sample cp2k input with comments

```
&FORCE_EVAL
  METHOD Quickstep
  &DFT
    UKS
    BASIS_SET_FILE_NAME ./GTH_BASIS_SETS
    POTENTIAL_FILE_NAME ./GTH_POTENTIALS
    WFN_RESTART_FILE_NAME x-RESTART.wfn
    &MGRID
      CUTOFF 300
    &END MGRID
    &QS
      WF_INTERPOLATION ASPC
      EXTRAPOLATION_ORDER 3
    &END QS
    &SCF
     EPS_SCF 1.E-6
     SCF_GUESS RESTART
     MAX_SCF 400
     &OT T
       PRECONDITIONER FULL_SINGLE_INVERSE
       MINIMIZER DIIS
       LINESEARCH 3PNT
     &END OT
    &END SCF
    &XC
      &XC_FUNCTIONAL PBE
      &END XC_FUNCTIONAL
    &END XC
  &PRINT
#  &TOPOLOGY_INFO
#     XYZ_INFO T
#   &END TOPOLOGY_INFO
#   &V_HARTREE_CUBE
#   FILENAME ./rut_elpot
#  &END V_HARTREE_CUBE
#  &E_DENSITY_CUBE
#   FILENAME ./rut_density
#  &END E_DENSITY_CUBE
#   &MO_CUBES
#      WRITE_CUBE T
#      NHOMO 2
#      NLUMO 1
#  &END MO_CUBES
  &END PRINT
  &END DFT
  &SUBSYS
    &CELL
      ABC 8.4 8.4 8.4
      UNIT SCALED_ANGSTROM
    &END CELL
    &COORD
 Mg 0 0 0
Mg 0.25 0.25 0
Mg 0.25 0 0.25
Mg 0 0.25 0.25
O 0.25 0 0
O 0 0.25 0
O 0 0 0.25
O 0.25 0.25 0.25
Mg 0.5 0 0
```

```
Mg 0.75 0.25 0
Mg 0.75 0 0.25
Mg 0.5 0.25 0.25
O 0.75 0 0
O 0.5 0.25 0
O 0.5 0 0.25
O 0.75 0.25 0.25
Mg 0 0.5 0
Mg 0.25 0.75 0
Mg 0.25 0.5 0.25
Mg 0 0.75 0.25
O 0.25 0.5 0
O 0 0.75 0
O 0 0.5 0.25
O 0.25 0.75 0.25
Mg 0.5 0.5 0
Mg 0.75 0.75 0
Mg 0.75 0.5 0.25
Mg 0.5 0.75 0.25
O 0.75 0.5 0
O 0.5 0.75 0
O 0.5 0.5 0.25
O 0.75 0.75 0.25
Mg 0 0 0.5
Mg 0.25 0.25 0.5
Mg 0.25 0 0.75
Mg 0 0.25 0.75
O 0.25 0 0.5
O 0 0.25 0.5
O 0 0 0.75
O 0.25 0.25 0.75
Mg 0.5 0 0.5
Mg 0.75 0.25 0.5
Mg 0.75 0 0.75
Mg 0.5 0.25 0.75
O 0.75 0 0.5
O 0.5 0.25 0.5
O 0.5 0 0.75
O 0.75 0.25 0.75
Mg 0 0.5 0.5
Mg 0.25 0.75 0.5
Mg 0.25 0.5 0.75
Mg 0 0.75 0.75
O 0.25 0.5 0.5
O 0 0.75 0.5
O 0 0.5 0.75
O 0.25 0.75 0.75
Mg 0.5 0.5 0.5
Mg 0.75 0.75 0.5
Mg 0.75 0.5 0.75
Mg 0.5 0.75 0.75
O 0.75 0.5 0.5
O 0.5 0.75 0.5
O 0.5 0.5 0.75
O 0.75 0.75 0.75
    &END COORD
    &KIND Mg
      BASIS_SET DZVP-GTH
      POTENTIAL GTH-PBE-q10
    &END KIND
```

```
    &KIND O
      BASIS_SET DZVP-MOLOPT-GTH
      POTENTIAL GTH-PBE-q6
    &END KIND
    &KIND H
      BASIS_SET DZVP-MOLOPT-GTH
      POTENTIAL GTH-PBE-q1
    &END KIND
    &KIND C
      BASIS_SET DZVP-MOLOPT-GTH
      POTENTIAL GTH-PBE-q4
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
&GLOBAL
  PROJECT MgO-bulk
  RUN_TYPE GEO_OPT
#  RUN_TYPE ENERGY
  PRINT_LEVEL LOW
&END GLOBAL
 &MOTION
  &GEO_OPT
    MAX_ITER 200
    MAX_FORCE 0.0009725
    OPTIMIZER BFGS
  &END GEO_OPT
# &CONSTRAINT
#   &FIXED_ATOMS
#    RANGE 145 192
#   &END FIXED_ATOMS
#  &END CONSTRAINT
 &END MOTION
```