```
nadeskins@compute-0-3.local has created process number              0      4577

 **** **** ******  **  PROGRAM STARTED AT                   20100512 133252.776
***** ** ***  *** **   PROGRAM STARTED ON                     compute-0-3.local
**    ****   ******    PROGRAM STARTED BY                              nadeskins
***** **    ** ** **   PROGRAM PROCESS ID                              4577
 **** **  *******  **  PROGRAM STARTED IN          /home/nadeskins/work9/tmp3

CP2K| version string:                  CP2K version 2.0.0 (Development Version)
CP2K| is freely available from                      http://cp2k.berlios.de/
CP2K| Program compiled at                Fri Feb 19 16:21:11 EST 2010
CP2K| Program compiled on                                ccc-cluster.wpi.edu
CP2K| Program compiled for                             Linux-x86-64-gfortran
CP2K| Last CVS entry        F/1.22/Fri Feb 19 17:17:31 2010//D2008.04.24.04.00
CP2K| Input file name                  /home/nadeskins/work9/tmp3/HfO2-bulk.inp

GLOBAL| Force Environment number                                            1
GLOBAL| Basis set file name                          ./GTH_BASIS_SETS_5-12-10
GLOBAL| Potential file name                          ./GTH_POTENTIALS_5-12-10
GLOBAL| MM Potential file name                                  MM_POTENTIAL
GLOBAL| Coordinate file name                                   __STD_INPUT__
GLOBAL| Method name                                                    CP2K
GLOBAL| Project name                                          HfO2-tet-bulk
GLOBAL| Preferred FFT library                                         FFTW3
GLOBAL| Run type                                                    GEO_OPT
GLOBAL| All-to-all communication in single precision                      F
GLOBAL| FFTs using library dependent lengths                              F
GLOBAL| Global print level                                                1
GLOBAL| Total number of message passing processes                         1
GLOBAL| Number of threads for this process                                1
GLOBAL| This output is from process                                       0

WARNING : FFT library FFTW3 is not available  Trying FFTSG as a default

GENERATE|  Preliminary Number of Bonds generated:                          0
GENERATE|  Achieved consistency in connectivity generation.
GENERATE|  Number of Bonds generated:                                      0
GENERATE|  Preliminary Number of Bends generated:                         0
GENERATE|  Number of Bends generated:                                     0
GENERATE|  Number of UB generated:                                        0
GENERATE|  Preliminary Number of Torsions generated:                      0
GENERATE|  Number of Torsions generated:                                  0
GENERATE|  Number of Impropers generated:                                 0
GENERATE|  Number of 1-4 interactions generated:                          0

*******************************************************************************
*******************************************************************************
**                                                                           **
**      #####                          ##              ##                    **
**     ##   ##             ##          ##              ##                    **
**    ##     ##                        ##            ######                  **
**    ##     ##  ##   ##  ##   #####   ##  ##   ####   ##    #####    #####   **
**    ##     ##  ##   ##  ##  ##       ## ##   ##      ##   ##   ##  ##   ##  **
**    ##  ## ##  ##   ##  ##  ##       ####     ###    ##   ######   ######   **
**     ##  ###   ##   ##  ##  ##       ## ##      ##   ##   ##       ##       **
**      #######   #####   ##   #####   ##  ##  ####    ##    #####   ##       **
**            ##                                                     ##       **
**                                                                           **
**                                        ... make the atoms dance           **
**                                                                           **
```

```
**            Copyright (C) by CP2K Developers Group (2000 - 2008)           **
**                                                                           **
*******************************************************************************


SCF PARAMETERS         Density guess:                                RESTART
                       ------------------------------------------------------
                       max_scf:                                          800
                       max_scf_history:                                    0
                       max_diis:                                           4
                       ------------------------------------------------------
                       eps_scf:                                     1.00E-06
                       eps_scf_history:                             0.00E+00
                       eps_diis:                                    1.00E-01
                       eps_eigval:                                  1.00E-05
                       eps_jacobi:                                  0.00E+00
                       jacobi_threshold:                            1.00E-07
                       ------------------------------------------------------
                       p_mix:                                            0.40
                       G-space mixing a:                                 1.00
                       G-space mixing b:                                 0.00
                       work_syevx:                                       1.00
                       level_shift [a.u.]:                               0.00
                       smear [a.u.]:                                     0.00
                       added MOs                                      0    0
                       ------------------------------------------------------
                       No outer SCF

2D_MC| Monte Carlo annealing to optimize the distribution_2d
2D_MC| Number of moves                                              400000
2D_MC| Number of annealing cycles                                       10
2D_MC| Number of reduction steps per cycle                               5
2D_MC| Reduction factor per step                              0.8000000000
2D_MC| Termination tolerance                                 0.0200000000
2D_MC| Maximum temperature                                    0.5000000000
2D_MC| Swap probability                                       0.9000000000
2D_MC| Number of processor rows                                          1
2D_MC| Number of processor cols                                          1
2D_MC| Number of elements                                              108
2D_MC| Cost of optimal distribution                                 1770444
2D_MC| Cost of found distribution                                   1770444
2D_MC| Difference in percent                                             0

*******************************************************************************
***                    STARTING GEOMETRY OPTIMIZATION                       ***
***                                 BFGS                                    ***
*******************************************************************************

 Number of electrons:                 864
 Number of occupied orbitals:         432
 Number of orbital functions:        1872

 Number of independent orbital functions:      1872

 Extrapolation method: initial_guess

*** 3652.852 WARNING in qs_initial_guess:calculate_first_density_matrix  ***
*** err=-300  User requested to restart the wavefunction from the file   ***
*** named: x-RESTART.wfn. This file does not exist. Please check the     ***
*** existence of the file or change properly the value of the keyword    ***
```

```
*** WFN_RESTART_FILE_NAME. Calculation continues using ATOMIC GUESS.     ***
*** /root/cp2k/makefiles/../src/qs_initial_guess.F line    202          ***


SCF WAVEFUNCTION OPTIMIZATION

 Step  Update method              Time         Convergence        Total energy
 ---------------------------------------------------------------------------

 ---------------------------------- OT -------------------------------------

 Allowing for rotations:  F
 minimizer      : DIIS                : direct inversion
                                        in the iterative subspace
                          using       : -   7 diis vectors
                                        - safer DIIS on
 preconditioner : FULL_SINGLE_INVERSE : cholesky inversion of H + eS
 stepsize       :    0.15000000
 energy_gap     :    0.20000000
 eps_taylor     :   0.10000E-15
 max_taylor     :             4

 ---------------------------------- OT -------------------------------------
    1  OT DIIS         0.15E+00  102.76        0.0157142425    -2858.3573814073
    2  OT DIIS         0.15E+00  102.90        0.0107123907    -2883.0132594354
    3  OT DIIS         0.15E+00  100.76        0.0067168298    -2903.1331919873
    4  OT DIIS         0.15E+00  101.84        0.0050072639    -2911.9603138437
    5  OT DIIS         0.15E+00  104.38        0.0037330914    -2918.7908722592
    6  OT DIIS         0.15E+00  106.04        0.0031999817    -2922.3901980371
    7  OT DIIS         0.15E+00  102.68        0.0023065914    -2928.0154192276
    8  OT DIIS         0.15E+00  101.23        0.0019499894    -2930.1968314617
    9  OT DIIS         0.15E+00  101.08        0.0016868453    -2931.2153012205
   10  OT DIIS         0.15E+00  102.81        0.0014951459    -2932.2340828807
   11  OT DIIS         0.15E+00  102.62        0.0011625925    -2933.4631269849
   12  OT DIIS         0.15E+00  101.06        0.0009731237    -2934.0468056554
   13  OT DIIS         0.15E+00  101.16        0.0007808877    -2934.7006777102
   14  OT DIIS         0.15E+00  103.60        0.0007158218    -2934.9600829413
   15  OT DIIS         0.15E+00  106.45        0.0006702106    -2935.2163011791
   16  OT DIIS         0.15E+00  102.62        0.0006025840    -2935.4304005184
   17  OT DIIS         0.15E+00  100.85        0.0007055646    -2935.4281461781
   18  OT DIIS         0.15E+00  101.18        0.0005774002    -2935.6266185405
   19  OT DIIS         0.15E+00  102.59        0.0005232208    -2935.7348792116
   20  OT DIIS         0.15E+00  102.44        0.0004680790    -2935.9022424872
   21  OT DIIS         0.15E+00  100.80        0.0003933279    -2935.9956220659
   22  OT DIIS         0.15E+00  101.42        0.0003793967    -2936.0337752306
   23  OT DIIS         0.15E+00  103.52        0.0003157092    -2936.0884250350
   24  OT DIIS         0.15E+00  106.13        0.0002655965    -2936.1384962149
   25  OT DIIS         0.15E+00  102.93        0.0002077996    -2936.1875218750
   26  OT DIIS         0.15E+00  101.17        0.0001682919    -2936.2113353219
   27  OT DIIS         0.15E+00  101.04        0.0001156176    -2936.2362773479
   28  OT DIIS         0.15E+00  102.49        0.0001056182    -2936.2436622451
   29  OT DIIS         0.15E+00  102.64        0.0000836901    -2936.2498069814
   30  OT DIIS         0.15E+00  100.91        0.0000712921    -2936.2554523036
   31  OT DIIS         0.15E+00  101.10        0.0000591045    -2936.2590218053
   32  OT DIIS         0.15E+00  103.69        0.0000476032    -2936.2626778695
   33  OT DIIS         0.15E+00  106.37        0.0000424123    -2936.2647221917
   34  OT DIIS         0.15E+00  102.64        0.0000405385    -2936.2660246635
   35  OT DIIS         0.15E+00  100.82        0.0000330659    -2936.2675352589
   36  OT DIIS         0.15E+00  101.19        0.0000291449    -2936.2688398447
   37  OT DIIS         0.15E+00  102.37        0.0000262993    -2936.2696900437
```

| | | | | | |
|---|---|---|---|---|---|
| 38 | OT DIIS | 0.15E+00 | 102.50 | 0.0000223323 | -2936.2708977470 |
| 39 | OT DIIS | 0.15E+00 | 101.06 | 0.0000205328 | -2936.2714644540 |
| 40 | OT DIIS | 0.15E+00 | 101.27 | 0.0000187632 | -2936.2719085543 |
| 41 | OT DIIS | 0.15E+00 | 103.73 | 0.0000169177 | -2936.2724972830 |
| 42 | OT DIIS | 0.15E+00 | 106.79 | 0.0000159921 | -2936.2727708611 |
| 43 | OT DIIS | 0.15E+00 | 102.98 | 0.0000152618 | -2936.2729987825 |
| 44 | OT DIIS | 0.15E+00 | 101.05 | 0.0000135567 | -2936.2734376015 |
| 45 | OT DIIS | 0.15E+00 | 100.59 | 0.0000128674 | -2936.2736259999 |
| 46 | OT DIIS | 0.15E+00 | 100.76 | 0.0000122055 | -2936.2738081338 |
| 47 | OT DIIS | 0.15E+00 | 100.62 | 0.0000110543 | -2936.2740647641 |
| 48 | OT DIIS | 0.15E+00 | 100.62 | 0.0000104197 | -2936.2742107262 |
| 49 | OT DIIS | 0.15E+00 | 100.42 | 0.0000097830 | -2936.2743664410 |
| 50 | OT DIIS | 0.15E+00 | 100.62 | 0.0000092178 | -2936.2744911293 |
| 51 | OT DIIS | 0.15E+00 | 100.48 | 0.0000075513 | -2936.2747418085 |
| 52 | OT DIIS | 0.15E+00 | 100.45 | 0.0000072231 | -2936.2748061227 |
| 53 | OT DIIS | 0.15E+00 | 100.74 | 0.0000068089 | -2936.2748951179 |
| 54 | OT DIIS | 0.15E+00 | 100.63 | 0.0000063994 | -2936.2749913967 |
| 55 | OT DIIS | 0.15E+00 | 100.47 | 0.0000061031 | -2936.2750752454 |
| 56 | OT DIIS | 0.15E+00 | 100.44 | 0.0000056017 | -2936.2751853134 |
| 57 | OT DIIS | 0.15E+00 | 100.61 | 0.0000052025 | -2936.2752663600 |
| 58 | OT DIIS | 0.15E+00 | 100.48 | 0.0000048079 | -2936.2753349818 |
| 59 | OT DIIS | 0.15E+00 | 100.45 | 0.0000045935 | -2936.2753609360 |
| 60 | OT DIIS | 0.15E+00 | 100.61 | 0.0000044832 | -2936.2753754145 |
| 61 | OT DIIS | 0.15E+00 | 100.82 | 0.0000041163 | -2936.2754470702 |
| 62 | OT DIIS | 0.15E+00 | 100.61 | 0.0000038626 | -2936.2754848811 |
| 63 | OT DIIS | 0.15E+00 | 100.55 | 0.0000037294 | -2936.2755096103 |
| 64 | OT DIIS | 0.15E+00 | 100.66 | 0.0000035602 | -2936.2755288918 |
| 65 | OT DIIS | 0.15E+00 | 100.47 | 0.0000033481 | -2936.2755822418 |
| 66 | OT DIIS | 0.15E+00 | 100.47 | 0.0000031967 | -2936.2755921725 |
| 67 | OT DIIS | 0.15E+00 | 100.64 | 0.0000029514 | -2936.2756443323 |
| 68 | OT DIIS | 0.15E+00 | 100.75 | 0.0000028273 | -2936.2756649861 |
| 69 | OT DIIS | 0.15E+00 | 100.50 | 0.0000027547 | -2936.2756812213 |
| 70 | OT DIIS | 0.15E+00 | 100.45 | 0.0000026056 | -2936.2757076056 |
| 71 | OT DIIS | 0.15E+00 | 100.61 | 0.0000024857 | -2936.2757311590 |
| 72 | OT DIIS | 0.15E+00 | 100.48 | 0.0000024000 | -2936.2757441775 |
| 73 | OT DIIS | 0.15E+00 | 100.42 | 0.0000022787 | -2936.2757680208 |
| 74 | OT DIIS | 0.15E+00 | 100.62 | 0.0000022338 | -2936.2757759464 |
| 75 | OT DIIS | 0.15E+00 | 100.61 | 0.0000021483 | -2936.2757906987 |
| 76 | OT DIIS | 0.15E+00 | 100.48 | 0.0000020668 | -2936.2758032392 |
| 77 | OT DIIS | 0.15E+00 | 100.42 | 0.0000020175 | -2936.2758107121 |
| 78 | OT DIIS | 0.15E+00 | 100.62 | 0.0000019409 | -2936.2758235877 |
| 79 | OT DIIS | 0.15E+00 | 100.50 | 0.0000018566 | -2936.2758355780 |
| 80 | OT DIIS | 0.15E+00 | 100.45 | 0.0000017387 | -2936.2758477138 |
| 81 | OT DIIS | 0.15E+00 | 100.94 | 0.0000017107 | -2936.2758508040 |
| 82 | OT DIIS | 0.15E+00 | 100.76 | 0.0000016367 | -2936.2758586491 |
| 83 | OT DIIS | 0.15E+00 | 100.62 | 0.0000015736 | -2936.2758644477 |
| 84 | OT DIIS | 0.15E+00 | 100.57 | 0.0000015325 | -2936.2758702348 |
| 85 | OT DIIS | 0.15E+00 | 100.75 | 0.0000015013 | -2936.2758755140 |
| 86 | OT DIIS | 0.15E+00 | 100.47 | 0.0000014437 | -2936.2758858471 |
| 87 | OT DIIS | 0.15E+00 | 100.58 | 0.0000013832 | -2936.2758946996 |
| 88 | OT DIIS | 0.15E+00 | 100.76 | 0.0000013551 | -2936.2758977707 |
| 89 | OT DIIS | 0.15E+00 | 100.64 | 0.0000013104 | -2936.2759028999 |
| 90 | OT DIIS | 0.15E+00 | 100.47 | 0.0000012927 | -2936.2759052921 |
| 91 | OT DIIS | 0.15E+00 | 100.44 | 0.0000012584 | -2936.2759100434 |
| 92 | OT DIIS | 0.15E+00 | 100.63 | 0.0000012255 | -2936.2759149870 |
| 93 | OT DIIS | 0.15E+00 | 100.48 | 0.0000012020 | -2936.2759183328 |
| 94 | OT DIIS | 0.15E+00 | 100.45 | 0.0000011895 | -2936.2759200520 |
| 95 | OT DIIS | 0.15E+00 | 100.64 | 0.0000011550 | -2936.2759248428 |
| 96 | OT DIIS | 0.15E+00 | 100.63 | 0.0000011340 | -2936.2759281307 |
| 97 | OT DIIS | 0.15E+00 | 100.52 | 0.0000011099 | -2936.2759320622 |

```
   98  OT DIIS        0.15E+00  100.59        0.0000010921    -2936.2759350439
   99  OT DIIS        0.15E+00  100.63        0.0000010357    -2936.2759459115
  100  OT DIIS        0.15E+00  100.48        0.0000009998    -2936.2759519512

 *** SCF run converged in   100 steps ***


 Total electronic density (r-space):       -863.9999894559     0.0000105441
 Total core charge density (r-space):       863.9999999346    -0.0000000654
 Total charge density (r-space):                                0.0000104787
 Total charge density (g-space):                                0.0000104787

 Overlap energy of the core charge distribution:              0.00000025798990
 Self energy of the core charge distribution:             -5601.27869639467644
 Core Hamiltonian energy:                                  1407.22232386328733
 Hartree energy:                                           1732.00401181841016
 Exchange-correlation energy:                              -474.22359149624782

 Total energy:                                            -2936.27595195123649

ENERGY| Total FORCE_EVAL ( QS ) energy (a.u.):            -2936.275958248451388


--------  Informations at step =     0 ------------
 Optimization Method        =                 BFGS
 Total Energy               =     -2936.2759582485
-------------------------------------------------


---------------------------
OPTIMIZATION STEP:      1
---------------------------

 Number of electrons:              864
 Number of occupied orbitals:      432
 Number of orbital functions:     1872

 Number of independent orbital functions:      1872

 Parameters for the always stable predictor-corrector (ASPC) method:

 ASPC order: 0

 B(1) =   1.000000

 Extrapolation method: ASPC


SCF WAVEFUNCTION OPTIMIZATION

 Step  Update method              Time         Convergence        Total energy
 ---------------------------------------------------------------------------

 ---------------------------------- OT -------------------------------------

 Allowing for rotations:  F
 minimizer      : DIIS                : direct inversion
                                        in the iterative subspace
                           using      : -   7 diis vectors
                                        - safer DIIS on
 preconditioner : FULL_SINGLE_INVERSE : cholesky inversion of H + eS
```

```
 stepsize       :    0.15000000
 energy_gap     :    0.20000000
 eps_taylor     :   0.10000E-15
 max_taylor     :             4

 ---------------------------------- OT ----------------------------------
    1  OT DIIS        0.15E+00  101.65        0.0000181125    -2936.2759972463
    2  OT DIIS        0.15E+00  101.03        0.0000138552    -2936.2760316341
    3  OT DIIS        0.15E+00  101.07        0.0000092173    -2936.2760715659
    4  OT DIIS        0.15E+00  101.54        0.0000051364    -2936.2760982299
    5  OT DIIS        0.15E+00  101.78        0.0000022306    -2936.2761079727
    6  OT DIIS        0.15E+00  101.93        0.0000012463    -2936.2761094213
    7  OT DIIS        0.15E+00  101.73        0.0000008481    -2936.2761098642

 *** SCF run converged in     7 steps ***


 Total electronic density (r-space):       -863.9999895230        0.0000104770
 Total core charge density (r-space):       863.9999999346       -0.0000000654
 Total charge density (r-space):                                  0.0000104116
 Total charge density (g-space):                                  0.0000104116

 Overlap energy of the core charge distribution:              0.00000025905408
 Self energy of the core charge distribution:             -5601.27869639467644
 Core Hamiltonian energy:                                  1407.23350147506335
 Hartree energy:                                           1731.99483496400626
 Exchange-correlation energy:                              -474.22575016767735

 Total energy:                                            -2936.27610986422997

ENERGY| Total FORCE_EVAL ( QS ) energy (a.u.):            -2936.276110159385098


--------  Informations at step =     1 ------------
 Optimization Method        =                  BFGS
 Total Energy               =     -2936.2761101594
 Real energy change         =        -0.0001519109
 Predicted change in energy =        -0.0000206944
 Scaling factor             =         0.0000000000
 Step size                  =         0.0045113842
 Trust radius               =         0.1000000000
 Decrease in energy         =                  YES

 Convergence check :
 Max. step size             =         0.0008138857
 Conv. limit for step size  =         0.0030000000
 Convergence in step size   =                  YES
 RMS step size              =         0.0003573973
 Conv. limit for RMS step   =         0.0015000000
 Convergence in RMS step    =                  YES
 Max. gradient              =         0.0007871494
 Conv. limit for gradients  =         0.0009725000
 Conv. in gradients         =                  YES
 RMS gradient               =         0.0003673384
 Conv. limit for RMS grad.  =         0.0003000000
 Conv. for gradients        =                   NO
 -----------------------------------------------------

...............
...............
```

```
.............. Intermediate steps not shown here
.............. but will be present in real output file
..............
..............
```

```
 --------------------------
 OPTIMIZATION STEP:     12
 --------------------------

  Number of electrons:                864
  Number of occupied orbitals:        432
  Number of orbital functions:       1872

  Number of independent orbital functions:      1872

  Parameters for the always stable predictor-corrector (ASPC) method:

  ASPC order: 3

  B(1) =   3.000000
  B(2) =  -3.428571
  B(3) =   1.928571
  B(4) =  -0.571429
  B(5) =   0.071429

  Extrapolation method: ASPC


 SCF WAVEFUNCTION OPTIMIZATION

  Step  Update method              Time         Convergence        Total energy
  ------------------------------------------------------------------------------

  ----------------------------------- OT -------------------------------------

  Allowing for rotations:  F
  minimizer      : DIIS                : direct inversion
                                         in the iterative subspace
                           using       : -   7 diis vectors
                                         - safer DIIS on
  preconditioner : FULL_SINGLE_INVERSE : cholesky inversion of H + eS
  stepsize       :    0.15000000
  energy_gap     :    0.20000000
  eps_taylor     :   0.10000E-15
  max_taylor     :             4

  ----------------------------------- OT -------------------------------------
     1  OT DIIS        0.15E+00  103.09        0.0000300341    -2936.3075420728
     2  OT DIIS        0.15E+00  102.98        0.0000212896    -2936.3076341668
     3  OT DIIS        0.15E+00  102.82        0.0000117748    -2936.3077276448
     4  OT DIIS        0.15E+00  103.20        0.0000063712    -2936.3077674392
     5  OT DIIS        0.15E+00  103.11        0.0000027558    -2936.3077811097
     6  OT DIIS        0.15E+00  103.08        0.0000015615    -2936.3077830609
     7  OT DIIS        0.15E+00  102.91        0.0000009244    -2936.3077837255

  *** SCF run converged in     7 steps ***


  Total electronic density (r-space):       -863.9999862125        0.0000137875
```

```
 Total core charge density (r-space):       863.9999999349       -0.0000000651
 Total charge density (r-space):                                  0.0000137224
 Total charge density (g-space):                                  0.0000137224

 Overlap energy of the core charge distribution:                0.00000046876769
 Self energy of the core charge distribution:               -5601.27869639467644
 Core Hamiltonian energy:                                    1409.26427946303306
 Hartree energy:                                             1730.37165547226300
 Exchange-correlation energy:                                 -474.66502273490249

 Total energy:                                              -2936.30778372551458

ENERGY| Total FORCE_EVAL ( QS ) energy (a.u.):              -2936.307784004529822


--------  Informations at step =    12 ------------
 Optimization Method        =                  BFGS
 Total Energy               =     -2936.3077840045
 Real energy change         =        -0.0000147132
 Predicted change in energy =        -0.0000148520
 Scaling factor             =         0.4104841534
 Step size                  =         0.0070297495
 Trust radius               =         0.1000000000
 Decrease in energy         =                  YES

 Convergence check :
 Max. step size             =         0.0013342515
 Conv. limit for step size  =         0.0030000000
 Convergence in step size   =                  YES
 RMS step size              =         0.0005569052
 Conv. limit for RMS step   =         0.0015000000
 Convergence in RMS step    =                  YES
 Max. gradient              =         0.0001731547
 Conv. limit for gradients  =         0.0009725000
 Conv. in gradients         =                  YES
 RMS gradient               =         0.0000437903
 Conv. limit for RMS grad.  =         0.0003000000
 Conv. in RMS gradients     =                  YES
---------------------------------------------------

*******************************************************************************
***                    GEOMETRY OPTIMIZATION COMPLETED                      ***
*******************************************************************************

                  Reevaluating energy at the minimum

 Number of electrons:              864
 Number of occupied orbitals:      432
 Number of orbital functions:     1872

 Number of independent orbital functions:      1872

 Parameters for the always stable predictor-corrector (ASPC) method:

 ASPC order: 3

 B(1) =   3.000000
 B(2) =  -3.428571
 B(3) =   1.928571
 B(4) =  -0.571429
```

```
 B(5) =   0.071429

 Extrapolation method: ASPC


SCF WAVEFUNCTION OPTIMIZATION

 Step  Update method              Time         Convergence        Total energy
 ---------------------------------------------------------------------------

 ---------------------------------- OT -------------------------------------

 Allowing for rotations:  F
 minimizer      : DIIS                : direct inversion
                                        in the iterative subspace
                           using      : -   7 diis vectors
                                        - safer DIIS on
 preconditioner : FULL_SINGLE_INVERSE : cholesky inversion of H + eS
 stepsize       :    0.15000000
 energy_gap     :    0.20000000
 eps_taylor     :   0.10000E-15
 max_taylor     :             4

 ---------------------------------- OT -------------------------------------
    1  OT DIIS        0.15E+00  102.85        0.0000082169    -2936.3077613357
    2  OT DIIS        0.15E+00  102.95        0.0000061282    -2936.3077683749
    3  OT DIIS        0.15E+00  102.91        0.0000037746    -2936.3077766768
    4  OT DIIS        0.15E+00  103.28        0.0000023402    -2936.3077811950
    5  OT DIIS        0.15E+00  103.15        0.0000012238    -2936.3077833846
    6  OT DIIS        0.15E+00  102.97        0.0000006673    -2936.3077839031

 *** SCF run converged in     6 steps ***


 Total electronic density (r-space):       -863.9999862125        0.0000137875
 Total core charge density (r-space):       863.9999999349       -0.0000000651
 Total charge density (r-space):                                  0.0000137224
 Total charge density (g-space):                                  0.0000137224

 Overlap energy of the core charge distribution:              0.00000046876769
 Self energy of the core charge distribution:             -5601.27869639467644
 Core Hamiltonian energy:                                  1409.26468064107280
 Hartree energy:                                           1730.37126869789108
 Exchange-correlation energy:                              -474.66503731615683

 Total energy:                                            -2936.30778390310115

ENERGY| Total FORCE_EVAL ( QS ) energy (a.u.):            -2936.307783903101154


-----------------------------------------------------------------------------
-                                                                           -
-                           R E F E R E N C E S                             -
-                                                                           -
-----------------------------------------------------------------------------

CP2K version 2.0.0 (Development Version), the CP2K developers group (2008).
CP2K is freely available from http://cp2k.berlios.de/ .

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## T I M I N G

```
-                                                                              -
-------------------------------------------------------------------------------
SUBROUTINE                       CALLS  ASD   CPU TIME T  PERFORMANCE ELAPSED TIME
CP2K                                 1  1.0   47899.53 I       ---        47922.84
cp_geo_opt                           1  2.0   47897.82 I       ---        47920.38
geoopt_bfgs                          1  3.0   47897.82 I       ---        47920.38
cp_eval_at                          14  4.0   47892.35 I       ---        47910.47
qs_forces                           13  5.0   46935.22 I       ---        46952.69
qs_energies                         14  5.9   23732.91 I       ---        23746.75
build_core_hamiltonian_matri       13e 6.0   23029.40 I       ---        23033.50
scf_env_do_scf                      201  7.9   20972.33 I       ---        20992.68
qs_ks_build_kohn_sham_matrix        200  9.8   10612.79 I       ---        10614.66
qs_ks_update_qs_env                 201  9.0    9522.05 I       ---         9523.75
integrate_v_rspace                  200 10.8    9342.55 I       ---         9344.15
calculate_rho_elec                  201  9.0    6709.81 I       ---         6711.04
build_core_hamiltonian_matri         14  6.9    3464.70 I       ---         3465.26
ot_scf_mini                         187  9.0    3099.29 I       ---         3099.83
cp_fm_gemm                         3344 12.2    2871.78 I   0.8 Gflops      2872.34
ot_mini                             187 10.0    2200.40 I       ---         2200.75
init_scf_loop                        14  7.9    1165.30 I       ---         1165.51
qs_ot_get_derivative                187 11.0    1134.69 I       ---         1134.88
apply_preconditioner                201 11.0    1115.23 I       ---         1115.40
qs_ks_update_qs_env (forces)         13  6.0    1092.70 I       ---         1092.88
cp_sm_fm_multiply_general           515 10.3    1067.19 I       ---         1067.41
sparse_times_local                  515 11.3    1051.47 I   1.5 Gflops      1051.65
-------------------------------------------------------------------------------

 **** **** ******  **  PROGRAM ENDED AT                   20100513 025135.615
***** ** ***  *** **   PROGRAM RAN ON                     compute-0-3.local
**    ****   ******    PROGRAM RAN BY                            nadeskins
***** **    ** ** **   PROGRAM PROCESS ID                            4577
 **** **  *******  **  PROGRAM STARTED IN          /home/nadeskins/work9/tmp3
```