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Program PWSCF v.6.3 starts on 31Aug2019 at 23:50:13

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
    "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
    "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
     URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Parallel version (MPI), running on     4 processors

MPI processes distributed on     1 nodes
R & G space division:  proc/nbgrp/npool/nimage =       4
Waiting for input...
Reading input from standard input
Message from routine read_cards :
DEPRECATED: no units specified in ATOMIC_POSITIONS card
Message from routine read_cards :
ATOMIC_POSITIONS: units set to alat

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

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


Parallelization info
--------------------
sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
Min         124     124     37                 1845     1845     309
Max         125     125     38                 1849     1849     312
Sum         499     499    151                 7391     7391    1243



bravais-lattice index     =            2
lattice parameter (alat)  =       9.5000  a.u.
unit-cell volume          =     214.3438 (a.u.)^3
number of atoms/cell      =            2
number of atomic types    =            1
number of electrons       =         8.00
number of Kohn-Sham states=            4
kinetic-energy cutoff     =      40.0000  Ry
charge density cutoff     =     160.0000  Ry
convergence threshold     =      1.0E-08
mixing beta               =       0.7000
number of iterations used =            8  plain     mixing
Exchange-correlation      = SLA PZ NOGX NOGC ( 1  1  0  0 0 0)
nstep                     =           50


celldm(1)=   9.500000  celldm(2)=   0.000000  celldm(3)=   0.000000
celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

crystal axes: (cart. coord. in units of alat)
          a(1) = (  -0.500000   0.000000   0.500000 )
          a(2) = (   0.000000   0.500000   0.500000 )
          a(3) = (  -0.500000   0.500000   0.000000 )
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      reciprocal axes: (cart. coord. in units 2 pi/alat)
                b(1) = ( -1.000000 -1.000000  1.000000 )
                b(2) = (  1.000000  1.000000  1.000000 )
                b(3) = ( -1.000000  1.000000 -1.000000 )


      PseudoPot. # 1 for Si read from file:
      /qe-6.3/pseudo/Si.pz-vbc.UPF
      MD5 check sum: a974d1b8727157e37210f3f86afb6210
      Pseudo is Norm-conserving, Zval =  4.0
      Generated by new atomic code, or converted to UPF format
      Using radial grid of  431 points,  2 beta functions with:
                 l(1) =   0
                 l(2) =   1

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

      No symmetry found



    Cartesian axes

      site n.     atom                  positions (alat units)
          1           Si  tau(   1) = (   0.0000000   0.0000000   0.0000000  )
          2           Si  tau(   2) = (   0.2600000   0.2500000   0.2700000  )

      number of k points=    36
                        cart. coord. in units 2pi/alat
         k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
         k(    2) = (  -0.2500000   0.2500000  -0.2500000), wk =   0.0625000
         k(    3) = (   0.5000000  -0.5000000   0.5000000), wk =   0.0312500
         k(    4) = (   0.0000000   0.5000000   0.0000000), wk =   0.0625000
         k(    5) = (   0.7500000  -0.2500000   0.7500000), wk =   0.0625000
         k(    6) = (   0.5000000   0.0000000   0.5000000), wk =   0.0625000
         k(    7) = (   0.0000000  -1.0000000   0.0000000), wk =   0.0312500
         k(    8) = (  -0.5000000  -1.0000000   0.0000000), wk =   0.0625000
         k(    9) = (   0.2500000  -0.2500000  -0.2500000), wk =   0.0625000
         k(   10) = (   0.2500000   0.2500000   0.2500000), wk =   0.0625000
         k(   11) = (  -0.2500000  -0.2500000   0.2500000), wk =   0.0625000
         k(   12) = (  -0.5000000   0.5000000   0.5000000), wk =   0.0312500
         k(   13) = (  -0.5000000  -0.5000000  -0.5000000), wk =   0.0312500
         k(   14) = (   0.5000000   0.5000000  -0.5000000), wk =   0.0312500
         k(   15) = (   0.5000000   0.0000000   0.0000000), wk =   0.0625000
         k(   16) = (   0.0000000   0.0000000   0.5000000), wk =   0.0625000
         k(   17) = (  -0.7500000   0.2500000   0.7500000), wk =   0.0625000
         k(   18) = (  -0.7500000  -0.2500000  -0.7500000), wk =   0.0625000
         k(   19) = (   0.7500000   0.2500000  -0.7500000), wk =   0.0625000
         k(   20) = (  -0.2500000   0.7500000  -0.7500000), wk =   0.0625000
         k(   21) = (   0.2500000  -0.7500000  -0.7500000), wk =   0.0625000
         k(   22) = (  -0.2500000  -0.7500000   0.7500000), wk =   0.0625000
         k(   23) = (   0.2500000   0.7500000   0.7500000), wk =   0.0625000
         k(   24) = (  -0.7500000   0.7500000  -0.2500000), wk =   0.0625000
         k(   25) = (  -0.7500000  -0.7500000   0.2500000), wk =   0.0625000
         k(   26) = (   0.7500000   0.7500000   0.2500000), wk =   0.0625000
         k(   27) = (   0.7500000  -0.7500000  -0.2500000), wk =   0.0625000
         k(   28) = (  -0.5000000   0.0000000   0.5000000), wk =   0.0625000
         k(   29) = (   0.0000000   0.5000000  -0.5000000), wk =   0.0625000
         k(   30) = (   0.0000000  -0.5000000  -0.5000000), wk =   0.0625000
         k(   31) = (  -0.5000000   0.5000000   0.0000000), wk =   0.0625000
         k(   32) = (  -0.5000000  -0.5000000   0.0000000), wk =   0.0625000
         k(   33) = (  -1.0000000   0.0000000   0.0000000), wk =   0.0312500
         k(   34) = (   0.0000000   0.0000000  -1.0000000), wk =   0.0312500
         k(   35) = (  -1.0000000  -0.5000000   0.0000000), wk =   0.0625000
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     k(   36) = (   0.0000000   1.0000000  -0.5000000), wk =   0.0625000

   Dense  grid:     7391 G-vectors     FFT dimensions: (  27,  27,  27)

   Estimated max dynamical RAM per process >       2.05 MB

   Estimated total dynamical RAM >       8.21 MB

   Initial potential from superposition of free atoms

   starting charge    7.99901, renormalised to    8.00000
   Starting wfcs are    8 randomized atomic wfcs

   total cpu time spent up to now is        0.4 secs

   Self-consistent Calculation

   iteration #  1     ecut=    40.00 Ry     beta= 0.70
   Davidson diagonalization with overlap
   ethr =  1.00E-02,  avg # of iterations =  2.0

   total cpu time spent up to now is        0.8 secs

   total energy              =     -15.77016731 Ry
   Harris-Foulkes estimate   =     -15.81014258 Ry
   estimated scf accuracy    <       0.09862980 Ry

   iteration #  2     ecut=    40.00 Ry     beta= 0.70
   Davidson diagonalization with overlap
   ethr =  1.23E-03,  avg # of iterations =  2.0

   total cpu time spent up to now is        1.1 secs

   total energy              =     -15.77950523 Ry
   Harris-Foulkes estimate   =     -15.77965025 Ry
   estimated scf accuracy    <       0.00223170 Ry

   iteration #  3     ecut=    40.00 Ry     beta= 0.70
   Davidson diagonalization with overlap
   ethr =  2.79E-05,  avg # of iterations =  2.2

   total cpu time spent up to now is        1.4 secs

   total energy              =     -15.77993811 Ry
   Harris-Foulkes estimate   =     -15.77994333 Ry
   estimated scf accuracy    <       0.00008504 Ry

   iteration #  4     ecut=    40.00 Ry     beta= 0.70
   Davidson diagonalization with overlap
   ethr =  1.06E-06,  avg # of iterations =  2.4

   total cpu time spent up to now is        1.7 secs

   total energy              =     -15.77996070 Ry
   Harris-Foulkes estimate   =     -15.77996110 Ry
   estimated scf accuracy    <       0.00000154 Ry

   iteration #  5     ecut=    40.00 Ry     beta= 0.70
   Davidson diagonalization with overlap
   ethr =  1.93E-08,  avg # of iterations =  2.7

   total cpu time spent up to now is        2.0 secs

   total energy              =     -15.77996139 Ry
   Harris-Foulkes estimate   =     -15.77996138 Ry
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     estimated scf accuracy    <       0.00000002 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.06E-10,  avg # of iterations =  2.8

     total cpu time spent up to now is        2.3 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -4.9497   8.1520   8.7654   9.3496

          k =-0.2500 0.2500-0.2500 (   917 PWs)   bands (ev):

    -3.9575   4.0538   7.7289   8.1810

          k = 0.5000-0.5000 0.5000 (   912 PWs)   bands (ev):

    -1.7700   0.1625   7.2048   7.6606

          k = 0.0000 0.5000 0.0000 (   902 PWs)   bands (ev):

    -3.6393   5.1100   6.3831   6.5169

          k = 0.7500-0.2500 0.7500 (   917 PWs)   bands (ev):

    -1.4815   1.2928   4.6651   6.0065

          k = 0.5000 0.0000 0.5000 (   907 PWs)   bands (ev):

    -2.4347   2.7331   4.0229   7.1438

          k = 0.0000-1.0000 0.0000 (   934 PWs)   bands (ev):

     0.0591   0.1103   5.2297   5.2711

          k =-0.5000-1.0000 0.0000 (   932 PWs)   bands (ev):

     0.1650   0.6445   3.6219   3.9250

          k = 0.2500-0.2500-0.2500 (   917 PWs)   bands (ev):

    -3.9693   4.1908   7.5289   8.2379

          k = 0.2500 0.2500 0.2500 (   917 PWs)   bands (ev):

    -3.9928   4.4778   7.4320   7.9544

          k =-0.2500-0.2500 0.2500 (   917 PWs)   bands (ev):

    -3.9812   4.3357   7.4047   8.1834

          k =-0.5000 0.5000 0.5000 (   912 PWs)   bands (ev):

    -1.9021   0.3925   7.0273   7.7456

          k =-0.5000-0.5000-0.5000 (   912 PWs)   bands (ev):

    -2.1108   0.8032   6.9818   7.5026

          k = 0.5000 0.5000-0.5000 (   912 PWs)   bands (ev):

    -2.0144   0.6063   6.9337   7.7095
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```
      k = 0.5000 0.0000 0.0000 (   902 PWs)   bands (ev):

-3.6396   5.1356   6.3190   6.5468

      k = 0.0000 0.0000 0.5000 (   902 PWs)   bands (ev):

-3.6406   5.2260   6.1540   6.5957

      k =-0.7500 0.2500 0.7500 (   917 PWs)   bands (ev):

-1.5520   1.5000   4.4591   6.0814

      k =-0.7500-0.2500-0.7500 (   917 PWs)   bands (ev):

-1.6752   1.9361   4.1205   6.0534

      k = 0.7500 0.2500-0.7500 (   917 PWs)   bands (ev):

-1.6168   1.7159   4.2767   6.0963

      k =-0.2500 0.7500-0.7500 (   917 PWs)   bands (ev):

-1.4893   1.3394   4.4949   6.1377

      k = 0.2500-0.7500-0.7500 (   917 PWs)   bands (ev):

-1.5481   1.4603   4.6383   5.9284

      k =-0.2500-0.7500 0.7500 (   917 PWs)   bands (ev):

-1.6230   1.7750   4.1320   6.1701

      k = 0.2500 0.7500 0.7500 (   917 PWs)   bands (ev):

-1.6722   1.8828   4.2755   5.9571

      k =-0.7500 0.7500-0.2500 (   917 PWs)   bands (ev):

-1.5004   1.3984   4.3458   6.2215

      k =-0.7500-0.7500 0.2500 (   917 PWs)   bands (ev):

-1.6128   1.6371   4.6375   5.7894

      k = 0.7500 0.7500 0.2500 (   917 PWs)   bands (ev):

-1.6718   1.8433   4.4571   5.8034

      k = 0.7500-0.7500-0.2500 (   917 PWs)   bands (ev):

-1.5689   1.6172   4.1663   6.2385

      k =-0.5000 0.0000 0.5000 (   907 PWs)   bands (ev):

-2.4353   2.7708   3.9608   7.1952

      k = 0.0000 0.5000-0.5000 (   907 PWs)   bands (ev):

-2.4060   2.6033   4.0143   7.3087

      k = 0.0000-0.5000-0.5000 (   907 PWs)   bands (ev):

-2.4631   2.9042   3.9788   7.0088
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          k =-0.5000 0.5000 0.0000 (   907 PWs)   bands (ev):

    -2.3757   2.4558   4.0468   7.4298

          k =-0.5000-0.5000 0.0000 (   907 PWs)   bands (ev):

    -2.4908   3.0672   3.9718   6.8223

          k =-1.0000 0.0000 0.0000 (   934 PWs)   bands (ev):

    -0.0564   0.2347   5.1531   5.3300

          k = 0.0000 0.0000-1.0000 (   934 PWs)   bands (ev):

    -0.1867   0.3925   5.0347   5.3948

          k =-1.0000-0.5000 0.0000 (   932 PWs)   bands (ev):

     0.1407   0.6767   3.5995   3.9382

          k = 0.0000 1.0000-0.5000 (   932 PWs)   bands (ev):

     0.2712   0.5152   3.7112   3.8634

     highest occupied level (ev):     9.3496

!    total energy              =     -15.77996140 Ry
     Harris-Foulkes estimate   =     -15.77996140 Ry
     estimated scf accuracy    <          4.4E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       6.48775106 Ry
     hartree contribution      =       0.93609525 Ry
     xc contribution           =      -5.07289652 Ry
     ewald contribution        =     -18.13091120 Ry

     convergence has been achieved in   6 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.04142378   -0.01251719    0.08126431
     atom    2 type  1   force =    -0.04142378    0.01251719   -0.08126431

     Total force =     0.130204     Total SCF correction =     0.000002


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=  335.53
   0.00229929  -0.00070229   0.00006140        338.24   -103.31      9.03
  -0.00070229   0.00232826  -0.00035237       -103.31    342.50    -51.83
   0.00006140  -0.00035237   0.00221506          9.03    -51.83    325.85


     BFGS Geometry Optimization

     number of scf cycles    =   1
     number of bfgs steps    =   0

     enthalpy new            =     -15.7799614042 Ry

     new trust radius        =       0.1798782374 bohr
     new conv_thr            =       0.0000000100 Ry
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      new unit-cell volume =    253.05286 a.u.^3 (    37.49856 Ang^3 )
      density =      2.48745 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.527973628   0.004374014   0.526920830
   -0.008011109   0.524698739   0.523283735
   -0.537519689   0.537881894  -0.005172047

 ATOMIC_POSITIONS (alat)
 Si       0.004647307  -0.001546203   0.009046137
 Si       0.266323212   0.259154525   0.274102350



      Writing output data file Si_relax.save/
      NEW-OLD atomic charge density approx. for the potential
      extrapolated charge    9.22360, renormalised to    8.00000

      total cpu time spent up to now is        2.6 secs

      Self-consistent Calculation

      iteration #  1     ecut=    40.00 Ry     beta= 0.70
      Davidson diagonalization with overlap
      ethr =  1.00E-06,  avg # of iterations =  6.3

      total cpu time spent up to now is        3.2 secs

      total energy              =     -15.82102300 Ry
      Harris-Foulkes estimate   =     -16.49520503 Ry
      estimated scf accuracy    <       0.00676587 Ry

      iteration #  2     ecut=    40.00 Ry     beta= 0.70
      Davidson diagonalization with overlap
      ethr =  8.46E-05,  avg # of iterations =  3.1

      total cpu time spent up to now is        3.6 secs

      total energy              =     -15.83550931 Ry
      Harris-Foulkes estimate   =     -15.83789921 Ry
      estimated scf accuracy    <       0.00733480 Ry

      iteration #  3     ecut=    40.00 Ry     beta= 0.70
      Davidson diagonalization with overlap
      ethr =  8.46E-05,  avg # of iterations =  1.0

      total cpu time spent up to now is        3.8 secs

      total energy              =     -15.83452782 Ry
      Harris-Foulkes estimate   =     -15.83569864 Ry
      estimated scf accuracy    <       0.00218383 Ry

      iteration #  4     ecut=    40.00 Ry     beta= 0.70
      Davidson diagonalization with overlap
      ethr =  2.73E-05,  avg # of iterations =  2.0

      total cpu time spent up to now is        4.1 secs

      total energy              =     -15.83484518 Ry
      Harris-Foulkes estimate   =     -15.83485087 Ry
      estimated scf accuracy    <       0.00001194 Ry

      iteration #  5     ecut=    40.00 Ry     beta= 0.70
      Davidson diagonalization with overlap
      ethr =  1.49E-07,  avg # of iterations =  2.4
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     total cpu time spent up to now is        4.4 secs

     total energy              =     -15.83485163 Ry
     Harris-Foulkes estimate   =     -15.83485168 Ry
     estimated scf accuracy    <       0.00000037 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  4.66E-09,  avg # of iterations =  2.0

     total cpu time spent up to now is        4.7 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.6172   6.6559   6.7422   6.9460

          k =-0.2322 0.2304-0.2346 (   917 PWs)   bands (ev):

    -4.8087   2.5822   6.0163   6.1681

          k = 0.4645-0.4609 0.4692 (   912 PWs)   bands (ev):

    -3.2677  -0.5138   5.6065   5.7217

          k = 0.0078 0.4727 0.0039 (   902 PWs)   bands (ev):

    -4.4730   3.2936   4.7483   4.7771

          k = 0.7046-0.2187 0.7078 (   917 PWs)   bands (ev):

    -2.8350   0.2940   3.0496   4.4591

          k = 0.4723 0.0118 0.4732 (   907 PWs)   bands (ev):

    -3.4567   1.2315   2.7434   5.3504

          k =-0.0157-0.9453-0.0079 (   934 PWs)   bands (ev):

    -1.2795  -1.1748   3.7403   3.7614

          k =-0.4886-0.9532-0.0072 (   932 PWs)   bands (ev):

    -1.1439  -0.8902   2.5768   2.6409

          k = 0.2329-0.2344-0.2392 (   917 PWs)   bands (ev):

    -4.7757   2.6561   5.9504   6.0947

          k = 0.2401 0.2422 0.2386 (   917 PWs)   bands (ev):

    -4.7359   2.8986   5.8203   5.8842

          k =-0.2407-0.2383 0.2352 (   917 PWs)   bands (ev):

    -4.7522   2.7650   5.8511   6.0290

          k =-0.4657 0.4688 0.4784 (   912 PWs)   bands (ev):

    -3.1181  -0.5707   5.5262   5.6230

          k =-0.4802-0.4844-0.4771 (   912 PWs)   bands (ev):
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-2.9696  -0.4732   5.3623   5.4081

      k = 0.4814 0.4766-0.4705 (   912 PWs)   bands (ev):

-3.0217  -0.5509   5.4100   5.5481

      k = 0.4730 0.0078-0.0006 (   902 PWs)   bands (ev):

-4.4720   3.2930   4.6618   4.8610

      k =-0.0006 0.0039 0.4738 (   902 PWs)   bands (ev):

-4.4694   3.2958   4.5542   4.9546

      k =-0.7064 0.2305 0.7136 (   917 PWs)   bands (ev):

-2.7378   0.2275   2.9936   4.4685

      k =-0.7124-0.2540-0.7117 (   917 PWs)   bands (ev):

-2.6237   0.1933   3.0107   4.3868

      k = 0.7143 0.2422-0.7097 (   917 PWs)   bands (ev):

-2.6698   0.2014   2.9748   4.4443

      k =-0.2238 0.6992-0.7045 (   917 PWs)   bands (ev):

-2.8262   0.2660   3.0050   4.5568

      k = 0.2256-0.7110-0.7169 (   917 PWs)   bands (ev):

-2.7449   0.2554   3.0412   4.3657

      k =-0.2492-0.7070 0.7051 (   917 PWs)   bands (ev):

-2.6532   0.1324   3.0246   4.4996

      k = 0.2473 0.7188 0.7163 (   917 PWs)   bands (ev):

-2.6377   0.2627   2.9635   4.3256

      k =-0.6974 0.6953-0.2301 (   917 PWs)   bands (ev):

-2.8134   0.2217   3.0033   4.6311

      k =-0.7215-0.7188 0.2319 (   917 PWs)   bands (ev):

-2.6856   0.2765   3.0346   4.2460

      k = 0.7209 0.7227 0.2419 (   917 PWs)   bands (ev):

-2.6461   0.3103   2.9752   4.2301

      k = 0.6980-0.6992-0.2437 (   917 PWs)   bands (ev):

-2.7080   0.1145   3.0417   4.5977

      k =-0.4736-0.0039 0.4744 (   907 PWs)   bands (ev):

-3.4202   1.1448   2.7447   5.4165

      k = 0.0085 0.4687-0.4699 (   907 PWs)   bands (ev):

-3.4856   1.2016   2.7265   5.4429
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          k =-0.0072-0.4766-0.4777 (   907 PWs)   bands (ev):

    -3.3924   1.1803   2.7640   5.3186

          k =-0.4651 0.4648 0.0046 (   907 PWs)   bands (ev):

    -3.5308   1.2104   2.7146   5.5037

          k =-0.4808-0.4805-0.0033 (   907 PWs)   bands (ev):

    -3.3500   1.1874   2.7865   5.2372

          k =-0.9459-0.0157 0.0012 (   934 PWs)   bands (ev):

    -1.2701  -1.1794   3.6423   3.8525

          k = 0.0012-0.0079-0.9476 (   934 PWs)   bands (ev):

    -1.3028  -1.1300   3.5195   3.9510

          k =-0.9537-0.4883-0.0027 (   932 PWs)   bands (ev):

    -1.1505  -0.8822   2.5806   2.6384

          k = 0.0163 0.9414-0.4659 (   932 PWs)   bands (ev):

    -1.0963  -0.9435   2.5858   2.6302

     highest occupied level (ev):     6.9460

!    total energy              =     -15.83485167 Ry
     Harris-Foulkes estimate   =     -15.83485167 Ry
     estimated scf accuracy    <          6.8E-09 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       5.14583436 Ry
     hartree contribution      =       1.06476675 Ry
     xc contribution           =      -4.87872002 Ry
     ewald contribution        =     -17.16673276 Ry

     convergence has been achieved in   6 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =    -0.00293467    0.00875997   -0.00537003
     atom    2 type  1   force =     0.00293467   -0.00875997    0.00537003

     Total force =     0.015112     Total SCF correction =     0.000037


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   58.75
   0.00039742   0.00020998  -0.00006483         58.46     30.89     -9.54
   0.00020998   0.00039288   0.00010464         30.89     57.80     15.39
  -0.00006483   0.00010464   0.00040780         -9.54     15.39     59.99


     number of scf cycles    =   2
     number of bfgs steps    =   1

     enthalpy old            =     -15.7799614042 Ry
     enthalpy new            =     -15.8348516689 Ry
```

```
     CASE: enthalpy_new < enthalpy_old

     new trust radius        =       0.0492639697 bohr
     new conv_thr            =       0.0000000009 Ry

     new unit-cell volume =    263.80400 a.u.^3 (    39.09172 Ang^3 )
     density =      2.38608 g/cm^3

CELL_PARAMETERS (alat=  9.50000000)
  -0.536284820   0.002803835   0.535329325
  -0.005873519   0.533533631   0.532253629
  -0.541727286   0.542031341  -0.002647516

ATOMIC_POSITIONS (alat)
Si       0.004415131  -0.000354305   0.008731179
Si       0.271395521   0.264068841   0.278688918



     Writing output data file Si_relax.save/
     NEW-OLD atomic charge density approx. for the potential
     extrapolated charge    8.32599, renormalised to    8.00000

     total cpu time spent up to now is        5.0 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  4.4

     total cpu time spent up to now is        5.6 secs

     total energy              =     -15.83700437 Ry
     Harris-Foulkes estimate   =     -16.00622602 Ry
     estimated scf accuracy    <       0.00057613 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  7.20E-06,  avg # of iterations =  3.1

     total cpu time spent up to now is        5.9 secs

     total energy              =     -15.83817323 Ry
     Harris-Foulkes estimate   =     -15.83835297 Ry
     estimated scf accuracy    <       0.00053833 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  6.73E-06,  avg # of iterations =  1.0

     total cpu time spent up to now is        6.1 secs

     total energy              =     -15.83810652 Ry
     Harris-Foulkes estimate   =     -15.83818846 Ry
     estimated scf accuracy    <       0.00014812 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.85E-06,  avg # of iterations =  2.0

     total cpu time spent up to now is        6.4 secs

     total energy              =     -15.83813211 Ry
```

```
     Harris-Foulkes estimate   =     -15.83813512 Ry
     estimated scf accuracy    <       0.00000797 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  9.96E-08,  avg # of iterations =  1.5

     total cpu time spent up to now is        6.6 secs

     total energy              =     -15.83813194 Ry
     Harris-Foulkes estimate   =     -15.83813271 Ry
     estimated scf accuracy    <       0.00000150 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.87E-08,  avg # of iterations =  2.0

     total cpu time spent up to now is        6.9 secs

     total energy              =     -15.83813214 Ry
     Harris-Foulkes estimate   =     -15.83813214 Ry
     estimated scf accuracy    <          1.1E-09 Ry

     iteration #  7     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.36E-11,  avg # of iterations =  3.6

     total cpu time spent up to now is        7.3 secs

     total energy              =     -15.83813214 Ry
     Harris-Foulkes estimate   =     -15.83813214 Ry
     estimated scf accuracy    <          2.2E-09 Ry

     iteration #  8     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.36E-11,  avg # of iterations =  2.0

     total cpu time spent up to now is        7.5 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.7691   6.1979   6.3305   6.4725

          k =-0.2309 0.2294-0.2325 (   917 PWs)   bands (ev):

    -4.9700   2.2466   5.5869   5.6899

          k = 0.4617-0.4587 0.4649 (   912 PWs)   bands (ev):

    -3.4313  -0.8104   5.1654   5.2406

          k = 0.0049 0.4662 0.0025 (   902 PWs)   bands (ev):

    -4.6645   2.8367   4.3866   4.4055

          k = 0.6975-0.2220 0.6999 (   917 PWs)   bands (ev):

    -3.0336  -0.0967   2.7333   4.0880

          k = 0.4666 0.0074 0.4674 (   907 PWs)   bands (ev):

    -3.6701   0.8253   2.4579   4.9732
```

```
      k =-0.0098-0.9323-0.0050 (   934 PWs)   bands (ev):

-1.5388  -1.5315   3.4028   3.4211

      k =-0.4762-0.9372-0.0052 (   932 PWs)   bands (ev):

-1.3954  -1.2980   2.3106   2.3718

      k = 0.2306-0.2319-0.2347 (   917 PWs)   bands (ev):

-4.9570   2.3144   5.5138   5.6616

      k = 0.2358 0.2368 0.2349 (   917 PWs)   bands (ev):

-4.9296   2.4862   5.4138   5.5215

      k =-0.2356-0.2343 0.2323 (   917 PWs)   bands (ev):

-4.9440   2.3951   5.4450   5.6155

      k =-0.4613 0.4637 0.4695 (   912 PWs)   bands (ev):

-3.3814  -0.7903   5.0926   5.2010

      k =-0.4715-0.4736-0.4699 (   912 PWs)   bands (ev):

-3.2820  -0.7164   4.9696   5.0593

      k = 0.4711 0.4686-0.4645 (   912 PWs)   bands (ev):

-3.3342  -0.7562   5.0138   5.1539

      k = 0.4664 0.0049 0.0002 (   902 PWs)   bands (ev):

-4.6635   2.8398   4.3219   4.4644

      k = 0.0002 0.0025 0.4672 (   902 PWs)   bands (ev):

-4.6606   2.8496   4.2411   4.5264

      k =-0.6968 0.2294 0.7017 (   917 PWs)   bands (ev):

-2.9970  -0.1054   2.7038   4.0922

      k =-0.7024-0.2442-0.7024 (   917 PWs)   bands (ev):

-2.9256  -0.0942   2.6580   4.0484

      k = 0.7018 0.2367-0.6992 (   917 PWs)   bands (ev):

-2.9627  -0.1012   2.6763   4.0792

      k =-0.2262 0.6930-0.6972 (   917 PWs)   bands (ev):

-3.0257  -0.1218   2.7129   4.1536

      k = 0.2255-0.7005-0.7044 (   917 PWs)   bands (ev):

-3.0025  -0.0797   2.7282   4.0193

      k =-0.2403-0.6979 0.6970 (   917 PWs)   bands (ev):

-2.9555  -0.1240   2.6674   4.1279

      k = 0.2409 0.7054 0.7046 (   917 PWs)   bands (ev):
```

```
     -2.9303  -0.0704   2.6706   3.9922

          k =-0.6923 0.6906-0.2302 (   917 PWs)   bands (ev):

     -3.0160  -0.1435   2.6998   4.2036

          k =-0.7069-0.7054 0.2296 (   917 PWs)   bands (ev):

     -2.9702  -0.0516   2.7262   3.9334

          k = 0.7071 0.7079 0.2376 (   917 PWs)   bands (ev):

     -2.9324  -0.0463   2.6958   3.9193

          k = 0.6921-0.6931-0.2370 (   917 PWs)   bands (ev):

     -2.9800  -0.1498   2.6816   4.1908

          k =-0.4662-0.0024 0.4670 (   907 PWs)   bands (ev):

     -3.6720   0.8200   2.4507   4.9899

          k = 0.0047 0.4637-0.4647 (   907 PWs)   bands (ev):

     -3.6966   0.8148   2.4466   5.0320

          k =-0.0051-0.4686-0.4697 (   907 PWs)   bands (ev):

     -3.6467   0.8354   2.4662   4.9236

          k =-0.4615 0.4612 0.0023 (   907 PWs)   bands (ev):

     -3.7220   0.8086   2.4445   5.0763

          k =-0.4713-0.4711-0.0027 (   907 PWs)   bands (ev):

     -3.6253   0.8570   2.4816   4.8560

          k =-0.9328-0.0098-0.0004 (   934 PWs)   bands (ev):

     -1.5459  -1.5185   3.3335   3.4825

          k =-0.0004-0.0050-0.9344 (   934 PWs)   bands (ev):

     -1.5472  -1.4989   3.2471   3.5449

          k =-0.9377-0.4760-0.0029 (   932 PWs)   bands (ev):

     -1.4008  -1.2907   2.3077   2.3756

          k = 0.0096 0.9298-0.4622 (   932 PWs)   bands (ev):

     -1.3754  -1.3236   2.3250   2.3548

      highest occupied level (ev):     6.4725

!     total energy              =     -15.83813214 Ry
      Harris-Foulkes estimate   =     -15.83813214 Ry
      estimated scf accuracy    <          1.2E-10 Ry

      The total energy is the sum of the following terms:

      one-electron contribution =       4.83014317 Ry
      hartree contribution      =       1.09672163 Ry
```

```
     xc contribution           =      -4.83246156 Ry
     ewald contribution        =     -16.93253538 Ry

     convergence has been achieved in   8 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.00123317    0.00087066    0.00301369
     atom    2 type  1   force =    -0.00123317   -0.00087066   -0.00301369

     Total force =     0.004767     Total SCF correction =     0.000002


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   12.59
    0.00008347   0.00009683  -0.00000139         12.28     14.24     -0.21
    0.00009683   0.00008029   0.00005024         14.24     11.81      7.39
   -0.00000139   0.00005024   0.00009289         -0.21      7.39     13.67


     number of scf cycles    =   3
     number of bfgs steps    =   2

     enthalpy old            =     -15.8348516689 Ry
     enthalpy new            =     -15.8381321427 Ry

     CASE: enthalpy_new < enthalpy_old

     new trust radius        =       0.0199064925 bohr
     new conv_thr            =       0.0000000003 Ry

     new unit-cell volume =    267.44031 a.u.^3 (    39.63057 Ang^3 )
     density =      2.35363 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.538763930   0.001843016   0.537972576
   -0.003959969   0.536910722   0.535848486
   -0.542134598   0.542380913  -0.001538588

 ATOMIC_POSITIONS (alat)
 Si       0.004653198  -0.000120658   0.009309405
 Si       0.273359057   0.266602042   0.279969800



     Writing output data file Si_relax.save/
     NEW-OLD atomic charge density approx. for the potential
     extrapolated charge    8.10876, renormalised to    8.00000

     total cpu time spent up to now is        7.9 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  3.5

     total cpu time spent up to now is        8.3 secs

     total energy              =     -15.83837733 Ry
     Harris-Foulkes estimate   =     -15.89386155 Ry
     estimated scf accuracy    <       0.00007596 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
```

```
     Davidson diagonalization with overlap
     ethr =  9.49E-07,  avg # of iterations =  3.0

     total cpu time spent up to now is        8.6 secs

     total energy              =     -15.83851209 Ry
     Harris-Foulkes estimate   =     -15.83853262 Ry
     estimated scf accuracy    <       0.00005992 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  7.49E-07,  avg # of iterations =  1.0

     total cpu time spent up to now is        8.7 secs

     total energy              =     -15.83850565 Ry
     Harris-Foulkes estimate   =     -15.83851395 Ry
     estimated scf accuracy    <       0.00001523 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.90E-07,  avg # of iterations =  2.0

     total cpu time spent up to now is        9.0 secs

     total energy              =     -15.83850822 Ry
     Harris-Foulkes estimate   =     -15.83850847 Ry
     estimated scf accuracy    <       0.00000063 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  7.89E-09,  avg # of iterations =  1.9

     total cpu time spent up to now is        9.2 secs

     total energy              =     -15.83850823 Ry
     Harris-Foulkes estimate   =     -15.83850828 Ry
     estimated scf accuracy    <       0.00000009 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.13E-09,  avg # of iterations =  2.0

     total cpu time spent up to now is        9.5 secs

     total energy              =     -15.83850825 Ry
     Harris-Foulkes estimate   =     -15.83850825 Ry
     estimated scf accuracy    <          4.5E-10 Ry

     iteration #  7     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  5.69E-12,  avg # of iterations =  2.5

     total cpu time spent up to now is        9.8 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.8187   6.0903   6.1916   6.2845

          k =-0.2307 0.2297-0.2318 (   917 PWs)   bands (ev):

    -5.0212   2.1641   5.4412   5.5069
```

```
      k = 0.4614-0.4593 0.4637 (   912 PWs)   bands (ev):
-3.4830  -0.8840   5.0137   5.0602

      k = 0.0032 0.4641 0.0016 (   902 PWs)   bands (ev):
-4.7268   2.6909   4.2691   4.2822

      k = 0.6953-0.2249 0.6971 (   917 PWs)   bands (ev):
-3.0956  -0.2119   2.6209   3.9650

      k = 0.4646 0.0047 0.4652 (   907 PWs)   bands (ev):
-3.7442   0.7033   2.3627   4.8472

      k =-0.0063-0.9282-0.0031 (   934 PWs)   bands (ev):
-1.6381  -1.6316   3.2948   3.3085

      k =-0.4706-0.9313-0.0034 (   932 PWs)   bands (ev):
-1.4806  -1.4265   2.2324   2.2763

      k = 0.2304-0.2313-0.2331 (   917 PWs)   bands (ev):
-5.0146   2.2116   5.3887   5.4932

      k = 0.2339 0.2344 0.2334 (   917 PWs)   bands (ev):
-4.9965   2.3254   5.3195   5.4031

      k =-0.2336-0.2328 0.2316 (   917 PWs)   bands (ev):
-5.0063   2.2651   5.3414   5.4652

      k =-0.4609 0.4625 0.4663 (   912 PWs)   bands (ev):
-3.4608  -0.8595   4.9623   5.0413

      k =-0.4677-0.4688-0.4668 (   912 PWs)   bands (ev):
-3.3955  -0.8101   4.8775   4.9509

      k = 0.4672 0.4657-0.4631 (   912 PWs)   bands (ev):
-3.4313  -0.8353   4.9085   5.0130

      k = 0.4643 0.0032 0.0003 (   902 PWs)   bands (ev):
-4.7260   2.6940   4.2257   4.3202

      k = 0.0003 0.0016 0.4650 (   902 PWs)   bands (ev):
-4.7234   2.7034   4.1704   4.3590

      k =-0.6945 0.2297 0.6978 (   917 PWs)   bands (ev):
-3.0777  -0.2099   2.6019   3.9687

      k =-0.6984-0.2392-0.6986 (   917 PWs)   bands (ev):
-3.0317  -0.1973   2.5630   3.9409

      k = 0.6976 0.2344-0.6963 (   917 PWs)   bands (ev):
```

```
-3.0563  -0.2055   2.5828   3.9605
      k =-0.2278 0.6922-0.6952 (   917 PWs)   bands (ev):
-3.0900  -0.2287   2.6084   4.0077
      k = 0.2270-0.6969-0.6997 (   917 PWs)   bands (ev):
-3.0811  -0.1925   2.6179   3.9194
      k =-0.2365-0.6953 0.6950 (   917 PWs)   bands (ev):
-3.0521  -0.2159   2.5696   3.9932
      k = 0.2373 0.7001 0.6999 (   917 PWs)   bands (ev):
-3.0336  -0.1860   2.5794   3.9017
      k =-0.6919 0.6906-0.2305 (   917 PWs)   bands (ev):
-3.0827  -0.2417   2.5998   4.0382
      k =-0.7010-0.7001 0.2297 (   917 PWs)   bands (ev):
-3.0599  -0.1727   2.6181   3.8605
      k = 0.7013 0.7017 0.2352 (   917 PWs)   bands (ev):
-3.0339  -0.1706   2.5986   3.8508
      k = 0.6916-0.6922-0.2344 (   917 PWs)   bands (ev):
-3.0663  -0.2333   2.5801   4.0318
      k =-0.4640-0.0016 0.4647 (   907 PWs)   bands (ev):
-3.7503   0.7077   2.3576   4.8546
      k = 0.0029 0.4625-0.4634 (   907 PWs)   bands (ev):
-3.7625   0.6967   2.3567   4.8852
      k =-0.0034-0.4657-0.4665 (   907 PWs)   bands (ev):
-3.7331   0.7181   2.3679   4.8098
      k =-0.4611 0.4609 0.0013 (   907 PWs)   bands (ev):
-3.7791   0.6923   2.3579   4.9119
      k =-0.4675-0.4672-0.0018 (   907 PWs)   bands (ev):
-3.7201   0.7342   2.3801   4.7620
      k =-0.9286-0.0063-0.0005 (   934 PWs)   bands (ev):
-1.6369  -1.6274   3.2494   3.3472
      k =-0.0005-0.0032-0.9299 (   934 PWs)   bands (ev):
-1.6342  -1.6139   3.1901   3.3854
      k =-0.9318-0.4704-0.0021 (   932 PWs)   bands (ev):
```

```
     -1.4824  -1.4230   2.2300   2.2793

          k = 0.0060 0.9266-0.4618 (   932 PWs)   bands (ev):

     -1.4699  -1.4424   2.2423   2.2645

      highest occupied level (ev):     6.2845

!     total energy              =     -15.83850825 Ry
      Harris-Foulkes estimate   =     -15.83850825 Ry
      estimated scf accuracy    <          2.8E-10 Ry

      The total energy is the sum of the following terms:

      one-electron contribution =       4.72619896 Ry
      hartree contribution      =       1.10800139 Ry
      xc contribution           =      -4.81763513 Ry
      ewald contribution        =     -16.85507347 Ry

      convergence has been achieved in   7 iterations

      Forces acting on atoms (cartesian axes, Ry/au):

      atom    1 type  1   force =     0.00152741   -0.00018595    0.00298559
      atom    2 type  1   force =    -0.00152741    0.00018595   -0.00298559

      Total force =     0.004750     Total SCF correction =     0.000003


      Computing stress (Cartesian axis) and pressure

           total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.73
   -0.00000692   0.00005711   0.00000579         -1.02      8.40      0.85
    0.00005711  -0.00000971   0.00002831          8.40     -1.43      4.16
    0.00000579   0.00002831   0.00000168          0.85      4.16      0.25


      number of scf cycles    =   4
      number of bfgs steps    =   3

      enthalpy old            =     -15.8381321427 Ry
      enthalpy new            =     -15.8385082468 Ry

      CASE: enthalpy_new < enthalpy_old

      new trust radius        =       0.0112057553 bohr
      new conv_thr            =       0.0000000003 Ry

      new unit-cell volume =    268.37791 a.u.^3 (    39.76950 Ang^3 )
      density =      2.34541 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.539262649   0.001058207   0.538667865
   -0.002306234   0.538214082   0.537412135
   -0.541136707   0.541317623  -0.000827390

 ATOMIC_POSITIONS (alat)
 Si       0.004958827  -0.000062866   0.009929819
 Si       0.274183624   0.268046945   0.280203028



      Writing output data file Si_relax.save/
      NEW-OLD atomic charge density approx. for the potential
      extrapolated charge    8.02795, renormalised to    8.00000
```

```
     total cpu time spent up to now is       10.1 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  3.1

     total cpu time spent up to now is       10.4 secs

     total energy              =     -15.83860560 Ry
     Harris-Foulkes estimate   =     -15.85278864 Ry
     estimated scf accuracy    <       0.00001238 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.55E-07,  avg # of iterations =  2.9

     total cpu time spent up to now is       10.7 secs

     total energy              =     -15.83861606 Ry
     Harris-Foulkes estimate   =     -15.83861766 Ry
     estimated scf accuracy    <       0.00000403 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  5.04E-08,  avg # of iterations =  1.0

     total cpu time spent up to now is       10.9 secs

     total energy              =     -15.83861600 Ry
     Harris-Foulkes estimate   =     -15.83861629 Ry
     estimated scf accuracy    <       0.00000058 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  7.26E-09,  avg # of iterations =  2.0

     total cpu time spent up to now is       11.2 secs

     total energy              =     -15.83861610 Ry
     Harris-Foulkes estimate   =     -15.83861611 Ry
     estimated scf accuracy    <       0.00000001 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.73E-10,  avg # of iterations =  2.2

     total cpu time spent up to now is       11.4 secs

     total energy              =     -15.83861610 Ry
     Harris-Foulkes estimate   =     -15.83861610 Ry
     estimated scf accuracy    <          8.8E-10 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.11E-11,  avg # of iterations =  2.3

     total cpu time spent up to now is       11.7 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):
```

```
-5.8314   6.0941   6.1545   6.2066

      k =-0.2311 0.2305-0.2318 (   917 PWs)   bands (ev):

-5.0313   2.1670   5.3978   5.4335

      k = 0.4622-0.4609 0.4636 (   912 PWs)   bands (ev):

-3.4865  -0.8894   4.9650   4.9890

      k = 0.0018 0.4636 0.0009 (   902 PWs)   bands (ev):

-4.7426   2.6552   4.2392   4.2480

      k = 0.6951-0.2278 0.6963 (   917 PWs)   bands (ev):

-3.1035  -0.2373   2.5835   3.9302

      k = 0.4640 0.0027 0.4645 (   907 PWs)   bands (ev):

-3.7648   0.6752   2.3375   4.8139

      k =-0.0036-0.9273-0.0018 (   934 PWs)   bands (ev):

-1.6623  -1.6569   3.2676   3.2770

      k =-0.4674-0.9291-0.0020 (   932 PWs)   bands (ev):

-1.4961  -1.4660   2.2192   2.2447

      k = 0.2309-0.2314-0.2325 (   917 PWs)   bands (ev):

-5.0279   2.1937   5.3681   5.4267

      k = 0.2329 0.2332 0.2327 (   917 PWs)   bands (ev):

-5.0174   2.2594   5.3259   5.3766

      k =-0.2327-0.2323 0.2316 (   917 PWs)   bands (ev):

-5.0232   2.2242   5.3388   5.4130

      k =-0.4618 0.4627 0.4650 (   912 PWs)   bands (ev):

-3.4756  -0.8742   4.9360   4.9797

      k =-0.4658-0.4663-0.4654 (   912 PWs)   bands (ev):

-3.4378  -0.8458   4.8843   4.9301

      k = 0.4654 0.4645-0.4632 (   912 PWs)   bands (ev):

-3.4588  -0.8604   4.9025   4.9663

      k = 0.4638 0.0018 0.0002 (   902 PWs)   bands (ev):

-4.7419   2.6576   4.2145   4.2686

      k = 0.0002 0.0009 0.4643 (   902 PWs)   bands (ev):

-4.7399   2.6651   4.1813   4.2890

      k =-0.6945 0.2305 0.6966 (   917 PWs)   bands (ev):

-3.0944  -0.2357   2.5726   3.9336
```

```
      k =-0.6969-0.2359-0.6972 (   917 PWs)   bands (ev):

-3.0679  -0.2275   2.5495   3.9167

      k = 0.6963 0.2332-0.6957 (   917 PWs)   bands (ev):

-3.0821  -0.2331   2.5617   3.9290

      k =-0.2295 0.6932-0.6952 (   917 PWs)   bands (ev):

-3.1000  -0.2470   2.5766   3.9544

      k = 0.2289-0.6959-0.6977 (   917 PWs)   bands (ev):

-3.0961  -0.2254   2.5823   3.9042

      k =-0.2343-0.6950 0.6950 (   917 PWs)   bands (ev):

-3.0796  -0.2382   2.5538   3.9465

      k = 0.2349 0.6977 0.6979 (   917 PWs)   bands (ev):

-3.0686  -0.2217   2.5601   3.8940

      k =-0.6931 0.6923-0.2311 (   917 PWs)   bands (ev):

-3.0951  -0.2541   2.5727   3.9697

      k =-0.6983-0.6977 0.2305 (   917 PWs)   bands (ev):

-3.0832  -0.2138   2.5836   3.8684

      k = 0.6985 0.6986 0.2338 (   917 PWs)   bands (ev):

-3.0680  -0.2127   2.5722   3.8628

      k = 0.6929-0.6932-0.2332 (   917 PWs)   bands (ev):

-3.0870  -0.2478   2.5609   3.9664

      k =-0.4636-0.0009 0.4641 (   907 PWs)   bands (ev):

-3.7693   0.6779   2.3349   4.8188

      k = 0.0016 0.4627-0.4634 (   907 PWs)   bands (ev):

-3.7756   0.6713   2.3349   4.8354

      k =-0.0020-0.4645-0.4652 (   907 PWs)   bands (ev):

-3.7593   0.6845   2.3411   4.7919

      k =-0.4620 0.4618 0.0007 (   907 PWs)   bands (ev):

-3.7855   0.6695   2.3374   4.8483

      k =-0.4656-0.4654-0.0011 (   907 PWs)   bands (ev):

-3.7523   0.6945   2.3499   4.7623

      k =-0.9276-0.0036-0.0004 (   934 PWs)   bands (ev):

-1.6597  -1.6554   3.2418   3.2975
```

```
          k =-0.0004-0.0018-0.9286 (   934 PWs)   bands (ev):

    -1.6564  -1.6459   3.2058   3.3172

          k =-0.9294-0.4672-0.0013 (   932 PWs)   bands (ev):

    -1.4966  -1.4641   2.2178   2.2464

          k = 0.0034 0.9264-0.4625 (   932 PWs)   bands (ev):

    -1.4908  -1.4755   2.2248   2.2378

     highest occupied level (ev):     6.2066

!    total energy              =     -15.83861610 Ry
     Harris-Foulkes estimate   =     -15.83861610 Ry
     estimated scf accuracy    <          6.5E-11 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       4.69940239 Ry
     hartree contribution      =       1.11100538 Ry
     xc contribution           =      -4.81391465 Ry
     ewald contribution        =     -16.83510922 Ry

     convergence has been achieved in   6 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.00096204   -0.00017856    0.00180530
     atom    2 type  1   force =    -0.00096204    0.00017856   -0.00180530

     Total force =     0.002904     Total SCF correction =     0.000001


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   -3.98
  -0.00002864   0.00003199   0.00000471         -4.21      4.71      0.69
   0.00003199  -0.00003087   0.00001555          4.71     -4.54      2.29
   0.00000471   0.00001555  -0.00002171          0.69      2.29     -3.19


     number of scf cycles    =   5
     number of bfgs steps    =   4

     enthalpy old            =     -15.8385082468 Ry
     enthalpy new            =     -15.8386161044 Ry

     CASE: enthalpy_new < enthalpy_old

     new trust radius        =       0.0110753297 bohr
     new conv_thr            =       0.0000000001 Ry

     new unit-cell volume =    268.17917 a.u.^3 (    39.74005 Ang^3 )
     density =      2.34715 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.538935910   0.000246138   0.538602175
   -0.000561129   0.538735663   0.538279029
   -0.539328407   0.539423802  -0.000158290

 ATOMIC_POSITIONS (alat)
 Si       0.005291912  -0.000029744   0.010585886
 Si       0.274626979   0.269145824   0.280051556
```

```
     Writing output data file Si_relax.save/
     NEW-OLD atomic charge density approx. for the potential
     extrapolated charge    7.99407, renormalised to    8.00000

     total cpu time spent up to now is       12.0 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  3.1

     total cpu time spent up to now is       12.3 secs

     total energy              =     -15.83867617 Ry
     Harris-Foulkes estimate   =     -15.83567507 Ry
     estimated scf accuracy    <       0.00000877 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.10E-07,  avg # of iterations =  2.1

     total cpu time spent up to now is       12.6 secs

     total energy              =     -15.83867853 Ry
     Harris-Foulkes estimate   =     -15.83867864 Ry
     estimated scf accuracy    <       0.00000034 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  4.19E-09,  avg # of iterations =  2.1

     total cpu time spent up to now is       12.8 secs

     total energy              =     -15.83867859 Ry
     Harris-Foulkes estimate   =     -15.83867859 Ry
     estimated scf accuracy    <       0.00000002 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.95E-10,  avg # of iterations =  2.1

     total cpu time spent up to now is       13.1 secs

     total energy              =     -15.83867859 Ry
     Harris-Foulkes estimate   =     -15.83867859 Ry
     estimated scf accuracy    <          2.5E-10 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.08E-12,  avg # of iterations =  3.1

     total cpu time spent up to now is       13.4 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.8289   6.1458   6.1604   6.1715

          k =-0.2318 0.2316-0.2321 (   917 PWs)   bands (ev):
```

```
-5.0233   2.2079   5.3956   5.4015

      k = 0.4636-0.4632 0.4641 (   912 PWs)   bands (ev):

-3.4651  -0.8678   4.9562   4.9594

      k = 0.0004 0.4639 0.0002 (   902 PWs)   bands (ev):

-4.7389   2.6649   4.2460   4.2500

      k = 0.6958-0.2310 0.6964 (   917 PWs)   bands (ev):

-3.0857  -0.2280   2.5767   3.9311

      k = 0.4640 0.0006 0.4643 (   907 PWs)   bands (ev):

-3.7628   0.6842   2.3421   4.8196

      k =-0.0008-0.9277-0.0004 (   934 PWs)   bands (ev):

-1.6536  -1.6524   3.2738   3.2778

      k =-0.4648-0.9281-0.0005 (   932 PWs)   bands (ev):

-1.4794  -1.4722   2.2334   2.2391

      k = 0.2317-0.2318-0.2322 (   917 PWs)   bands (ev):

-5.0227   2.2128   5.3899   5.4006

      k = 0.2322 0.2322 0.2322 (   917 PWs)   bands (ev):

-5.0202   2.2285   5.3773   5.3910

      k =-0.2321-0.2320 0.2320 (   917 PWs)   bands (ev):

-5.0216   2.2196   5.3805   5.4003

      k =-0.4635 0.4637 0.4644 (   912 PWs)   bands (ev):

-3.4632  -0.8651   4.9506   4.9580

      k =-0.4644-0.4645-0.4645 (   912 PWs)   bands (ev):

-3.4540  -0.8583   4.9353   4.9490

      k = 0.4643 0.4641-0.4640 (   912 PWs)   bands (ev):

-3.4592  -0.8621   4.9398   4.9582

      k = 0.4640 0.0004 0.0001 (   902 PWs)   bands (ev):

-4.7386   2.6663   4.2407   4.2530

      k = 0.0001 0.0002 0.4642 (   902 PWs)   bands (ev):

-4.7374   2.6707   4.2311   4.2553

      k =-0.6956 0.2316 0.6963 (   917 PWs)   bands (ev):

-3.0838  -0.2284   2.5740   3.9337

      k =-0.6962-0.2329-0.6966 (   917 PWs)   bands (ev):

-3.0775  -0.2261   2.5692   3.9280
```

```
      k = 0.6960 0.2322-0.6961 (   917 PWs)   bands (ev):
-3.0810  -0.2280   2.5717   3.9326
      k =-0.2315 0.6953-0.6961 (   917 PWs)   bands (ev):
-3.0845  -0.2303   2.5752   3.9365
      k = 0.2313-0.6959-0.6966 (   917 PWs)   bands (ev):
-3.0840  -0.2257   2.5770   3.9254
      k =-0.2325-0.6957 0.6960 (   917 PWs)   bands (ev):
-3.0802  -0.2288   2.5708   3.9348
      k = 0.2327 0.6963 0.6967 (   917 PWs)   bands (ev):
-3.0773  -0.2249   2.5717   3.9229
      k =-0.6954 0.6951-0.2319 (   917 PWs)   bands (ev):
-3.0824  -0.2316   2.5760   3.9371
      k =-0.6965-0.6963 0.2317 (   917 PWs)   bands (ev):
-3.0800  -0.2229   2.5788   3.9145
      k = 0.6966 0.6965 0.2325 (   917 PWs)   bands (ev):
-3.0762  -0.2224   2.5757   3.9131
      k = 0.6953-0.6953-0.2323 (   917 PWs)   bands (ev):
-3.0809  -0.2305   2.5738   3.9365
      k =-0.4639-0.0002 0.4642 (   907 PWs)   bands (ev):
-3.7643   0.6840   2.3415   4.8223
      k = 0.0003 0.4637-0.4640 (   907 PWs)   bands (ev):
-3.7656   0.6833   2.3422   4.8243
      k =-0.0005-0.4641-0.4644 (   907 PWs)   bands (ev):
-3.7619   0.6863   2.3435   4.8146
      k =-0.4635 0.4634 0.0001 (   907 PWs)   bands (ev):
-3.7684   0.6843   2.3448   4.8241
      k =-0.4644-0.4643-0.0003 (   907 PWs)   bands (ev):
-3.7608   0.6897   2.3477   4.8049
      k =-0.9279-0.0008-0.0001 (   934 PWs)   bands (ev):
-1.6523  -1.6513   3.2681   3.2806
      k =-0.0001-0.0004-0.9285 (   934 PWs)   bands (ev):
-1.6495  -1.6468   3.2571   3.2821
```

```
          k =-0.9283-0.4647-0.0003 (   932 PWs)   bands (ev):

    -1.4792  -1.4716   2.2332   2.2395

          k = 0.0007 0.9275-0.4639 (   932 PWs)   bands (ev):

    -1.4789  -1.4753   2.2344   2.2374

     highest occupied level (ev):     6.1715

!    total energy              =     -15.83867859 Ry
     Harris-Foulkes estimate   =     -15.83867859 Ry
     estimated scf accuracy    <          1.3E-11 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       4.70473503 Ry
     hartree contribution      =       1.11046132 Ry
     xc contribution           =      -4.81476075 Ry
     ewald contribution        =     -16.83911419 Ry

     convergence has been achieved in   5 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.00021161    0.00000279    0.00037747
     atom    2 type  1   force =    -0.00021161   -0.00000279   -0.00037747

     Total force =     0.000612     Total SCF correction =     0.000001


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   -3.27
  -0.00002312   0.00000740   0.00000159         -3.40      1.09      0.23
   0.00000740  -0.00002442   0.00000351          1.09     -3.59      0.52
   0.00000159   0.00000351  -0.00001905          0.23      0.52     -2.80


     number of scf cycles    =   6
     number of bfgs steps    =   5

     enthalpy old            =     -15.8386161044 Ry
     enthalpy new            =     -15.8386785925 Ry

     CASE: enthalpy_new < enthalpy_old

     new trust radius        =       0.0045974770 bohr
     new conv_thr            =            1.0E-10 Ry

     new unit-cell volume =    267.54031 a.u.^3 (    39.64538 Ang^3 )
     density =      2.35275 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.538417539  -0.000011952   0.538216794
    0.000007709   0.538485432   0.538204304
   -0.538361020   0.538413664   0.000032578

 ATOMIC_POSITIONS (alat)
 Si       0.005394448  -0.000019504   0.010784379
 Si       0.274572860   0.269285184   0.279833826


     Writing output data file Si_relax.save/
```

```
     NEW-OLD atomic charge density approx. for the potential
     extrapolated charge    7.98090, renormalised to    8.00000

     total cpu time spent up to now is       13.7 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  2.1

     Threshold (ethr) on eigenvalues was too large:
     Diagonalizing with lowered threshold

     Davidson diagonalization with overlap
     ethr =  3.39E-08,  avg # of iterations =  1.9

     total cpu time spent up to now is       14.1 secs

     total energy              =     -15.83868705 Ry
     Harris-Foulkes estimate   =     -15.82898856 Ry
     estimated scf accuracy    <       0.00000277 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.46E-08,  avg # of iterations =  3.0

     total cpu time spent up to now is       14.4 secs

     total energy              =     -15.83869119 Ry
     Harris-Foulkes estimate   =     -15.83869182 Ry
     estimated scf accuracy    <       0.00000178 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  2.23E-08,  avg # of iterations =  1.0

     total cpu time spent up to now is       14.7 secs

     total energy              =     -15.83869104 Ry
     Harris-Foulkes estimate   =     -15.83869125 Ry
     estimated scf accuracy    <       0.00000041 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  5.10E-09,  avg # of iterations =  2.0

     total cpu time spent up to now is       14.9 secs

     total energy              =     -15.83869110 Ry
     Harris-Foulkes estimate   =     -15.83869111 Ry
     estimated scf accuracy    <       0.00000001 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.30E-10,  avg # of iterations =  2.1

     total cpu time spent up to now is       15.2 secs

     total energy              =     -15.83869110 Ry
     Harris-Foulkes estimate   =     -15.83869110 Ry
     estimated scf accuracy    <          7.6E-10 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
```

```
     ethr =  9.47E-12,  avg # of iterations =  2.0

     total cpu time spent up to now is       15.4 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.8204   6.1819   6.1837   6.1868

          k =-0.2322 0.2322-0.2323 (   917 PWs)   bands (ev):

    -5.0116   2.2392   5.4127   5.4162

          k = 0.4644-0.4643 0.4646 (   912 PWs)   bands (ev):

    -3.4454  -0.8487   4.9704   4.9748

          k =-0.0000 0.4643-0.0000 (   902 PWs)   bands (ev):

    -4.7279   2.6912   4.2667   4.2686

          k = 0.6966-0.2322 0.6968 (   917 PWs)   bands (ev):

    -3.0667  -0.2085   2.5904   3.9495

          k = 0.4644-0.0000 0.4645 (   907 PWs)   bands (ev):

    -3.7505   0.7056   2.3584   4.8413

          k = 0.0001-0.9286 0.0001 (   934 PWs)   bands (ev):

    -1.6353  -1.6347   3.2926   3.2943

          k =-0.4643-0.9286 0.0000 (   932 PWs)   bands (ev):

    -1.4578  -1.4575   2.2506   2.2515

          k = 0.2322-0.2322-0.2322 (   917 PWs)   bands (ev):

    -5.0117   2.2374   5.4129   5.4183

          k = 0.2322 0.2321 0.2323 (   917 PWs)   bands (ev):

    -5.0118   2.2372   5.4149   5.4167

          k =-0.2321-0.2321 0.2323 (   917 PWs)   bands (ev):

    -5.0118   2.2368   5.4144   5.4176

          k =-0.4644 0.4643 0.4645 (   912 PWs)   bands (ev):

    -3.4457  -0.8500   4.9707   4.9768

          k =-0.4643-0.4643-0.4645 (   912 PWs)   bands (ev):

    -3.4461  -0.8499   4.9726   4.9754

          k = 0.4643 0.4643-0.4645 (   912 PWs)   bands (ev):

    -3.4459  -0.8503   4.9722   4.9762

          k = 0.4643-0.0000 0.0000 (   902 PWs)   bands (ev):

    -4.7277   2.6921   4.2662   4.2678
```

```
      k = 0.0000-0.0000 0.4645 (   902 PWs)   bands (ev):
-4.7270   2.6947   4.2637   4.2659

      k =-0.6965 0.2322 0.6967 (   917 PWs)   bands (ev):
-3.0669  -0.2094   2.5903   3.9512

      k =-0.6965-0.2321-0.6968 (   917 PWs)   bands (ev):
-3.0672  -0.2090   2.5914   3.9497

      k = 0.6965 0.2321-0.6968 (   917 PWs)   bands (ev):
-3.0670  -0.2096   2.5906   3.9513

      k =-0.2323 0.6965-0.6968 (   917 PWs)   bands (ev):
-3.0664  -0.2083   2.5906   3.9489

      k = 0.2322-0.6964-0.6967 (   917 PWs)   bands (ev):
-3.0666  -0.2093   2.5911   3.9501

      k =-0.2321-0.6964 0.6968 (   917 PWs)   bands (ev):
-3.0668  -0.2093   2.5919   3.9491

      k = 0.2321 0.6964 0.6967 (   917 PWs)   bands (ev):
-3.0668  -0.2091   2.5910   3.9501

      k =-0.6966 0.6965-0.2323 (   917 PWs)   bands (ev):
-3.0654  -0.2079   2.5923   3.9457

      k =-0.6965-0.6964 0.2323 (   917 PWs)   bands (ev):
-3.0657  -0.2093   2.5926   3.9478

      k = 0.6965 0.6964 0.2323 (   917 PWs)   bands (ev):
-3.0658  -0.2089   2.5922   3.9478

      k = 0.6966-0.6965-0.2322 (   917 PWs)   bands (ev):
-3.0657  -0.2086   2.5933   3.9458

      k =-0.4643 0.0000 0.4645 (   907 PWs)   bands (ev):
-3.7507   0.7046   2.3583   4.8429

      k =-0.0001 0.4643-0.4645 (   907 PWs)   bands (ev):
-3.7506   0.7058   2.3591   4.8407

      k = 0.0000-0.4643-0.4645 (   907 PWs)   bands (ev):
-3.7509   0.7053   2.3589   4.8417

      k =-0.4644 0.4643-0.0000 (   907 PWs)   bands (ev):
-3.7510   0.7073   2.3612   4.8373
```

```
          k =-0.4643-0.4643 0.0000 (   907 PWs)   bands (ev):

    -3.7515   0.7064   2.3610   4.8392

          k =-0.9287 0.0001-0.0000 (   934 PWs)   bands (ev):

    -1.6344  -1.6343   3.2920   3.2932

          k =-0.0000 0.0000-0.9290 (   934 PWs)   bands (ev):

    -1.6322  -1.6320   3.2886   3.2908

          k =-0.9287-0.4642-0.0000 (   932 PWs)   bands (ev):

    -1.4575  -1.4572   2.2508   2.2515

          k =-0.0001 0.9286-0.4646 (   932 PWs)   bands (ev):

    -1.4585  -1.4583   2.2505   2.2512

     highest occupied level (ev):     6.1868

!    total energy              =     -15.83869110 Ry
     Harris-Foulkes estimate   =     -15.83869110 Ry
     estimated scf accuracy    <          6.5E-11 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       4.72266050 Ry
     hartree contribution      =       1.10850410 Ry
     xc contribution           =      -4.81735721 Ry
     ewald contribution        =     -16.85249850 Ry

     convergence has been achieved in   6 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =    -0.00003321    0.00007977   -0.00006323
     atom    2 type  1   force =     0.00003321   -0.00007977    0.00006323

     Total force =     0.000151     Total SCF correction =     0.000000


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   -1.01
  -0.00000746  -0.00000042   0.00000009         -1.10     -0.06      0.01
  -0.00000042  -0.00000823  -0.00000024         -0.06     -1.21     -0.03
   0.00000009  -0.00000024  -0.00000501          0.01     -0.03     -0.74


     number of scf cycles    =   7
     number of bfgs steps    =   6

     enthalpy old            =     -15.8386785925 Ry
     enthalpy new            =     -15.8386911033 Ry

     CASE: enthalpy_new < enthalpy_old

     new trust radius        =       0.0012320249 bohr
     new conv_thr            =            1.0E-10 Ry

     new unit-cell volume =    267.27687 a.u.^3 (    39.60635 Ang^3 )
     density =      2.35507 g/cm^3
```

```
 CELL_PARAMETERS (alat=  9.50000000)
   -0.538222773  -0.000010409   0.538069908
    0.000010487   0.538279948   0.538061763
   -0.538177577   0.538215240   0.000022835

 ATOMIC_POSITIONS (alat)
 Si       0.005390412  -0.000011825   0.010776741
 Si       0.274480955   0.269172415   0.279768262



     Writing output data file Si_relax.save/
     NEW-OLD atomic charge density approx. for the potential
     extrapolated charge    7.99212, renormalised to    8.00000

     total cpu time spent up to now is       15.7 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  1.0

     Threshold (ethr) on eigenvalues was too large:
     Diagonalizing with lowered threshold

     Davidson diagonalization with overlap
     ethr =  3.93E-09,  avg # of iterations =  2.2

     total cpu time spent up to now is       16.2 secs

     total energy              =     -15.83869148 Ry
     Harris-Foulkes estimate   =     -15.83468370 Ry
     estimated scf accuracy    <       0.00000033 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  4.07E-09,  avg # of iterations =  3.0

     total cpu time spent up to now is       16.5 secs

     total energy              =     -15.83869217 Ry
     Harris-Foulkes estimate   =     -15.83869227 Ry
     estimated scf accuracy    <       0.00000030 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.77E-09,  avg # of iterations =  1.0

     total cpu time spent up to now is       16.7 secs

     total energy              =     -15.83869213 Ry
     Harris-Foulkes estimate   =     -15.83869218 Ry
     estimated scf accuracy    <       0.00000008 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.04E-09,  avg # of iterations =  2.0

     total cpu time spent up to now is       16.9 secs

     total energy              =     -15.83869214 Ry
     Harris-Foulkes estimate   =     -15.83869215 Ry
     estimated scf accuracy    <          6.1E-09 Ry
```

```
     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  7.67E-11,  avg # of iterations =  1.2

     total cpu time spent up to now is       17.1 secs

     total energy              =     -15.83869214 Ry
     Harris-Foulkes estimate   =     -15.83869214 Ry
     estimated scf accuracy    <          1.1E-09 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.39E-11,  avg # of iterations =  2.0

     total cpu time spent up to now is       17.4 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (   941 PWs)   bands (ev):

    -5.8169   6.1927   6.1942   6.1964

          k =-0.2323 0.2322-0.2323 (   917 PWs)   bands (ev):

    -5.0074   2.2473   5.4230   5.4257

          k = 0.4646-0.4645 0.4647 (   912 PWs)   bands (ev):

    -3.4394  -0.8434   4.9806   4.9840

          k =-0.0000 0.4645-0.0000 (   902 PWs)   bands (ev):

    -4.7234   2.7020   4.2752   4.2765

          k = 0.6968-0.2323 0.6970 (   917 PWs)   bands (ev):

    -3.0605  -0.2011   2.5978   3.9577

          k = 0.4645-0.0000 0.4647 (   907 PWs)   bands (ev):

    -3.7452   0.7141   2.3652   4.8504

          k = 0.0001-0.9289 0.0000 (   934 PWs)   bands (ev):

    -1.6278  -1.6275   3.3002   3.3013

          k =-0.4644-0.9289 0.0000 (   932 PWs)   bands (ev):

    -1.4503  -1.4499   2.2569   2.2575

          k = 0.2323-0.2322-0.2323 (   917 PWs)   bands (ev):

    -5.0075   2.2460   5.4232   5.4272

          k = 0.2322 0.2322 0.2323 (   917 PWs)   bands (ev):

    -5.0076   2.2456   5.4247   5.4262

          k =-0.2322-0.2322 0.2323 (   917 PWs)   bands (ev):

    -5.0076   2.2455   5.4244   5.4267

          k =-0.4645 0.4645 0.4646 (   912 PWs)   bands (ev):

    -3.4397  -0.8442   4.9809   4.9854
```

```
      k =-0.4645-0.4644-0.4646 (   912 PWs)   bands (ev):
-3.4400  -0.8443   4.9823   4.9846
      k = 0.4645 0.4644-0.4646 (   912 PWs)   bands (ev):
-3.4399  -0.8445   4.9820   4.9850
      k = 0.4645-0.0000 0.0000 (   902 PWs)   bands (ev):
-4.7233   2.7027   4.2747   4.2760
      k = 0.0000-0.0000 0.4646 (   902 PWs)   bands (ev):
-4.7227   2.7047   4.2727   4.2746
      k =-0.6968 0.2323 0.6969 (   917 PWs)   bands (ev):
-3.0607  -0.2017   2.5978   3.9589
      k =-0.6968-0.2322-0.6970 (   917 PWs)   bands (ev):
-3.0610  -0.2014   2.5985   3.9579
      k = 0.6967 0.2322-0.6969 (   917 PWs)   bands (ev):
-3.0609  -0.2018   2.5980   3.9589
      k =-0.2323 0.6967-0.6970 (   917 PWs)   bands (ev):
-3.0603  -0.2009   2.5980   3.9571
      k = 0.2323-0.6967-0.6969 (   917 PWs)   bands (ev):
-3.0605  -0.2016   2.5983   3.9581
      k =-0.2322-0.6967 0.6970 (   917 PWs)   bands (ev):
-3.0607  -0.2015   2.5989   3.9573
      k = 0.2322 0.6967 0.6969 (   917 PWs)   bands (ev):
-3.0607  -0.2015   2.5983   3.9582
      k =-0.6968 0.6967-0.2324 (   917 PWs)   bands (ev):
-3.0595  -0.2006   2.5993   3.9547
      k =-0.6967-0.6967 0.2323 (   917 PWs)   bands (ev):
-3.0598  -0.2016   2.5994   3.9564
      k = 0.6967 0.6967 0.2323 (   917 PWs)   bands (ev):
-3.0599  -0.2014   2.5993   3.9565
      k = 0.6968-0.6967-0.2323 (   917 PWs)   bands (ev):
-3.0598  -0.2010   2.5999   3.9548
      k =-0.4645 0.0000 0.4646 (   907 PWs)   bands (ev):
-3.7454   0.7135   2.3651   4.8514
```

```
           k =-0.0000 0.4645-0.4647 (   907 PWs)   bands (ev):

     -3.7453   0.7142   2.3657   4.8498

           k = 0.0000-0.4645-0.4646 (   907 PWs)   bands (ev):

     -3.7456   0.7139   2.3656   4.8506

           k =-0.4645 0.4645-0.0000 (   907 PWs)   bands (ev):

     -3.7456   0.7154   2.3673   4.8472

           k =-0.4645-0.4644 0.0000 (   907 PWs)   bands (ev):

     -3.7460   0.7148   2.3671   4.8487

           k =-0.9290 0.0000-0.0000 (   934 PWs)   bands (ev):

     -1.6271  -1.6271   3.2996   3.3006

           k =-0.0000 0.0000-0.9293 (   934 PWs)   bands (ev):

     -1.6254  -1.6254   3.2970   3.2989

           k =-0.9290-0.4644-0.0000 (   932 PWs)   bands (ev):

     -1.4501  -1.4497   2.2570   2.2575

           k =-0.0001 0.9289-0.4647 (   932 PWs)   bands (ev):

     -1.4508  -1.4506   2.2568   2.2573

      highest occupied level (ev):     6.1964

!     total energy              =     -15.83869214 Ry
      Harris-Foulkes estimate   =     -15.83869214 Ry
      estimated scf accuracy    <          7.9E-12 Ry

      The total energy is the sum of the following terms:

      one-electron contribution =       4.73007304 Ry
      hartree contribution      =       1.10769943 Ry
      xc contribution           =      -4.81843140 Ry
      ewald contribution        =     -16.85803322 Ry

      convergence has been achieved in   6 iterations

      Forces acting on atoms (cartesian axes, Ry/au):

      atom    1 type  1   force =    -0.00002442    0.00004718   -0.00004243
      atom    2 type  1   force =     0.00002442   -0.00004718    0.00004243

      Total force =     0.000096     Total SCF correction =     0.000000


      Computing stress (Cartesian axis) and pressure

           total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.08
    -0.00000094  -0.00000044   0.00000010         -0.14     -0.06      0.01
    -0.00000044  -0.00000153  -0.00000022         -0.06     -0.22     -0.03
     0.00000010  -0.00000022   0.00000092          0.01     -0.03      0.14


      bfgs converged in   8 scf cycles and   7 bfgs steps
      (criteria: energy <  1.0E-04 Ry, force <  1.0E-03Ry/Bohr, cell <  5.0E-01kbar)
```

```
     End of BFGS Geometry Optimization

     Final enthalpy =     -15.8386921438 Ry
 Begin final coordinates
     new unit-cell volume =    267.27687 a.u.^3 (    39.60635 Ang^3 )
     density =      2.35507 g/cm^3

 CELL_PARAMETERS (alat=  9.50000000)
   -0.538222773  -0.000010409   0.538069908
    0.000010487   0.538279948   0.538061763
   -0.538177577   0.538215240   0.000022835

 ATOMIC_POSITIONS (alat)
 Si       0.005390412  -0.000011825   0.010776741
 Si       0.274480955   0.269172415   0.279768262
 End final coordinates



     Writing output data file Si_relax.save/

     A final scf calculation at the relaxed structure.
     The G-vectors are recalculated for the final unit cell
     Results may differ from those at the preceding step.

     Parallelization info
     --------------------
     sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
     Min         145     145     42                 2296     2296     367
     Max         146     146     43                 2297     2297     368
     Sum         583     583    169                 9185     9185    1471



     bravais-lattice index     =            2
     lattice parameter (alat)  =       9.5000  a.u.
     unit-cell volume          =     267.2769 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            1
     number of electrons       =         8.00
     number of Kohn-Sham states=            4
     kinetic-energy cutoff     =      40.0000  Ry
     charge density cutoff     =     160.0000  Ry
     convergence threshold     =      1.0E-10
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation      = SLA PZ NOGX NOGC ( 1  1  0  0 0 0)

     celldm(1)=   9.500000  celldm(2)=   0.000000  celldm(3)=   0.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (  -0.538223  -0.000010   0.538070 )
               a(2) = (   0.000010   0.538280   0.538062 )
               a(3) = (  -0.538178   0.538215   0.000023 )

     reciprocal axes: (cart. coord. in units 2 pi/alat)
               b(1) = ( -0.928922 -0.928896  0.929291 )
               b(2) = (  0.928975  0.928871  0.929257 )
               b(3) = ( -0.929105  0.928992 -0.929351 )


     PseudoPot. # 1 for Si read from file:
     /qe-6.3/pseudo/Si.pz-vbc.UPF
```

```
      MD5 check sum: a974d1b8727157e37210f3f86afb6210
      Pseudo is Norm-conserving, Zval =  4.0
      Generated by new atomic code, or converted to UPF format
      Using radial grid of  431 points,  2 beta functions with:
                 l(1) =   0
                 l(2) =   1

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

      No symmetry found



    Cartesian axes

      site n.     atom                  positions (alat units)
          1           Si  tau(   1) = (   0.0053904  -0.0000118   0.0107767  )
          2           Si  tau(   2) = (   0.2744810   0.2691724   0.2797683  )

      number of k points=    36
                        cart. coord. in units 2pi/alat
         k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0312500
         k(    2) = (  -0.2322762   0.2322481  -0.2323377), wk =   0.0625000
         k(    3) = (   0.4645524  -0.4644961   0.4646754), wk =   0.0312500
         k(    4) = (  -0.0000324   0.4644658  -0.0000234), wk =   0.0625000
         k(    5) = (   0.6967963  -0.2322784   0.6969897), wk =   0.0625000
         k(    6) = (   0.4645200  -0.0000304   0.4646520), wk =   0.0625000
         k(    7) = (   0.0000648  -0.9289315   0.0000469), wk =   0.0312500
         k(    8) = (  -0.4644418  -0.9289075   0.0000319), wk =   0.0625000
         k(    9) = (   0.2322628  -0.2322417  -0.2322993), wk =   0.0625000
         k(   10) = (   0.2322438   0.2322177   0.2323143), wk =   0.0625000
         k(   11) = (  -0.2322304  -0.2322240   0.2323227), wk =   0.0625000
         k(   12) = (  -0.4645257   0.4644835   0.4645986), wk =   0.0312500
         k(   13) = (  -0.4644876  -0.4644354  -0.4646286), wk =   0.0312500
         k(   14) = (   0.4644609   0.4644481  -0.4646455), wk =   0.0312500
         k(   15) = (   0.4645067  -0.0000240   0.0000150), wk =   0.0625000
         k(   16) = (   0.0000134  -0.0000063   0.4646370), wk =   0.0625000
         k(   17) = (  -0.6967561   0.2322594   0.6969213), wk =   0.0625000
         k(   18) = (  -0.6967638  -0.2321873  -0.6969663), wk =   0.0625000
         k(   19) = (   0.6967237   0.2322064  -0.6969448), wk =   0.0625000
         k(   20) = (  -0.2323220   0.6967202  -0.6969982), wk =   0.0625000
         k(   21) = (   0.2322819  -0.6967012  -0.6969129), wk =   0.0625000
         k(   22) = (  -0.2321847  -0.6966962   0.6969832), wk =   0.0625000
         k(   23) = (   0.2322248   0.6966771   0.6969279), wk =   0.0625000
         k(   24) = (  -0.6968153   0.6967379  -0.2323761), wk =   0.0625000
         k(   25) = (  -0.6967047  -0.6966658   0.2323312), wk =   0.0625000
         k(   26) = (   0.6967181   0.6966594   0.2323058), wk =   0.0625000
         k(   27) = (   0.6968019  -0.6967315  -0.2322609), wk =   0.0625000
         k(   28) = (  -0.4644933   0.0000177   0.4646220), wk =   0.0625000
         k(   29) = (  -0.0000458   0.4644721  -0.4646605), wk =   0.0625000
         k(   30) = (   0.0000190  -0.4644594  -0.4646136), wk =   0.0625000
         k(   31) = (  -0.4645391   0.4644898  -0.0000384), wk =   0.0625000
         k(   32) = (  -0.4644742  -0.4644417   0.0000085), wk =   0.0625000
         k(   33) = (  -0.9290133   0.0000481  -0.0000300), wk =   0.0312500
         k(   34) = (  -0.0000267   0.0000127  -0.9292740), wk =   0.0312500
         k(   35) = (  -0.9289809  -0.4644177  -0.0000065), wk =   0.0625000
         k(   36) = (  -0.0000782   0.9289379  -0.4646839), wk =   0.0625000

      Dense  grid:     9185 G-vectors     FFT dimensions: (  30,  30,  30)

      Estimated max dynamical RAM per process >       2.56 MB

      Estimated total dynamical RAM >      10.22 MB
```

```
     Initial potential from superposition of free atoms

     starting charge    7.99901, renormalised to    8.00000
     Starting wfcs are    8 randomized atomic wfcs

     total cpu time spent up to now is       17.8 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-06,  avg # of iterations =  6.1

     total cpu time spent up to now is       18.5 secs

     total energy              =     -15.83496105 Ry
     Harris-Foulkes estimate   =     -15.85869595 Ry
     estimated scf accuracy    <       0.06886871 Ry

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  8.61E-04,  avg # of iterations =  1.0

     total cpu time spent up to now is       18.8 secs

     total energy              =     -15.83855759 Ry
     Harris-Foulkes estimate   =     -15.83885947 Ry
     estimated scf accuracy    <       0.00230449 Ry

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  2.88E-05,  avg # of iterations =  2.1

     total cpu time spent up to now is       19.2 secs

     total energy              =     -15.83903464 Ry
     Harris-Foulkes estimate   =     -15.83905898 Ry
     estimated scf accuracy    <       0.00006536 Ry

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  8.17E-07,  avg # of iterations =  2.0

     total cpu time spent up to now is       19.6 secs

     total energy              =     -15.83904781 Ry
     Harris-Foulkes estimate   =     -15.83904963 Ry
     estimated scf accuracy    <       0.00000469 Ry

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  5.86E-08,  avg # of iterations =  2.0

     total cpu time spent up to now is       20.0 secs

     total energy              =     -15.83904849 Ry
     Harris-Foulkes estimate   =     -15.83904852 Ry
     estimated scf accuracy    <       0.00000007 Ry

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  8.36E-10,  avg # of iterations =  2.1

     total cpu time spent up to now is       20.4 secs
```

```
     total energy              =     -15.83904851 Ry
     Harris-Foulkes estimate   =     -15.83904851 Ry
     estimated scf accuracy    <          4.4E-10 Ry

     iteration #  7     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  5.55E-12,  avg # of iterations =  2.9

     total cpu time spent up to now is       20.9 secs

     End of self-consistent calculation

          k = 0.0000 0.0000 0.0000 (  1139 PWs)   bands (ev):

    -5.8174   6.1925   6.1941   6.1962

          k =-0.2323 0.2322-0.2323 (  1146 PWs)   bands (ev):

    -5.0080   2.2468   5.4229   5.4256

          k = 0.4646-0.4645 0.4647 (  1158 PWs)   bands (ev):

    -3.4402  -0.8438   4.9805   4.9839

          k =-0.0000 0.4645-0.0000 (  1118 PWs)   bands (ev):

    -4.7241   2.7011   4.2752   4.2765

          k = 0.6968-0.2323 0.6970 (  1141 PWs)   bands (ev):

    -3.0611  -0.2017   2.5976   3.9578

          k = 0.4645-0.0000 0.4647 (  1135 PWs)   bands (ev):

    -3.7459   0.7134   2.3651   4.8504

          k = 0.0001-0.9289 0.0000 (  1138 PWs)   bands (ev):

    -1.6285  -1.6281   3.3004   3.3015

          k =-0.4644-0.9289 0.0000 (  1144 PWs)   bands (ev):

    -1.4509  -1.4506   2.2569   2.2575

          k = 0.2323-0.2322-0.2323 (  1146 PWs)   bands (ev):

    -5.0082   2.2456   5.4231   5.4271

          k = 0.2322 0.2322 0.2323 (  1146 PWs)   bands (ev):

    -5.0083   2.2452   5.4247   5.4261

          k =-0.2322-0.2322 0.2323 (  1146 PWs)   bands (ev):

    -5.0082   2.2451   5.4243   5.4266

          k =-0.4645 0.4645 0.4646 (  1158 PWs)   bands (ev):

    -3.4406  -0.8446   4.9808   4.9854

          k =-0.4645-0.4644-0.4646 (  1158 PWs)   bands (ev):

    -3.4409  -0.8447   4.9823   4.9845

          k = 0.4645 0.4644-0.4646 (  1158 PWs)   bands (ev):
```

```
-3.4408  -0.8449   4.9820   4.9849
      k = 0.4645-0.0000 0.0000 (  1118 PWs)   bands (ev):
-4.7239   2.7017   4.2747   4.2760
      k = 0.0000-0.0000 0.4646 (  1118 PWs)   bands (ev):
-4.7234   2.7037   4.2727   4.2746
      k =-0.6968 0.2323 0.6969 (  1141 PWs)   bands (ev):
-3.0613  -0.2023   2.5976   3.9589
      k =-0.6968-0.2322-0.6970 (  1141 PWs)   bands (ev):
-3.0616  -0.2021   2.5983   3.9580
      k = 0.6967 0.2322-0.6969 (  1141 PWs)   bands (ev):
-3.0615  -0.2024   2.5978   3.9590
      k =-0.2323 0.6967-0.6970 (  1141 PWs)   bands (ev):
-3.0608  -0.2016   2.5978   3.9572
      k = 0.2323-0.6967-0.6969 (  1141 PWs)   bands (ev):
-3.0610  -0.2023   2.5981   3.9582
      k =-0.2322-0.6967 0.6970 (  1141 PWs)   bands (ev):
-3.0613  -0.2022   2.5987   3.9574
      k = 0.2322 0.6967 0.6969 (  1141 PWs)   bands (ev):
-3.0613  -0.2022   2.5981   3.9583
      k =-0.6968 0.6967-0.2324 (  1141 PWs)   bands (ev):
-3.0601  -0.2012   2.5991   3.9547
      k =-0.6967-0.6967 0.2323 (  1141 PWs)   bands (ev):
-3.0604  -0.2022   2.5992   3.9565
      k = 0.6967 0.6967 0.2323 (  1141 PWs)   bands (ev):
-3.0605  -0.2020   2.5991   3.9565
      k = 0.6968-0.6967-0.2323 (  1141 PWs)   bands (ev):
-3.0604  -0.2017   2.5997   3.9548
      k =-0.4645 0.0000 0.4646 (  1135 PWs)   bands (ev):
-3.7461   0.7128   2.3651   4.8514
      k =-0.0000 0.4645-0.4647 (  1135 PWs)   bands (ev):
-3.7460   0.7136   2.3656   4.8498
      k = 0.0000-0.4645-0.4646 (  1135 PWs)   bands (ev):
```

```
     -3.7462   0.7132   2.3655   4.8506

          k =-0.4645 0.4645-0.0000 (  1135 PWs)   bands (ev):

     -3.7462   0.7147   2.3672   4.8472

          k =-0.4645-0.4644 0.0000 (  1135 PWs)   bands (ev):

     -3.7467   0.7141   2.3671   4.8487

          k =-0.9290 0.0000-0.0000 (  1138 PWs)   bands (ev):

     -1.6278  -1.6278   3.2997   3.3007

          k =-0.0000 0.0000-0.9293 (  1138 PWs)   bands (ev):

     -1.6261  -1.6261   3.2971   3.2990

          k =-0.9290-0.4644-0.0000 (  1144 PWs)   bands (ev):

     -1.4508  -1.4504   2.2570   2.2575

          k =-0.0001 0.9289-0.4647 (  1144 PWs)   bands (ev):

     -1.4514  -1.4513   2.2568   2.2573

      highest occupied level (ev):     6.1962

!     total energy              =     -15.83904851 Ry
      Harris-Foulkes estimate   =     -15.83904851 Ry
      estimated scf accuracy    <          1.2E-11 Ry

      The total energy is the sum of the following terms:

      one-electron contribution =       4.72954454 Ry
      hartree contribution      =       1.10785017 Ry
      xc contribution           =      -4.81841044 Ry
      ewald contribution        =     -16.85803278 Ry

      convergence has been achieved in   7 iterations

      Forces acting on atoms (cartesian axes, Ry/au):

      atom    1 type  1   force =    -0.00002435    0.00004714   -0.00004248
      atom    2 type  1   force =     0.00002435   -0.00004714    0.00004248

      Total force =     0.000096     Total SCF correction =     0.000000


      Computing stress (Cartesian axis) and pressure

           total   stress  (Ry/bohr**3)                   (kbar)     P=    0.20
    0.00000093  -0.00000044   0.00000010          0.14     -0.06      0.01
   -0.00000044   0.00000035  -0.00000022         -0.06      0.05     -0.03
    0.00000010  -0.00000022   0.00000280          0.01     -0.03      0.41


      Writing output data file Si_relax.save/

      init_run     :      0.62s CPU      0.65s WALL (       2 calls)
      electrons    :     16.63s CPU     17.90s WALL (       9 calls)
      update_pot   :      0.70s CPU      0.71s WALL (       7 calls)
      forces       :      0.45s CPU      0.48s WALL (       9 calls)
      stress       :      1.11s CPU      1.14s WALL (       9 calls)
```

```
     Called by init_run:
     wfcinit      :      0.31s CPU      0.34s WALL (       2 calls)
     potinit      :      0.09s CPU      0.09s WALL (       2 calls)
     hinit0       :      0.20s CPU      0.21s WALL (       2 calls)

     Called by electrons:
     c_bands      :     14.18s CPU     15.20s WALL (      59 calls)
     sum_band     :      2.22s CPU      2.41s WALL (      59 calls)
     v_of_rho     :      0.10s CPU      0.10s WALL (      66 calls)
     mix_rho      :      0.07s CPU      0.07s WALL (      59 calls)

     Called by c_bands:
     init_us_2    :      0.30s CPU      0.39s WALL (    4968 calls)
     cegterg      :     13.75s CPU     14.73s WALL (    2124 calls)

     Called by sum_band:

     Called by *egterg:
     h_psi        :     12.32s CPU     13.24s WALL (    7133 calls)
     g_psi        :      0.05s CPU      0.05s WALL (    4937 calls)
     cdiaghg      :      0.61s CPU      0.63s WALL (    6737 calls)

     Called by h_psi:
     h_psi:pot    :     12.28s CPU     13.18s WALL (    7133 calls)
     h_psi:calbec :      0.40s CPU      0.46s WALL (    7133 calls)
     vloc_psi     :     11.72s CPU     12.59s WALL (    7133 calls)
     add_vuspsi   :      0.12s CPU      0.09s WALL (    7133 calls)

     General routines
     calbec       :      0.66s CPU      0.71s WALL (    8753 calls)
     fft          :      0.35s CPU      0.33s WALL (     252 calls)
     ffts         :      0.02s CPU      0.04s WALL (      59 calls)
     fftw         :     13.12s CPU     14.15s WALL (   60998 calls)

     Parallel routines
     fft_scatt_xy :      0.61s CPU      0.66s WALL (   61309 calls)
     fft_scatt_yz :      6.78s CPU      7.16s WALL (   61309 calls)

     PWSCF        :    19.80s CPU        21.24s WALL


    This run was terminated on:  23:50:35  31Aug2019

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