

```

&CONTROL
  calculation = 'bands',
  restart_mode = 'from_scratch'
  prefix = 'A',
  outdir = './tmp-hetero/'
  pseudo_dir = './pseudo'
  tstress = .true.
  tprnfor = .true.
  verbosity = 'high'
  etot_conv_thr = 1.0D-4,
  forc_conv_thr = 1.0D-3,
/
&SYSTEM
 ibrav = 4,
nat = 2, ntyp = 1,
celldm(1) = 4.65,
celldm(3) = 3,
ecutwfc = 45,
ecutrho = 450,
starting_magnetization(1)=0.5,
starting_magnetization(2)=-0.5,
occupations = 'smearing',
nspin = 2,
degauss = 0.001 ,
smearing = 'm-v'
/
&ELECTRONS
diagonalization='david',
mixing_mode = 'plain',
mixing_beta = 0.7,
electron_maxstep = 200,
conv_thr = 1.0D-8,
/
&IONS
ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
  C 12.01 C.pbe-rrkjus.UPF

ATOMIC_POSITIONS (crystal)
C      0.0000000000    0.0000000000    0.5000000000
C      0.3333333300    0.6666666667    0.5000000000

K_POINTS crystal
  400
    0.0000000000    0.0000000000    0.0000000000    1.0
    0.0034246575    0.0000000000    0.0000000000    1.0
    0.0068493151    0.0000000000    0.0000000000    1.0
    0.0102739726    0.0000000000    0.0000000000    1.0
    0.0136986301    0.0000000000    0.0000000000    1.0
    0.0171232877    0.0000000000    0.0000000000    1.0
    0.0205479452    0.0000000000    0.0000000000    1.0
    0.0239726027    0.0000000000    0.0000000000    1.0
    0.0273972603    0.0000000000    0.0000000000    1.0
    0.0308219178    0.0000000000    0.0000000000    1.0
    0.0342465753    0.0000000000    0.0000000000    1.0
    0.0376712329    0.0000000000    0.0000000000    1.0
    0.0410958904    0.0000000000    0.0000000000    1.0
    0.0445205479    0.0000000000    0.0000000000    1.0
    0.0479452055    0.0000000000    0.0000000000    1.0
    0.0513698630    0.0000000000    0.0000000000    1.0
    0.0547945205    0.0000000000    0.0000000000    1.0

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0.0582191781	0.0000000000	0.0000000000	1.0
0.0616438356	0.0000000000	0.0000000000	1.0
0.0650684932	0.0000000000	0.0000000000	1.0
0.0684931507	0.0000000000	0.0000000000	1.0
0.0719178082	0.0000000000	0.0000000000	1.0
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0.0787671233	0.0000000000	0.0000000000	1.0
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0.0890410959	0.0000000000	0.0000000000	1.0
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0.1472602740	0.0000000000	0.0000000000	1.0
0.1506849315	0.0000000000	0.0000000000	1.0
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0.1712328767	0.0000000000	0.0000000000	1.0
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0.1780821918	0.0000000000	0.0000000000	1.0
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0.1735682840	0.1735682840	0.0000000000	1.0
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0.1676511834	0.1676511834	0.0000000000	1.0
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0.1360933136	0.1360933136	0.0000000000	1.0
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0.1321485799	0.1321485799	0.0000000000	1.0
0.1301762130	0.1301762130	0.0000000000	1.0
0.1282038462	0.1282038462	0.0000000000	1.0
0.1262314793	0.1262314793	0.0000000000	1.0
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0.0710052071	0.0710052071	0.0000000000	1.0
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0.0631157396	0.0631157396	0.0000000000	1.0
0.0611433728	0.0611433728	0.0000000000	1.0
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0.0236684024	0.0236684024	0.0000000000	1.0
0.0216960355	0.0216960355	0.0000000000	1.0

0.0197236686	0.0197236686	0.0000000000	1.0
0.0177513018	0.0177513018	0.0000000000	1.0
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0.0138065680	0.0138065680	0.0000000000	1.0
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0.0098618343	0.0098618343	0.0000000000	1.0
0.0078894675	0.0078894675	0.0000000000	1.0
0.0059171006	0.0059171006	0.0000000000	1.0
0.0039447337	0.0039447337	0.0000000000	1.0
0.0019723669	0.0019723669	0.0000000000	1.0
0.0000000000	0.0000000000	0.0000000000	1.0