./Job.out output for 176: Be S C30 (P1) ~ OBBe/Soptimisation_4x4x1_1 (VASP)

Status: finished

```
Startup is 'sourced'
Opening the database
 MedeA db: 'C:/MD/Databases/MedeA.db'


CALCULATION PROTOCOL:
=====================
1. Geometry optimization (atom positions)
     Saved properties in this step: charge density
2. Calculate superposed atomic charge densities for difference charge density
3. Total charge density and Bader charge analysis


VASP parameters
===============
This is a calculation based on density functional theory and the GGA-PBE exchange-correlation
functional for describing the interactions.

This is a non-magnetic calculation using 'normal' precision
and a default planewave cutoff energy of 400.000 eV.

The electronic iterations convergence is 1.00E-005 eV using the Fast (Davidson and RMM-DIIS)
algorithm
and real space projection operators.

Explicit k-mesh of 6x6x1 used
This corresponds to actual k-spacings of 0.123 x 0.123 x 0.449 per Angstrom.
The k-mesh is forced to be centered on the gamma point.

Using Gaussian smearing with a width of 0.2 eV.

Other non-default parameters:
        (Pseudo, difference,
spin) charge density is TRUE
=========================================

Using GGA-PBE / PAW potentials:
        C
        Be
        S

There are 13 symmetry-unique k-points
The plane wave cutoff is 400.00 eV

   VASP energy:            -277.426046 eV for BeSC30

   Initial VASP energy:    -271.721770 eV for BeSC30
   Relaxation energy:        -5.704276 eV gained after 23 optimization steps.

Electronic contributions:
                          Empirical Formula          Cell
                                BeSC30          BeSC30
                          --------------- ---------------
              VASP Energy      -26767.538      -26767.538 kJ/mol

Cell parameters:
 Parameter    Value
---------- ------------
         a     9.840000
         b     9.840000
         c    14.000000
     alpha    90.000000
      beta    90.000000
     gamma   120.000000
```

```
    Volume  1173.948010 Ang^3

        Density:     0.568 Mg/m^3

   The pressure given below is exerted by the system according to its volume.
   Positive pressure would cause expansion during full geometry optimization.
       Pressure:     4.397 GPa
              =    43.970 kbar

                      XX         YY         ZZ         XY         YZ         ZX
        Stress:    -6.451     -7.316      0.576     -0.000     -0.000      0.749 GPa
               =   -64.511    -73.164      5.759     -0.000     -0.000      7.494 kbar
   The stress tensor above is imposed on the system, i.e. negative values of diagonal components
   would cause expansion of the corresponding lattice parameter upon full geometry optimization.
   The pressure and stress include only electronic terms, i.e. the vibrational,
   temperature and other terms are not included here.

Fractional Coordinates:
        Atom          Initial Coordinates            Final Coordinates
        -----      -------- -------- --------      -------- -------- --------
        C1           0.0833   0.1667   0.5000        0.0849   0.1675   0.5000
        C2           0.1667   0.0833   0.5000        0.1633   0.0763   0.5000
        C3           0.0833   0.4167   0.5000        0.0818   0.4184   0.5000
        C4           0.1667   0.3333   0.5000        0.1633   0.3370   0.5000
        C5           0.0833   0.6667   0.5000        0.0829   0.6665   0.5000
        C6           0.1667   0.5833   0.5000        0.1664   0.5846   0.5000
        C7           0.0833   0.9167   0.5000        0.0818   0.9134   0.5000
        C8           0.1667   0.8333   0.5000        0.1664   0.8317   0.5000
        C9           0.3333   0.1667   0.5000        0.3243   0.1439   0.5000
        C10          0.4167   0.0833   0.5000        0.4154   0.0750   0.5000
        C11          0.3333   0.4167   0.5000        0.3243   0.4304   0.5000
        Be1          0.4167   0.3333   0.5000        0.3839   0.3169   0.5000
        C13          0.3333   0.6667   0.5000        0.3327   0.6709   0.5000
        C14          0.4167   0.5833   0.5000        0.4154   0.5903   0.5000
        C15          0.3333   0.9167   0.5000        0.3327   0.9118   0.5000
        C16          0.4167   0.8333   0.5000        0.4179   0.8339   0.5000
        C17          0.5833   0.1667   0.5000        0.5849   0.1606   0.5000
        C18          0.6667   0.0833   0.5000        0.6698   0.0815   0.5000
        S1           0.5833   0.4167   0.5000        0.5820   0.4160   0.5000
        C20          0.6667   0.3333   0.5000        0.6792   0.3236   0.5000
        C21          0.5833   0.6667   0.5000        0.5849   0.6742   0.5000
        C22          0.6667   0.5833   0.5000        0.6792   0.6055   0.5000
        C23          0.5833   0.9167   0.5000        0.5846   0.9173   0.5000
        C24          0.6667   0.8333   0.5000        0.6698   0.8382   0.5000
        C25          0.8333   0.1667   0.5000        0.8358   0.1668   0.5000
        C26          0.9167   0.0833   0.5000        0.9201   0.0851   0.5000
        C27          0.8333   0.4167   0.5000        0.8402   0.4168   0.5000
        C28          0.9167   0.3333   0.5000        0.9190   0.3329   0.5000
        C29          0.8333   0.6667   0.5000        0.8402   0.6733   0.5000
        C30          0.9167   0.5833   0.5000        0.9183   0.5842   0.5000
        C31          0.8333   0.9167   0.5000        0.8358   0.9190   0.5000
        C32          0.9167   0.8333   0.5000        0.9190   0.8361   0.5000

Analytic Derivatives:
        Atom          Derivatives fractional      Derivatives Cartesian (eV/Ang)
        -----      -------- -------- --------     -------- -------- --------
        C1           -0.0000  -0.0000   0.0000      -0.0004  -0.0002   0.0000
        C2           -0.0004  -0.0005   0.0000      -0.0016  -0.0042   0.0000
        C3           -0.0001   0.0008   0.0000      -0.0045   0.0070   0.0000
        C4           -0.0004   0.0001   0.0000      -0.0044   0.0007   0.0000
        C5            0.0004   0.0002   0.0000       0.0028   0.0016   0.0000
        C6           -0.0002  -0.0001   0.0000      -0.0015  -0.0008   0.0000
        C7           -0.0001  -0.0009   0.0000       0.0038  -0.0074   0.0000
        C8           -0.0002  -0.0001   0.0000      -0.0014  -0.0009   0.0000
        C9           -0.0001  -0.0000   0.0000      -0.0009  -0.0003   0.0000
        C10          -0.0000  -0.0011   0.0000       0.0050  -0.0091   0.0000
        C11          -0.0001  -0.0001   0.0000      -0.0007  -0.0006   0.0000
        Be1           0.0001   0.0001   0.0000       0.0008   0.0004   0.0000
        C13           0.0003   0.0014   0.0000      -0.0041   0.0122   0.0000
        C14          -0.0000   0.0010   0.0000      -0.0054   0.0089   0.0000
        C15           0.0003  -0.0011   0.0000       0.0085  -0.0097   0.0000   maximum gradient =
0.0129
        C16          -0.0004  -0.0002   0.0000      -0.0029  -0.0016   0.0000
        C17          -0.0003   0.0003   0.0000      -0.0042   0.0027   0.0000
        C18           0.0004   0.0007   0.0000       0.0005   0.0055   0.0000
        S1            0.0007   0.0003   0.0000       0.0049   0.0028   0.0000
        C20           0.0013   0.0010   0.0000       0.0079   0.0084   0.0000
        C21          -0.0003  -0.0006   0.0000       0.0002  -0.0050   0.0000
        C22           0.0013   0.0003   0.0000       0.0112   0.0027   0.0000
        C23           0.0008   0.0004   0.0000       0.0056   0.0032   0.0000
        C24           0.0004  -0.0003   0.0000       0.0051  -0.0023   0.0000
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        C25          -0.0001   0.0002   0.0000     -0.0019   0.0019   0.0000
        C26          -0.0005  -0.0003   0.0000     -0.0039  -0.0023   0.0000
        C27          -0.0012  -0.0002   0.0000     -0.0105  -0.0017   0.0000
        C28          -0.0002  -0.0003   0.0000     -0.0008  -0.0023   0.0000
        C29          -0.0012  -0.0010   0.0000     -0.0067  -0.0082   0.0000
        C30           0.0002   0.0001   0.0000      0.0014   0.0008   0.0000
        C31          -0.0001  -0.0003   0.0000      0.0007  -0.0026   0.0000
        C32          -0.0002   0.0001   0.0000     -0.0025   0.0004   0.0000

SUPERPOSITION OF ATOMIC CHARGE DENSITIES
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TOTAL CHARGE DENSITY AND BADER CHARGE ANALYSIS
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Fourier grid for calculations, so far:   48 x 48 x 70
Smallest Fourier grid avoiding aliasing: 66 x 66 x 90
Increase the Fourier grid by 0%
Fourier grid for total charge density:   66 x 66 x 90

Restarting from 176:./CHGCAR

Bader valence electron charges, charge transfer (relative to atoms) and Bader volumes:
        Atom          Valence     Charge    Volume    Distance
                       charge    transfer   (Ang^3)     (Ang)
        -----        ---------  ---------  ---------  ---------
        C1              4.0304    -0.0304    13.0961     0.6426
        C2              3.8594     0.1406    12.1907     0.5893
        C3              4.1122    -0.1122    12.6918     0.6172
        C4              4.0759    -0.0759    12.7131     0.5893
        C5              3.8241     0.1759    11.7598     0.5911
        C6              3.9507     0.0493    12.4446     0.6358
        C7              4.1111    -0.1111    12.4848     0.6348
        C8              3.9438     0.0562    12.4333     0.6000
        C9              4.5616    -0.5616    17.5703     0.5325
        C10             3.9516     0.0484    12.2649     0.6395
        C11             4.5171    -0.5171    17.3879     0.5733
        Be1             0.4430     1.5570     1.9346     0.4191
        C13             4.1496    -0.1496    12.9434     0.6299
        C14             4.0213    -0.0213    12.6842     0.5793
        C15             4.1500    -0.1500    12.9866     0.6139
        C16             3.9920     0.0080    12.4037     0.5941
        C17             4.0208    -0.0208    12.7085     0.5796
        C18             3.9867     0.0133    12.4732     0.5692
        S1              5.8010     0.1990    25.2542     0.7164
        C20             4.4503    -0.4503    12.9823     0.6742
        C21             4.0301    -0.0301    12.6545     0.5796
        C22             4.3064    -0.3064    12.4692     0.6276
        C23             3.8278     0.1722    11.8832     0.5834
        C24             4.0020    -0.0020    12.2795     0.5692
        C25             3.9480     0.0520    12.4333     0.6292
        C26             4.0766    -0.0766    12.8921     0.6031
        C27             4.0264    -0.0264    12.2822     0.5867
        C28             3.9661     0.0339    12.4579     0.5513
        C29             4.1303    -0.1303    12.7161     0.6366
        C30             3.9241     0.0759    12.6545     0.5959
        C31             3.7493     0.2507    12.0676     0.5877
        C32             4.0111    -0.0111    12.3647     0.6127
        Vacuum          0.0496    -0.0496   761.3851
        -----        ---------  ---------  ---------
        Total         128.0000     0.0000    1173.95

Job completed on Tue 05 April 2016 at 00:26:25 +0200 after 4649 s (1:17:29)
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