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     Program PWSCF v.6.5 starts on  3Nov2023 at 10:48:13

     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     1 processors

     MPI processes distributed on     1 nodes
     Waiting for input...
     Reading input from standard input
Warning: card &IONS ignored
Warning: card ION_DYNAMICS = 'BFGS' ignored
Warning: card / ignored

     Current dimensions of program PWSCF are:
     Max number of different atomic species (ntypx) = 10
     Max number of k-points (npk) =  40000
     Max angular momentum in pseudopotentials (lmaxx) =  3

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


     G-vector sticks info
     --------------------
     sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
     Sum         625     253     85                37579     9597    1785



     bravais-lattice index     =            4
     lattice parameter (alat)  =       4.7500  a.u.
     unit-cell volume          =     278.4407 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            2
     number of electrons       =         8.00
     number of Kohn-Sham states=            8
     kinetic-energy cutoff     =      40.0000  Ry
     charge density cutoff     =     400.0000  Ry
     convergence threshold     =      1.0E-08
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation= PBE
                          (   1   4   3   4   0   0   0)

     celldm(1)=   4.750000  celldm(2)=   0.000000  celldm(3)=   3.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (   1.000000   0.000000   0.000000 )
               a(2) = (  -0.500000   0.866025   0.000000 )
               a(3) = (   0.000000   0.000000   3.000000 )

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


     PseudoPot. # 1 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. # 2 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
        B              3.00    10.81000     B ( 1.00)
        N              5.00    14.01000     N ( 1.00)

     Starting magnetic structure
     atomic species   magnetization
        B            0.500
        N           -0.500

     12 Sym. Ops. (no inversion) 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 )


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

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

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


     isym =  3     120 deg rotation - cryst. axis [0,0,1]

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

 cart.    s( 3) = ( -0.5000000 -0.8660254  0.0000000 )
                  (  0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )


     isym =  4     120 deg rotation - cryst. axis [0,0,-1]

 cryst.   s( 4) = (    -1         -1          0      )
                  (     1          0          0      )
                  (     0          0          1      )

 cart.    s( 4) = ( -0.5000000  0.8660254  0.0000000 )
                  ( -0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )


     isym =  5     180 deg rotation - cryst. axis [1,-1,0]

 cryst.   s( 5) = (     0         -1          0      )
                  (    -1          0          0      )
                  (     0          0         -1      )

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


     isym =  6     180 deg rotation - cryst. axis [2,1,0]

 cryst.   s( 6) = (     1          1          0      )
                  (     0         -1          0      )
                  (     0          0         -1      )

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


     isym =  7     inv. 180 deg rotation - cart. axis [0,0,1]

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

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


     isym =  8     inv. 180 deg rotation - cart. axis [1,0,0]

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

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


      isym =  9     inv.  60 deg rotation - cryst. axis [0,0,1]

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

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


      isym = 10     inv.  60 deg rotation - cryst. axis [0,0,-1]

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

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


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

 cryst.   s(11) = (     1          1          0      )
                  (     0         -1          0      )
                  (     0          0          1      )

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


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

 cryst.   s(12) = (     0         -1          0      )
                  (    -1          0          0      )
                  (     0          0          1      )

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


     point group D_3h (-62m)
     there are  6 classes
     the character table:

       E     2C3   3C2   s_h   2S3   3s_v
A'_1   1.00  1.00  1.00  1.00  1.00  1.00
A'_2   1.00  1.00 -1.00  1.00  1.00 -1.00
E'     2.00 -1.00  0.00  2.00 -1.00  0.00
A''1   1.00  1.00  1.00 -1.00 -1.00 -1.00
A''2   1.00  1.00 -1.00 -1.00 -1.00  1.00
E''    2.00 -1.00  0.00 -2.00  1.00  0.00
```

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

     E        1
          identity
     2C3      3    4
          120 deg rotation - cryst. axis [0,0,1]
     3C2      2    6    5
          180 deg rotation - cart. axis [0,1,0]
     s_h      7
          inv. 180 deg rotation - cart. axis [0,0,1]
     2S3      9   10
          inv.  60 deg rotation - cryst. axis [0,0,1]
     3s_v     8   11   12
          inv. 180 deg rotation - cart. axis [1,0,0]

   Cartesian axes

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

   Crystallographic axes

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

     number of k points=    37  Marzari-Vanderbilt smearing, width (Ry)=  0.0010
                       cart. coord. in units 2pi/alat
        k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0030864
        k(    2) = (   0.0000000   0.0641500   0.0000000), wk =   0.0185185
        k(    3) = (   0.0000000   0.1283001   0.0000000), wk =   0.0185185
        k(    4) = (   0.0000000   0.1924501   0.0000000), wk =   0.0185185
        k(    5) = (   0.0000000   0.2566001   0.0000000), wk =   0.0185185
        k(    6) = (   0.0000000   0.3207501   0.0000000), wk =   0.0185185
        k(    7) = (   0.0000000   0.3849002   0.0000000), wk =   0.0185185
        k(    8) = (   0.0000000   0.4490502   0.0000000), wk =   0.0185185
        k(    9) = (   0.0000000   0.5132002   0.0000000), wk =   0.0185185
        k(   10) = (   0.0000000  -0.5773503   0.0000000), wk =   0.0092593
        k(   11) = (   0.0555556   0.0962250   0.0000000), wk =   0.0185185
        k(   12) = (   0.0555556   0.1603751   0.0000000), wk =   0.0370370
        k(   13) = (   0.0555556   0.2245251   0.0000000), wk =   0.0370370
        k(   14) = (   0.0555556   0.2886751   0.0000000), wk =   0.0370370
        k(   15) = (   0.0555556   0.3528252   0.0000000), wk =   0.0370370
        k(   16) = (   0.0555556   0.4169752   0.0000000), wk =   0.0370370
        k(   17) = (   0.0555556   0.4811252   0.0000000), wk =   0.0370370
        k(   18) = (   0.0555556   0.5452753   0.0000000), wk =   0.0370370
        k(   19) = (   0.1111111   0.1924501   0.0000000), wk =   0.0185185
        k(   20) = (   0.1111111   0.2566001   0.0000000), wk =   0.0370370
        k(   21) = (   0.1111111   0.3207501   0.0000000), wk =   0.0370370
        k(   22) = (   0.1111111   0.3849002   0.0000000), wk =   0.0370370
        k(   23) = (   0.1111111   0.4490502   0.0000000), wk =   0.0370370
        k(   24) = (   0.1111111   0.5132002   0.0000000), wk =   0.0370370
        k(   25) = (   0.1111111   0.5773503   0.0000000), wk =   0.0185185
        k(   26) = (   0.1666667   0.2886751   0.0000000), wk =   0.0185185
        k(   27) = (   0.1666667   0.3528252   0.0000000), wk =   0.0370370
        k(   28) = (   0.1666667   0.4169752   0.0000000), wk =   0.0370370
        k(   29) = (   0.1666667   0.4811252   0.0000000), wk =   0.0370370
        k(   30) = (   0.1666667   0.5452753   0.0000000), wk =   0.0370370
        k(   31) = (   0.2222222   0.3849002   0.0000000), wk =   0.0185185
        k(   32) = (   0.2222222   0.4490502   0.0000000), wk =   0.0370370
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      k(   33) = (   0.2222222   0.5132002   0.0000000), wk =   0.0370370
      k(   34) = (   0.2222222   0.5773503   0.0000000), wk =   0.0185185
      k(   35) = (   0.2777778   0.4811252   0.0000000), wk =   0.0185185
      k(   36) = (   0.2777778   0.5452753   0.0000000), wk =   0.0370370
      k(   37) = (   0.3333333   0.5773503   0.0000000), wk =   0.0061728

                     cryst. coord.
      k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0030864
      k(    2) = (   0.0000000   0.0555556   0.0000000), wk =   0.0185185
      k(    3) = (   0.0000000   0.1111111   0.0000000), wk =   0.0185185
      k(    4) = (   0.0000000   0.1666667   0.0000000), wk =   0.0185185
      k(    5) = (   0.0000000   0.2222222   0.0000000), wk =   0.0185185
      k(    6) = (   0.0000000   0.2777778   0.0000000), wk =   0.0185185
      k(    7) = (   0.0000000   0.3333333   0.0000000), wk =   0.0185185
      k(    8) = (   0.0000000   0.3888889   0.0000000), wk =   0.0185185
      k(    9) = (   0.0000000   0.4444444   0.0000000), wk =   0.0185185
      k(   10) = (   0.0000000  -0.5000000   0.0000000), wk =   0.0092593
      k(   11) = (   0.0555556   0.0555556   0.0000000), wk =   0.0185185
      k(   12) = (   0.0555556   0.1111111   0.0000000), wk =   0.0370370
      k(   13) = (   0.0555556   0.1666667   0.0000000), wk =   0.0370370
      k(   14) = (   0.0555556   0.2222222   0.0000000), wk =   0.0370370
      k(   15) = (   0.0555556   0.2777778   0.0000000), wk =   0.0370370
      k(   16) = (   0.0555556   0.3333333   0.0000000), wk =   0.0370370
      k(   17) = (   0.0555556   0.3888889   0.0000000), wk =   0.0370370
      k(   18) = (   0.0555556   0.4444444   0.0000000), wk =   0.0370370
      k(   19) = (   0.1111111   0.1111111   0.0000000), wk =   0.0185185
      k(   20) = (   0.1111111   0.1666667   0.0000000), wk =   0.0370370
      k(   21) = (   0.1111111   0.2222222   0.0000000), wk =   0.0370370
      k(   22) = (   0.1111111   0.2777778   0.0000000), wk =   0.0370370
      k(   23) = (   0.1111111   0.3333333   0.0000000), wk =   0.0370370
      k(   24) = (   0.1111111   0.3888889   0.0000000), wk =   0.0370370
      k(   25) = (   0.1111111   0.4444444   0.0000000), wk =   0.0185185
      k(   26) = (   0.1666667   0.1666667   0.0000000), wk =   0.0185185
      k(   27) = (   0.1666667   0.2222222   0.0000000), wk =   0.0370370
      k(   28) = (   0.1666667   0.2777778   0.0000000), wk =   0.0370370
      k(   29) = (   0.1666667   0.3333333   0.0000000), wk =   0.0370370
      k(   30) = (   0.1666667   0.3888889   0.0000000), wk =   0.0370370
      k(   31) = (   0.2222222   0.2222222   0.0000000), wk =   0.0185185
      k(   32) = (   0.2222222   0.2777778   0.0000000), wk =   0.0370370
      k(   33) = (   0.2222222   0.3333333   0.0000000), wk =   0.0370370
      k(   34) = (   0.2222222   0.3888889   0.0000000), wk =   0.0185185
      k(   35) = (   0.2777778   0.2777778   0.0000000), wk =   0.0185185
      k(   36) = (   0.2777778   0.3333333   0.0000000), wk =   0.0370370
      k(   37) = (   0.3333333   0.3333333   0.0000000), wk =   0.0061728

   Dense  grid:    37579 G-vectors     FFT dimensions: (  32,  32,  96)

   Smooth grid:     9597 G-vectors     FFT dimensions: (  20,  20,  60)

   Dynamical RAM for                 wfc:       0.15 MB

   Dynamical RAM for     wfc (w. buffer):      10.89 MB

   Dynamical RAM for           str. fact:       1.15 MB

   Dynamical RAM for           local pot:       0.00 MB

   Dynamical RAM for          nlocal pot:       0.29 MB

   Dynamical RAM for                qrad:       0.69 MB

   Dynamical RAM for          rho,v,vnew:       7.94 MB
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     Dynamical RAM for               rhoin:       2.65 MB

     Dynamical RAM for            rho*nmix:      18.35 MB

     Dynamical RAM for           G-vectors:       2.22 MB

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

     Dynamical RAM for          <psi|beta>:       0.00 MB

     Dynamical RAM for                 psi:       0.58 MB

     Dynamical RAM for                hpsi:       0.58 MB

     Dynamical RAM for                spsi:       0.58 MB

     Dynamical RAM for      wfcinit/wfcrot:       0.29 MB

     Dynamical RAM for           addusdens:      25.80 MB

     Dynamical RAM for          addusforce:      27.53 MB

     Dynamical RAM for         addusstress:      29.53 MB

     Estimated static dynamical RAM per process >      50.41 MB

     Estimated max dynamical RAM per process >      79.94 MB
     Generating pointlists ...
     new r_m :   0.2382 (alat units)  1.1312 (a.u.) for type    1
     new r_m :   0.2382 (alat units)  1.1312 (a.u.) for type    2

     Check: negative core charge=   -0.000009

     Initial potential from superposition of free atoms

     starting charge    7.99971, renormalised to    8.00000
     Starting wfcs are    8 randomized atomic wfcs

     total cpu time spent up to now is        4.3 secs

     Self-consistent Calculation

     iteration #  1     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-02,  avg # of iterations =  5.0

     total cpu time spent up to now is        7.3 secs

     total energy              =     -26.52810722 Ry
     Harris-Foulkes estimate   =     -26.68873458 Ry
     estimated scf accuracy    <       0.38799818 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.73 Bohr mag/cell

     iteration #  2     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  4.85E-03,  avg # of iterations =  3.0

     total cpu time spent up to now is        9.7 secs
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```
     total energy              =     -26.61627499 Ry
     Harris-Foulkes estimate   =     -26.68506594 Ry
     estimated scf accuracy    <       0.15010481 Ry

     total magnetization       =     0.00 Bohr mag/cell
     absolute magnetization    =     0.43 Bohr mag/cell

     iteration #  3     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.88E-03,  avg # of iterations =  2.1

     total cpu time spent up to now is       11.8 secs

     total energy              =     -26.65903116 Ry
     Harris-Foulkes estimate   =     -26.65158597 Ry
     estimated scf accuracy    <       0.00710224 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.26 Bohr mag/cell

     iteration #  4     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  8.88E-05,  avg # of iterations =  3.7

     total cpu time spent up to now is       14.3 secs

     total energy              =     -26.66288568 Ry
     Harris-Foulkes estimate   =     -26.66224673 Ry
     estimated scf accuracy    <       0.00103180 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.12 Bohr mag/cell

     iteration #  5     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.29E-05,  avg # of iterations =  2.7

     total cpu time spent up to now is       16.6 secs

     total energy              =     -26.66360787 Ry
     Harris-Foulkes estimate   =     -26.66357439 Ry
     estimated scf accuracy    <       0.00027493 Ry

     total magnetization       =     0.00 Bohr mag/cell
     absolute magnetization    =     0.05 Bohr mag/cell

     iteration #  6     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.44E-06,  avg # of iterations =  1.9

     total cpu time spent up to now is       18.6 secs

     total energy              =     -26.66371809 Ry
     Harris-Foulkes estimate   =     -26.66370906 Ry
     estimated scf accuracy    <       0.00000853 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.02 Bohr mag/cell

     iteration #  7     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.07E-07,  avg # of iterations =  3.2
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```
     total cpu time spent up to now is       21.0 secs

     total energy              =     -26.66373777 Ry
     Harris-Foulkes estimate   =     -26.66373781 Ry
     estimated scf accuracy    <       0.00000022 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.00 Bohr mag/cell

     iteration #  8     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  2.72E-09,  avg # of iterations =  1.9

     total cpu time spent up to now is       23.0 secs

     total energy              =     -26.66373781 Ry
     Harris-Foulkes estimate   =     -26.66373780 Ry
     estimated scf accuracy    <       0.00000001 Ry

     total magnetization       =     0.00 Bohr mag/cell
     absolute magnetization    =     0.00 Bohr mag/cell

     iteration #  9     ecut=    40.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.60E-10,  avg # of iterations =  2.5

     Magnetic moment per site:
     atom:    1    charge:    2.8716    magn:    0.0000    constr:    0.0000
     atom:    2    charge:    0.8840    magn:   -0.0000    constr:    0.0000

     total cpu time spent up to now is       25.3 secs

     End of self-consistent calculation

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


          k = 0.0000 0.0000 0.0000 (  1205 PWs)   bands (ev):

   -18.7872  -6.3755  -2.5511  -2.5511   3.0788   6.2376   7.8080  10.3197

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.0642 0.0000 (  1191 PWs)   bands (ev):

   -18.7282  -6.2962  -2.8050  -2.6681   3.1808   6.3118   7.9160  10.2892

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1283 0.0000 (  1187 PWs)   bands (ev):

   -18.5527  -6.0602  -3.5035  -2.9858   3.4805   6.5241   8.2080  10.2266

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1925 0.0000 (  1182 PWs)   bands (ev):

   -18.2652  -5.6724  -4.5068  -3.4274   3.9669   6.8275   8.5959  10.2153
```

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

       k = 0.0000 0.2566 0.0000 (  1174 PWs)   bands (ev):

-17.8747  -5.6724  -5.1428  -3.9112   4.6331   7.0536   8.9220   9.8276

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3208 0.0000 (  1184 PWs)   bands (ev):

-17.3978  -6.8838  -4.4896  -4.3730   5.4719   6.7683   9.0528   9.6583

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3849 0.0000 (  1196 PWs)   bands (ev):

-16.8649  -8.0422  -4.7679  -3.7475   5.8729   6.4640   9.0766  10.2046

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.4491 0.0000 (  1188 PWs)   bands (ev):

-16.3335  -9.0463  -5.0667  -2.9861   4.8165   7.5271   9.1709  11.1267

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.5132 0.0000 (  1194 PWs)   bands (ev):

-15.9089  -9.7642  -5.2523  -2.3498   3.9532   8.2787   9.7444  12.1859

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000-0.5774 0.0000 (  1192 PWs)   bands (ev):

-15.7393 -10.0330  -5.3150  -2.0842   3.6057   8.4454  10.8635  11.2725

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.0962 0.0000 (  1185 PWs)   bands (ev):

-18.6110  -6.1386  -3.2655  -2.9010   3.3817   6.4553   8.1204  10.2732

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.1604 0.0000 (  1187 PWs)   bands (ev):

-18.3794  -5.8266  -4.0829  -3.3145   3.7750   6.7162   8.4879  10.2809

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2245 0.0000 (  1181 PWs)   bands (ev):
```

```
-18.0400  -5.3675  -5.1360  -3.8089   4.3526   6.9994   8.9136  10.0826

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2887 0.0000 (  1183 PWs)   bands (ev):

-17.6052  -6.3025  -4.7748  -4.3048   5.1083   6.9956   9.2094   9.6411

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.3528 0.0000 (  1188 PWs)   bands (ev):

-17.0974  -7.4748  -4.7480  -4.0737   6.0323   6.3432   9.3020   9.9009

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4170 0.0000 (  1190 PWs)   bands (ev):

-16.5584  -8.5533  -5.1038  -3.3129   5.3257   7.0932   9.3354  10.6752

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4811 0.0000 (  1192 PWs)   bands (ev):

-16.0669  -9.4223  -5.3509  -2.5927   4.3405   8.1357   9.5380  11.6739

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.5453 0.0000 (  1194 PWs)   bands (ev):

-15.7538  -9.9291  -5.4774  -2.1106   3.7048   8.6469  10.4149  11.9494

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.1925 0.0000 (  1181 PWs)   bands (ev):

-18.0957  -5.4430  -4.8914  -3.8398   4.2604   6.9681   8.9507  10.1929

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.2566 0.0000 (  1187 PWs)   bands (ev):

-17.7108  -5.8732  -4.9196  -4.4196   4.9303   7.0716   9.4868   9.7094

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3208 0.0000 (  1187 PWs)   bands (ev):

-17.2418  -6.9486  -4.9520  -4.2751   5.7783   6.6551   9.7626   9.8591

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3849 0.0000 (  1188 PWs)   bands (ev):
```

```
-16.7194  -8.0147  -5.3905  -3.5445   5.7708   6.7924   9.9815  10.3691

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.4491 0.0000 (  1199 PWs)   bands (ev):

-16.2012  -8.9568  -5.7140  -2.7972   4.7759   7.9330  10.0364  11.2452

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5132 0.0000 (  1195 PWs)   bands (ev):

-15.7897  -9.6356  -5.9118  -2.1750   3.9644   8.9880  10.3030  12.1556

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5774 0.0000 (  1204 PWs)   bands (ev):

-15.6264  -9.8902  -5.9784  -1.9163   3.6362   9.3534  11.1234  11.6477

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.2887 0.0000 (  1185 PWs)   bands (ev):

-17.2907  -6.6967  -5.1044  -4.3431   5.6940   6.7621   9.7308  10.2184

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.3528 0.0000 (  1183 PWs)   bands (ev):

-16.8031  -7.5879  -5.7138  -3.6641   6.0368   6.6356  10.2187  10.7942

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4170 0.0000 (  1190 PWs)   bands (ev):

-16.2904  -8.4712  -6.1772  -2.9319   5.1324   7.7415  10.9584  10.9834

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4811 0.0000 (  1195 PWs)   bands (ev):

-15.8292  -9.2145  -6.4830  -2.2447   4.2776   8.9671  11.0422  11.7121

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.5453 0.0000 (  1200 PWs)   bands (ev):

-15.5398  -9.6551  -6.6345  -1.7892   3.7238  10.0506  11.2572  12.1842

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

```
          k = 0.2222 0.3849 0.0000 (  1175 PWs)   bands (ev):

   -16.3216  -8.2215  -6.4265  -2.9788   5.2731   7.6694  10.8558  11.7747

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.4491 0.0000 (  1193 PWs)   bands (ev):

   -15.8542  -8.8256  -6.9646  -2.2884   4.4958   8.8610  11.4378  12.0854

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.5132 0.0000 (  1193 PWs)   bands (ev):

   -15.4932  -9.2949  -7.2817  -1.7250   3.8688  10.1507  11.7077  12.0795

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.5774 0.0000 (  1207 PWs)   bands (ev):

   -15.3532  -9.4770  -7.3849  -1.4949   3.6150  11.0596  11.7454  11.9299

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.4811 0.0000 (  1197 PWs)   bands (ev):

   -15.4791  -9.0669  -7.6107  -1.7065   3.9389  10.1159  11.5131  12.6906

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.5453 0.0000 (  1197 PWs)   bands (ev):

   -15.2546  -9.1887  -7.9811  -1.3373   3.5896  11.3563  11.3806  12.6510

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.3333 0.5774 0.0000 (  1197 PWs)   bands (ev):

   -15.1677  -9.0406  -8.3389  -1.1906   3.4881  11.2183  11.9640  13.1072

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

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          k = 0.0000 0.0000 0.0000 (  1205 PWs)   bands (ev):

   -18.7872  -6.3755  -2.5511  -2.5511   3.0788   6.2376   7.8081  10.3197

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.0642 0.0000 (  1191 PWs)   bands (ev):

   -18.7282  -6.2962  -2.8049  -2.6681   3.1809   6.3118   7.9161  10.2891
```

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

       k = 0.0000 0.1283 0.0000 (  1187 PWs)   bands (ev):

-18.5527  -6.0602  -3.5035  -2.9857   3.4805   6.5241   8.2081  10.2265

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.1925 0.0000 (  1182 PWs)   bands (ev):

-18.2652  -5.6724  -4.5068  -3.4273   3.9669   6.8275   8.5959  10.2153

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.2566 0.0000 (  1174 PWs)   bands (ev):

-17.8747  -5.6723  -5.1428  -3.9112   4.6331   7.0536   8.9221   9.8277

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3208 0.0000 (  1184 PWs)   bands (ev):

-17.3978  -6.8837  -4.4896  -4.3730   5.4719   6.7683   9.0528   9.6584

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3849 0.0000 (  1196 PWs)   bands (ev):

-16.8649  -8.0422  -4.7679  -3.7476   5.8730   6.4640   9.0765  10.2046

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.4491 0.0000 (  1188 PWs)   bands (ev):

-16.3335  -9.0462  -5.0667  -2.9862   4.8166   7.5271   9.1709  11.1267

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.5132 0.0000 (  1194 PWs)   bands (ev):

-15.9089  -9.7642  -5.2523  -2.3498   3.9534   8.2787   9.7444  12.1859

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000-0.5774 0.0000 (  1192 PWs)   bands (ev):

-15.7393 -10.0330  -5.3150  -2.0842   3.6058   8.4454  10.8635  11.2725

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.0962 0.0000 (  1185 PWs)   bands (ev):
```

```
-18.6110  -6.1386  -3.2655  -2.9009   3.3817   6.4553   8.1205  10.2731

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.1604 0.0000 (  1187 PWs)   bands (ev):

-18.3794  -5.8266  -4.0828  -3.3144   3.7751   6.7162   8.4879  10.2808

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2245 0.0000 (  1181 PWs)   bands (ev):

-18.0400  -5.3675  -5.1360  -3.8089   4.3526   6.9994   8.9136  10.0827

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2887 0.0000 (  1183 PWs)   bands (ev):

-17.6052  -6.3025  -4.7748  -4.3047   5.1083   6.9956   9.2094   9.6412

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.3528 0.0000 (  1188 PWs)   bands (ev):

-17.0974  -7.4748  -4.7480  -4.0737   6.0323   6.3432   9.3020   9.9009

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4170 0.0000 (  1190 PWs)   bands (ev):

-16.5584  -8.5533  -5.1038  -3.3129   5.3257   7.0932   9.3354  10.6753

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4811 0.0000 (  1192 PWs)   bands (ev):

-16.0669  -9.4223  -5.3509  -2.5927   4.3406   8.1357   9.5380  11.6739

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.5453 0.0000 (  1194 PWs)   bands (ev):

-15.7538  -9.9291  -5.4774  -2.1106   3.7049   8.6469  10.4149  11.9494

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.1925 0.0000 (  1181 PWs)   bands (ev):

-18.0957  -5.4430  -4.8914  -3.8397   4.2604   6.9681   8.9507  10.1930

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.2566 0.0000 (  1187 PWs)   bands (ev):
```

```
-17.7108  -5.8732  -4.9196  -4.4196   4.9304   7.0716   9.4869   9.7094

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3208 0.0000 (  1187 PWs)   bands (ev):

-17.2418  -6.9486  -4.9520  -4.2751   5.7783   6.6552   9.7627   9.8591

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3849 0.0000 (  1188 PWs)   bands (ev):

-16.7194  -8.0146  -5.3904  -3.5445   5.7709   6.7924   9.9815  10.3692

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.4491 0.0000 (  1199 PWs)   bands (ev):

-16.2012  -8.9568  -5.7140  -2.7972   4.7760   7.9331  10.0364  11.2453

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5132 0.0000 (  1195 PWs)   bands (ev):

-15.7897  -9.6356  -5.9118  -2.1751   3.9645   8.9881  10.3030  12.1556

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5774 0.0000 (  1204 PWs)   bands (ev):

-15.6264  -9.8902  -5.9783  -1.9163   3.6363   9.3535  11.1235  11.6477

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.2887 0.0000 (  1185 PWs)   bands (ev):

-17.2907  -6.6967  -5.1044  -4.3431   5.6940   6.7622   9.7309  10.2184

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.3528 0.0000 (  1183 PWs)   bands (ev):

-16.8031  -7.5879  -5.7138  -3.6641   6.0368   6.6357  10.2187  10.7942

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4170 0.0000 (  1190 PWs)   bands (ev):

-16.2904  -8.4711  -6.1772  -2.9320   5.1325   7.7415  10.9584  10.9835

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

```
       k = 0.1667 0.4811 0.0000 (  1195 PWs)   bands (ev):

-15.8292  -9.2145  -6.4830  -2.2448   4.2777   8.9671  11.0423  11.7122

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.5453 0.0000 (  1200 PWs)   bands (ev):

-15.5398  -9.6551  -6.6344  -1.7893   3.7239  10.0506  11.2572  12.1842

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.3849 0.0000 (  1175 PWs)   bands (ev):

-16.3216  -8.2215  -6.4265  -2.9789   5.2732   7.6694  10.8558  11.7747

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.4491 0.0000 (  1193 PWs)   bands (ev):

-15.8542  -8.8256  -6.9646  -2.2884   4.4959   8.8611  11.4378  12.0854

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.5132 0.0000 (  1193 PWs)   bands (ev):

-15.4932  -9.2949  -7.2817  -1.7251   3.8690  10.1507  11.7077  12.0796

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.5774 0.0000 (  1207 PWs)   bands (ev):

-15.3532  -9.4769  -7.3849  -1.4950   3.6151  11.0598  11.7454  11.9299

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2778 0.4811 0.0000 (  1197 PWs)   bands (ev):

-15.4791  -9.0669  -7.6107  -1.7066   3.9390  10.1160  11.5131  12.6907

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2778 0.5453 0.0000 (  1197 PWs)   bands (ev):

-15.2546  -9.1887  -7.9811  -1.3374   3.5898  11.3564  11.3806  12.6511

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.3333 0.5774 0.0000 (  1197 PWs)   bands (ev):

-15.1677  -9.0406  -8.3388  -1.1907   3.4882  11.2183  11.9641  13.1072

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

```
     the Fermi energy is     1.1536 ev

!    total energy              =     -26.66373781 Ry
     Harris-Foulkes estimate   =     -26.66373781 Ry
     estimated scf accuracy    <          2.1E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =     -59.30892899 Ry
     hartree contribution      =      32.08374363 Ry
     xc contribution           =      -8.41610138 Ry
     ewald contribution        =       8.97754893 Ry
     smearing contrib. (-TS)   =       0.00000000 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.00 Bohr mag/cell

     convergence has been achieved in   9 iterations

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

     atom    1 type  2   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     The non-local contrib.  to forces
     atom    1 type  2   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000   -0.00000000    0.00000000
     The ionic contribution  to forces
     atom    1 type  2   force =    -0.00000005    0.00000000   -0.00000000
     atom    2 type  1   force =     0.00000005   -0.00000000    0.00000000
     The local contribution  to forces
     atom    1 type  2   force =    -0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =    -0.00000003    0.00000000    0.00000000
     The core correction contribution to forces
     atom    1 type  2   force =    -0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =    -0.00000000    0.00000000    0.00000000
     The Hubbard contrib.    to forces
     atom    1 type  2   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     The SCF correction term to forces
     atom    1 type  2   force =    -0.00000000    0.00000000   -0.00000000
     atom    2 type  1   force =    -0.00000000    0.00000000    0.00000000

     Total force =     0.000000     Total SCF correction =     0.000000


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=       -5.05
  -0.00004900  -0.00000000   0.00000000           -7.21       -0.00        0.00
  -0.00000000  -0.00004900   0.00000000           -0.00       -7.21        0.00
   0.00000000   0.00000000  -0.00000496            0.00        0.00       -0.73

     kinetic stress (kbar)   5179.53      0.00      0.00
                                0.00   5179.53      0.00
                                0.00      0.00   5799.71

     local   stress (kbar) -36932.48      0.00     -0.00
                                0.00 -36932.48     -0.00
                               -0.00     -0.00  34278.43

     nonloc. stress (kbar)   1919.33     -0.00     -0.00
```

```
                           -0.00   1919.33      0.00
                           -0.00      0.00   1794.51

     hartree stress (kbar)  15837.97     -0.00      0.00
                              -0.00  15837.97      0.00
                               0.00      0.00 -14725.54

     exc-cor stress (kbar)   -733.46     -0.00      0.00
                              -0.00   -733.46      0.00
                               0.00      0.00   -784.43

     corecor stress (kbar)   -560.91      0.00      0.00
                               0.00   -560.91     -0.00
                               0.00     -0.00   -540.79

     ewald   stress (kbar)  15282.81     -0.00     -0.00
                              -0.00  15282.81     -0.00
                              -0.00     -0.00 -25822.63

     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

     DFT-D3  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

     TS-vdW  stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00


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

     init_run     :      2.60s CPU      2.68s WALL (       1 calls)
     electrons    :     24.51s CPU     21.06s WALL (       1 calls)
     forces       :      1.03s CPU      1.03s WALL (       1 calls)
     stress       :      2.33s CPU      2.15s WALL (       1 calls)

     Called by init_run:
     wfcinit      :      0.69s CPU      0.63s WALL (       1 calls)
     wfcinit:atom :      0.05s CPU      0.04s WALL (      74 calls)
     wfcinit:wfcr :      0.48s CPU      0.44s WALL (      74 calls)
     potinit      :      0.65s CPU      0.73s WALL (       1 calls)
     hinit0       :      1.13s CPU      1.15s WALL (       1 calls)

     Called by electrons:
     c_bands      :     15.03s CPU     12.24s WALL (       9 calls)
     sum_band     :      4.01s CPU      3.13s WALL (       9 calls)
```

```
     v_of_rho     :      4.99s CPU      5.17s WALL (      10 calls)
     v_h          :      0.07s CPU      0.08s WALL (      10 calls)
     v_xc         :      5.85s CPU      6.07s WALL (      12 calls)
     newd         :      0.61s CPU      0.66s WALL (      10 calls)
     mix_rho      :      0.29s CPU      0.29s WALL (       9 calls)

     Called by c_bands:
     init_us_2    :      1.15s CPU      0.94s WALL (    1554 calls)
     cegterg      :     14.02s CPU     11.41s WALL (     666 calls)

     Called by sum_band:
     sum_band:bec :      0.01s CPU      0.01s WALL (     666 calls)
     addusdens    :      1.12s CPU      0.81s WALL (       9 calls)

     Called by *egterg:
     h_psi        :     10.17s CPU      8.37s WALL (    2660 calls)
     s_psi        :      0.45s CPU      0.37s WALL (    2660 calls)
     g_psi        :      0.14s CPU      0.10s WALL (    1920 calls)
     cdiaghg      :      1.35s CPU      1.18s WALL (    2586 calls)
     cegterg:over :      0.97s CPU      0.77s WALL (    1920 calls)
     cegterg:upda :      0.73s CPU      0.54s WALL (    1920 calls)
     cegterg:last :      0.19s CPU      0.15s WALL (     666 calls)

     Called by h_psi:
     h_psi:calbec :      0.58s CPU      0.51s WALL (    2660 calls)
     vloc_psi     :      9.02s CPU      7.40s WALL (    2660 calls)
     add_vuspsi   :      0.48s CPU      0.40s WALL (    2660 calls)

     General routines
     calbec       :      0.86s CPU      0.75s WALL (    3696 calls)
     fft          :      1.91s CPU      1.97s WALL (     288 calls)
     ffts         :      0.03s CPU      0.02s WALL (      38 calls)
     fftw         :      8.51s CPU      7.01s WALL (   35140 calls)
     interpolate  :      0.15s CPU      0.16s WALL (      20 calls)

     Parallel routines

     PWSCF        :     31.94s CPU     28.69s WALL


   This run was terminated on:  10:48:42   3Nov2023

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