -7.79517656
atom   60 type  3   force =    -0.30827926   -0.16998110  -13.01376299
atom   61 type  2   force =     0.09773825    0.42681921   -7.79390012
atom   62 type  3   force =    -0.00010090    0.14374994  -13.01328546
atom   63 type  2   force =    -0.09643278    0.42515040   -7.79523620
The local contribution  to forces
atom    1 type  1   force =    -0.02115803    0.01167052  -10.34196358
atom    2 type  1   force =     0.00154132   -0.00142980   -9.31711467
atom    3 type  1   force =     0.01422937    0.01339093   -9.15767471
atom    4 type  1   force =     0.01354705    0.00574788   -8.50566183
atom    5 type  1   force =    -0.00129415   -0.00339235   -9.34079788
atom    6 type  1   force =    -0.00340931   -0.01243408   -9.78455414
atom    7 type  1   force =    -0.01506453   -0.01564703   -9.89177419
atom    8 type  1   force =     0.03282375   -0.01776548  -11.06980054
atom    9 type  1   force =    -0.01114960    0.01089245   -8.90509534
atom   10 type  1   force =    -0.02188540    0.01891015   -7.94846198
atom   11 type  1   force =     0.00647213   -0.01493710   -8.21512745
atom   12 type  1   force =    -0.00151768   -0.02310816   -8.95524775
atom   13 type  1   force =    -0.00669488   -0.00694810   -8.91210761
atom   14 type  1   force =     0.00514941    0.00943556   -9.41613921
atom   15 type  1   force =    -0.00477000    0.01867096   -9.66499642
atom   16 type  1   force =     0.03807126   -0.01979065  -11.00375518
atom   17 type  1   force =     0.00699258   -0.00855309  -11.43539167
atom   18 type  1   force =    -0.00592434    0.01238627  -11.48809689
atom   19 type  1   force =     0.01501429    0.01297931  -10.34620857
atom   20 type  1   force =     0.00240844   -0.00295721  -10.53960348
atom   21 type  1   force =    -0.00512038    0.01246367  -10.89655308
atom   22 type  1   force =    -0.02688020   -0.01389612  -10.52912395
```

```
atom   23 type  1   force =    -0.00755496   -0.00632863  -10.79137330
atom   24 type  1   force =    -0.00733999   -0.01619951  -10.19017285
atom   25 type  1   force =     0.00817743   -0.00032569  -10.22843119
atom   26 type  1   force =     0.00060356    0.00198122  -10.23222011
atom   27 type  1   force =     0.01499903    0.01385719   -9.88891818
atom   28 type  1   force =    -0.00092121    0.00890178  -10.58116859
atom   29 type  1   force =    -0.00149493    0.02635904  -10.29388104
atom   30 type  1   force =    -0.01972956    0.00237057  -10.91677449
atom   31 type  1   force =     0.00114974    0.00205372  -10.60961194
atom   32 type  1   force =    -0.00250062   -0.01589478  -10.57934421
atom   33 type  2   force =     0.00238981   -0.00138777    7.79586486
atom   34 type  3   force =    -0.13361050    0.07784460   13.02047168
atom   35 type  2   force =    -0.33429307    0.36438440    7.79895774
atom   36 type  3   force =    -1.33599202   -0.63400205   13.02247120
atom   37 type  2   force =    -0.19622829   -0.11097194    7.79561852
atom   38 type  3   force =    -1.22436537   -0.83665171   13.01509525
atom   39 type  2   force =    -0.00305893   -3.65795916    7.80555840
atom   40 type  3   force =     1.21949768   -0.84046285   13.00870948
atom   41 type  2   force =    -3.17284220    1.83268913    7.81081522
atom   42 type  3   force =    -0.11833005    1.47499931   13.02407597
atom   43 type  2   force =    -0.48212942    0.10738465    7.79963516
atom   44 type  2   force =    -0.00196224    0.22552557    7.79694841
atom   45 type  3   force =     0.11191498    1.47903755   13.01713597
atom   46 type  2   force =     3.16621362    1.83242308    7.80617272
atom   47 type  3   force =     1.33728970   -0.63534513   13.00917164
atom   48 type  2   force =     0.19582609   -0.11303859    7.78918340
atom   49 type  3   force =     0.28911543   -0.16739951   13.00967539
atom   50 type  2   force =     0.48266130    0.11077126    7.79555909
atom   51 type  3   force =     0.13850552    0.08034404   13.01348023
atom   52 type  2   force =     0.33806257    0.36512130    7.79357263
atom   53 type  3   force =     0.00606428   -0.31962376   13.01242548
atom   54 type  2   force =     0.00251759   -0.09485701    7.79419930
atom   55 type  3   force =    -0.28384814   -0.16414297   13.01603062
atom   56 type  2   force =    -0.08202711    0.04675268    7.79589329
atom   57 type  3   force =    -0.28066483    0.16117458   13.01315475
atom   58 type  3   force =    -0.00008246    0.32652980   13.01763479
atom   59 type  2   force =     0.08337340    0.04476814    7.79483607
atom   60 type  3   force =     0.28042383    0.15409505   13.01358209
atom   61 type  2   force =    -0.14663105   -0.47565649    7.79354256
atom   62 type  3   force =     0.00014340   -0.16075912   13.01303794
atom   63 type  2   force =     0.14537212   -0.47410729    7.79488004
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 =     0.00009568   -0.00004070   -0.00004415
     atom   34 type  3   force =     0.00012041   -0.00006864   -0.00000022
     atom   35 type  2   force =    -0.00128253    0.00449845   -0.00004600
     atom   36 type  3   force =    -0.00058968   -0.00082932    0.00000161
     atom   37 type  2   force =     0.00234680    0.00127575   -0.00006672
     atom   38 type  3   force =    -0.00101252   -0.00009939    0.00000173
     atom   39 type  2   force =    -0.00001177   -0.02238915    0.00000485
     atom   40 type  3   force =     0.00101767   -0.00010142    0.00000166
     atom   41 type  2   force =    -0.01960411    0.01130133    0.00000564
     atom   42 type  3   force =     0.00042232    0.00092490    0.00000164
     atom   43 type  2   force =    -0.00452939   -0.00115439   -0.00004580
     atom   44 type  2   force =     0.00007988   -0.00265406   -0.00006751
     atom   45 type  3   force =    -0.00041956    0.00092688    0.00000175
     atom   46 type  2   force =     0.01936202    0.01117542    0.00000508
     atom   47 type  3   force =     0.00059759   -0.00083121    0.00000164
     atom   48 type  2   force =    -0.00226314    0.00132006   -0.00006362
     atom   49 type  3   force =     0.00018507   -0.00010665   -0.00000132
     atom   50 type  2   force =     0.00432296   -0.00121925   -0.00004517
     atom   51 type  3   force =    -0.00012125   -0.00007143   -0.00000008
     atom   52 type  2   force =     0.00096205    0.00449119   -0.00004446
     atom   53 type  3   force =     0.00000050   -0.00028565   -0.00000060
     atom   54 type  2   force =     0.00004760    0.00056701   -0.00004797
     atom   55 type  3   force =    -0.00018358   -0.00010686   -0.00000154
     atom   56 type  2   force =     0.00060150   -0.00033253   -0.00004230
     atom   57 type  3   force =    -0.00024664    0.00014272   -0.00000086
     atom   58 type  3   force =     0.00000140    0.00021159   -0.00000156
     atom   59 type  2   force =    -0.00045859   -0.00030281   -0.00004689
     atom   60 type  3   force =     0.00024649    0.00014224   -0.00000058
     atom   61 type  2   force =    -0.00339934   -0.00308546   -0.00004349
     atom   62 type  3   force =     0.00000133    0.00014076   -0.00000005
     atom   63 type  2   force =     0.00320395   -0.00315200   -0.00004541
     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  2   force =     0.00000000    0.00000000    0.00000000
atom   42 type  3   force =     0.00000000    0.00000000    0.00000000
atom   43 type  2   force =     0.00000000    0.00000000    0.00000000
atom   44 type  2   force =     0.00000000    0.00000000    0.00000000
atom   45 type  3   force =     0.00000000    0.00000000    0.00000000
atom   46 type  2   force =     0.00000000    0.00000000    0.00000000
atom   47 type  3   force =     0.00000000    0.00000000    0.00000000
atom   48 type  2   force =     0.00000000    0.00000000    0.00000000
atom   49 type  3   force =     0.00000000    0.00000000    0.00000000
atom   50 type  2   force =     0.00000000    0.00000000    0.00000000
atom   51 type  3   force =     0.00000000    0.00000000    0.00000000
atom   52 type  2   force =     0.00000000    0.00000000    0.00000000
atom   53 type  3   force =     0.00000000    0.00000000    0.00000000
atom   54 type  2   force =     0.00000000    0.00000000    0.00000000
atom   55 type  3   force =     0.00000000    0.00000000    0.00000000
atom   56 type  2   force =     0.00000000    0.00000000    0.00000000
atom   57 type  3   force =     0.00000000    0.00000000    0.00000000
atom   58 type  3   force =     0.00000000    0.00000000    0.00000000
atom   59 type  2   force =     0.00000000    0.00000000    0.00000000
atom   60 type  3   force =     0.00000000    0.00000000    0.00000000
atom   61 type  2   force =     0.00000000    0.00000000    0.00000000
atom   62 type  3   force =     0.00000000    0.00000000    0.00000000
atom   63 type  2   force =     0.00000000    0.00000000    0.00000000
The SCF correction term to forces
atom    1 type  1   force =     0.00000557    0.00000028   -0.00006223
atom    2 type  1   force =     0.00000783   -0.00000161   -0.00006941
atom    3 type  1   force =     0.00000637   -0.00000131   -0.00007070
atom    4 type  1   force =     0.00000808    0.00000093   -0.00007550
atom    5 type  1   force =     0.00000720    0.00000631   -0.00006986
atom    6 type  1   force =     0.00000822    0.00001144   -0.00006703
atom    7 type  1   force =     0.00000351    0.00000657   -0.00006677
atom    8 type  1   force =    -0.00000284    0.00000673   -0.00005876
atom    9 type  1   force =     0.00000152   -0.00000315   -0.00007334
atom   10 type  1   force =     0.00000560   -0.00000385   -0.00007937
atom   11 type  1   force =     0.00000114   -0.00000581   -0.00007734
atom   12 type  1   force =     0.00000378   -0.00000101   -0.00007185
atom   13 type  1   force =    -0.00000463   -0.00000744   -0.00007276
atom   14 type  1   force =    -0.00000769   -0.00001127   -0.00006960
atom   15 type  1   force =    -0.00000699   -0.00000832   -0.00006831
atom   16 type  1   force =    -0.00000971   -0.00000445   -0.00005908
```

```
     atom   17 type  1   force =    -0.00000865    0.00000134   -0.00005593
     atom   18 type  1   force =    -0.00000664    0.00000104   -0.00005465
     atom   19 type  1   force =    -0.00000546   -0.00000640   -0.00006280
     atom   20 type  1   force =    -0.00000026   -0.00000555   -0.00006091
     atom   21 type  1   force =    -0.00000573   -0.00000625   -0.00005878
     atom   22 type  1   force =     0.00000120   -0.00000134   -0.00006126
     atom   23 type  1   force =    -0.00000291    0.00000097   -0.00005905
     atom   24 type  1   force =     0.00000223    0.00000561   -0.00006350
     atom   25 type  1   force =    -0.00000379    0.00000216   -0.00006319
     atom   26 type  1   force =    -0.00000001    0.00000213   -0.00006314
     atom   27 type  1   force =    -0.00000611   -0.00000360   -0.00006550
     atom   28 type  1   force =    -0.00000567    0.00000009   -0.00006053
     atom   29 type  1   force =    -0.00000025    0.00000095   -0.00006278
     atom   30 type  1   force =     0.00000278    0.00000791   -0.00005879
     atom   31 type  1   force =     0.00000741    0.00000661   -0.00006043
     atom   32 type  1   force =     0.00000576    0.00000964   -0.00006116
     atom   33 type  2   force =     0.00000034   -0.00000029   -0.00005075
     atom   34 type  3   force =     0.00001139   -0.00000655   -0.00008374
     atom   35 type  2   force =     0.00002670   -0.00000171   -0.00005092
     atom   36 type  3   force =     0.00016219   -0.00000758   -0.00008434
     atom   37 type  2   force =     0.00005948    0.00003441   -0.00005096
     atom   38 type  3   force =     0.00007596    0.00014516   -0.00008403
     atom   39 type  2   force =     0.00000090    0.00011089   -0.00005097
     atom   40 type  3   force =    -0.00007478    0.00014502   -0.00008376
     atom   41 type  2   force =     0.00009658   -0.00005549   -0.00005110
     atom   42 type  3   force =     0.00008778   -0.00013670   -0.00008433
     atom   43 type  2   force =     0.00001496   -0.00002229   -0.00005091
     atom   44 type  2   force =    -0.00000002   -0.00006893   -0.00005097
     atom   45 type  3   force =    -0.00008767   -0.00013883   -0.00008411
     atom   46 type  2   force =    -0.00009554   -0.00005594   -0.00005101
     atom   47 type  3   force =    -0.00016324   -0.00000738   -0.00008395
     atom   48 type  2   force =    -0.00005978    0.00003458   -0.00005078
     atom   49 type  3   force =    -0.00004345    0.00002510   -0.00008594
     atom   50 type  2   force =    -0.00001533   -0.00002307   -0.00005085
     atom   51 type  3   force =    -0.00001115   -0.00000795   -0.00008348
     atom   52 type  2   force =    -0.00002745   -0.00000233   -0.00005080
     atom   53 type  3   force =    -0.00000088    0.00000968   -0.00008278
     atom   54 type  2   force =    -0.00000047    0.00001309   -0.00005139
     atom   55 type  3   force =     0.00004218    0.00002561   -0.00008610
     atom   56 type  2   force =     0.00001093   -0.00000636   -0.00005144
     atom   57 type  3   force =     0.00000849   -0.00000512   -0.00008293
     atom   58 type  3   force =    -0.00000110   -0.00004935   -0.00008605
     atom   59 type  2   force =    -0.00001156   -0.00000618   -0.00005137
     atom   60 type  3   force =    -0.00000873   -0.00000425   -0.00008271
     atom   61 type  2   force =    -0.00001156    0.00002488   -0.00005073
     atom   62 type  3   force =     0.00000139    0.00001345   -0.00008342
     atom   63 type  2   force =     0.00001220    0.00002465   -0.00005082

     Total force =     0.002681     Total SCF correction =     0.000715
     SCF correction compared to forces is large: reduce conv_thr to get better values


     entering subroutine stress ...


     negative rho (up, down):  7.044E-04 7.241E-04
          total   stress  (Ry/bohr**3)                   (kbar)     P=   73.39
  0.00075101   0.00000107   0.00000000        110.48      0.16      0.00
  0.00000107   0.00075159  -0.00000000          0.16    110.56     -0.00
  0.00000000  -0.00000000  -0.00000592          0.00     -0.00     -0.87

     kinetic stress (kbar)   2885.95      0.03      0.00
```

```
                            0.03   2885.95     -0.00
                            0.00     -0.00   3228.46

     local   stress (kbar) -89169.05     -4.78     -0.75
                           -4.78 -89171.69      0.57
                           -0.75      0.57  89466.05

     nonloc. stress (kbar)    481.49     -0.03     -0.00
                           -0.03    481.47      0.00
                           -0.00      0.00    440.02

     hartree stress (kbar)  43040.30      1.74      0.36
                            1.74  43041.25     -0.28
                            0.36     -0.28 -42602.34

     exc-cor stress (kbar)   -550.15      0.00     -0.00
                            0.00   -550.15      0.00
                           -0.00      0.00   -578.29

     corecor stress (kbar)   -162.85     -0.00      0.00
                           -0.00   -162.85     -0.00
                            0.00     -0.00   -156.38

     ewald   stress (kbar)  43584.79      3.19      0.38
                            3.19  43586.58     -0.29
                            0.38     -0.29 -49798.40

     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     :   1107.80s CPU   1119.65s WALL (       1 calls)
     electrons    :  36688.69s CPU  36944.68s WALL (       1 calls)
     forces       :    573.81s CPU    575.96s WALL (       1 calls)
     stress       :    824.78s CPU    828.80s WALL (       1 calls)

     Called by init_run:
     wfcinit      :   1072.22s CPU   1083.45s WALL (       1 calls)
     potinit      :      4.34s CPU      4.50s WALL (       1 calls)

     Called by electrons:
     c_bands      :  32647.33s CPU  32884.92s WALL (      17 calls)
     sum_band     :   3693.49s CPU   3709.38s WALL (      17 calls)
     v_of_rho     :     56.56s CPU     57.68s WALL (      18 calls)
     v_h          :      1.50s CPU      1.52s WALL (      18 calls)
     v_xc         :     61.08s CPU     62.31s WALL (      20 calls)
```

```
     newd         :    299.38s CPU    300.33s WALL (      18 calls)
     mix_rho      :      6.84s CPU      7.04s WALL (      17 calls)

     Called by c_bands:
     init_us_2    :     59.68s CPU     61.46s WALL (    1480 calls)
     cegterg      :  32466.32s CPU  32696.40s WALL (     680 calls)

     Called by sum_band:
     sum_band:bec :      2.39s CPU      2.41s WALL (     680 calls)
     addusdens    :    344.82s CPU    345.86s WALL (      17 calls)

     Called by *egterg:
     h_psi        :  15959.26s CPU  16025.58s WALL (    4184 calls)
     s_psi        :   5308.57s CPU   5322.12s WALL (    4184 calls)
     g_psi        :     14.24s CPU     14.30s WALL (    3464 calls)
     cdiaghg      :   2239.07s CPU   2245.73s WALL (    4144 calls)
     cegterg:over :   4220.19s CPU   4232.15s WALL (    3464 calls)
     cegterg:upda :   2683.95s CPU   2700.18s WALL (    3464 calls)
     cegterg:last :   1593.00s CPU   1599.26s WALL (     680 calls)
     cdiaghg:chol :    155.36s CPU    155.92s WALL (    4144 calls)
     cdiaghg:inve :     17.94s CPU     18.15s WALL (    4144 calls)
     cdiaghg:para :    731.86s CPU    733.70s WALL (    8288 calls)

     Called by h_psi:
     h_psi:vloc   :   5409.32s CPU   5443.32s WALL (    4184 calls)
     h_psi:vnl    :  10530.81s CPU  10561.51s WALL (    4184 calls)
     add_vuspsi   :   5308.35s CPU   5322.20s WALL (    4184 calls)

     General routines
     calbec       :   7488.86s CPU   7511.42s WALL (    4944 calls)
     fft          :     48.43s CPU     48.90s WALL (     592 calls)
     ffts         :      1.02s CPU      1.05s WALL (      70 calls)
     fftw         :   5036.48s CPU   5064.27s WALL (  629478 calls)
     interpolate  :      5.76s CPU      5.88s WALL (      70 calls)
     davcio       :      0.11s CPU      1.89s WALL (      40 calls)

     Parallel routines
     fft_scatter  :   1927.66s CPU   1943.98s WALL (  630140 calls)

     PWSCF        :    10h53m CPU       10h57m WALL


   This run was terminated on:   0: 5:59  15Feb2021

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