

```

#
# File Name
#

System.CurrentDirectory    ./ # default=./
System.Name                graphene
DATA.PATH                 ../../../../DFT_DATA13
level.of.stdout           1 # default=1 (1-3)
level.of.fileout          1 # default=1 (0-2)

#
# Definition of Atomic Species
#

Species.Number            1
<Definition.of.Atomic.Species
C C6.0-s2p1 C_PBE13
Definition.of.Atomic.Species>

#
# Atoms
#

Atoms.Number              4
Atoms.SpeciesAndCoordinates.Unit Ang # Ang|AU
<Atoms.SpeciesAndCoordinates
1 C 0.000000000 0.000000000 0.000000000 2.0 2.0
2 C 1.229756073 0.710000000 0.000000000 2.0 2.0
3 C 1.229756073 2.130000000 0.000000000 2.0 2.0
4 C 0.000000000 2.840000000 0.000000000 2.0 2.0
Atoms.SpeciesAndCoordinates>
Atoms.UnitVectors.Unit    Ang # Ang|AU
<Atoms.UnitVectors
2.45951214700000 0.000000000000000 0.000000000000000
0.000000000000000 4.26000000000000 0.000000000000000
0.000000000000000 0.000000000000000 20.000000000000000
Atoms.UnitVectors>

#
# SCF or Electronic System
#

scf.XcType                GGA-PBE # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization       on # On|Off|NC
scf.ElectronicTemperature 300.0 # default=300 (K)
scf.energycutoff           250.0 # default=150 (Ry)
scf.maxIter                200 # default=40
scf.EigenvalueSolver       Band # DC|GDC|Cluster|Band
scf.lapack.dste             dstevx # dstegr|dstedc|dstevx, default=dstegr
scf.Kgrid                  13 13 1 # means n1 x n2 x n3
scf.Mixing.Type            rmm-diisk # Simple|Rmm-Diis|Gr-Pulay|Kerker|Rmm-Diisk

```

```
scf.Init.Mixing.Weight 0.30 # default=0.30
scf.Min.Mixing.Weight 0.001 # default=0.001
scf.Max.Mixing.Weight 0.40 # default=0.40
scf.Mixing.History 5 # default=5
scf.Mixing.StartPulay 6 # default=6
scf.Mixing.EveryPulay 6 # default=6scf.criterion 1.0e-10 # default=1.0e-6
(Hartree)
```

```
#
# MD or Geometry Optimization
#
```

```
MD.Type Nomd # Opt|EF|BFGS|RF|DIIS
MD.Opt.DIIS.History 6 # default=3
MD.Opt.StartDIIS 7 # default=5
MD.Opt.EveryDIIS 6 # default=10
MD.maxIter 200 #
MD.Opt.criterion 1.0e-4 # default=1.0e-4 (a.u.)
```

```
#
# Band dispersion
#
```

```
Band.dispersion on # on|off, default=off
# if <Band.KPath.UnitCell does not exist,
# the reciprocal lattice vector is employed.
```

```
Band.Nkpath 6
<Band.kpath
 600 0.000000 0.000 0.0 0.3333333 0.000 0.0 G P
 600 0.3333333 0.000 0.0 0.5000000 0.000 0.0 P X
 600 0.5000000 0.000 0.0 0.5000000 0.500 0.0 X W
 600 0.5000000 0.500 0.0 0.0000000 0.500 0.0 W Y
 600 0.0000000 0.500 0.0 0.0000000 0.000 0.0 Y G
 600 0.0000000 0.000 0.0 0.5000000 0.500 0.0 G W
Band.kpath>
```

```
#
# DOS and PDOS
#
```

```
Dos.fileout off # on|off, default=off
Dos.Erange -15.0 25.0 # default = -20 20
Dos.Kgrid 300 300 1 # default = Kgrid1 Kgrid2 Kgrid3
```

```
DosGauss.fileout off
DosGauss.Num.Mesh 4000
DosGauss.Width 0.01
```