# self-consistent calculation

cat > fe2o3.scf.in << EOF

 &control

 calculation='scf'

 restart\_mode='from\_scratch',

 prefix='fe2o3'

 pseudo\_dir = '$PSEUDO\_DIR/',

 outdir='$TMP\_DIR/'

 /

 &system

 ibrav= 5, celldm(1)= 11.091428, celldm(4)=0.587237, nat= 10, ntyp= 3,

 ecutwfc =30.0, ecutrho=240.0,

 nbnd=40,

 starting\_magnetization(1)= 1.0,

 starting\_magnetization(2)= -1.0,

 starting\_magnetization(3)= 0.0,

 occupations='smearing', smearing='gauss', degauss=0.03,

 nspin=2,

 lda\_plus\_u=.true. Hubbard\_U(2)=4.3, Hubbard\_U(3)=4.3

 /

 &electrons

 mixing\_mode = 'plain'

 mixing\_beta = 0.3

 conv\_thr = 1.0d-6

 /

ATOMIC\_SPECIES

 Fe1 1. Fe.pbe-nd-rrkjus.UPF

 Fe2 1. Fe.pbe-nd-rrkjus.UPF

 O 1. O.pbe-rrkjus.UPF

ATOMIC\_POSITIONS {crystal}

 Fe1 0.1444 0.1444 0.1444

 Fe1 0.8556 0.8556 0.8556

 Fe2 0.3556 0.3556 0.3556

 Fe2 0.6443 0.6443 0.6443

 O 0.5565 0.9435 0.2500

 O 0.2500 0.5565 0.9435

 O 0.9435 0.2500 0.5565

 O 0.4435 0.0565 0.7500

 O 0.7500 0.4435 0.0565

 O 0.0565 0.7500 0.4435

 K\_POINTS {automatic}

2 2 2 1 1 1

EOF

$ECHO " running the scf calculation...\c"

$PW\_COMMAND < fe2o3.scf.in > fe2o3.scf.out

check\_failure $?

$ECHO " done"

# post-processing for charge density

cat > fe2o3.pp\_rho.in << EOF

 &inputpp

 prefix = 'fe2o3'

 outdir = '$TMP\_DIR/'

 filplot = 'fe2o3charge'

 plot\_num= 0

 /

 &plot

 nfile = 1

 filepp(1) = 'fe2o3charge'

 weight(1) = 1.0

 iflag = 2

 output\_format = 2

 fileout = 'fe2o3.rho.dat'

 e1(1) =1.0, e1(2)=0.0, e1(3) = 0.0,

 e2(1) =0.0, e2(2)=1.0, e2(3) = 0.0,

 nx=40, ny=40

/

EOF

$ECHO " running pp.x to do a 2-d plot of the charge density...\c"

$PP\_COMMAND < fe2o3.pp\_rho.in > fe2o3.pp\_rho.out

check\_failure $?

$ECHO " done"

# plotrho

cat > fe2o3.plotrho.in << EOF

fe2o3.rho.dat

fe2o3.rho.ps

n

0 0.09 6

EOF

$ECHO " running plotrho.x to generate rho.ps...\c"

$PLOTRHO\_COMMAND < fe2o3.plotrho.in > fe2o3.plotrho.out

$ECHO " done"

# band structure calculation along high-symmetry lines

cat > fe2o3.band.in << EOF

 &control

 calculation='bands'

 pseudo\_dir = '$PSEUDO\_DIR/',

 outdir='$TMP\_DIR/',

 prefix='fe2o3'

 /

 &system

 ibrav= 5, celldm(1)= 11.091428, celldm(4)=0.587237, nat= 10, ntyp= 3,

 ecutwfc =30.0, ecutrho=240.0,

 nbnd=40,

 starting\_magnetization(1)= 1.0,

 starting\_magnetization(2)= -1.0,

 occupations='smearing', smearing='gauss', degauss=0.03,

 nspin=2,

 lda\_plus\_u=.true. Hubbard\_U(2)=4.3, Hubbard\_U(3)=4.3

 /

 &electrons

 mixing\_mode = 'plain'

 mixing\_beta = 0.3

 conv\_thr = 1.0d-6

 /

ATOMIC\_SPECIES

 Fe1 1. Fe.pbe-nd-rrkjus.UPF

 Fe2 1. Fe.pbe-nd-rrkjus.UPF

 O 1. O.pbe-rrkjus.UPF

ATOMIC\_POSITIONS {crystal}

 Fe1 0.1444 0.1444 0.1444

 Fe1 0.8556 0.8556 0.8556

 Fe2 0.3556 0.3556 0.3556

 Fe2 0.6443 0.6443 0.6443

 O 0.5565 0.9435 0.2500

 O 0.2500 0.5565 0.9435

 O 0.9435 0.2500 0.5565

 O 0.4435 0.0565 0.7500

 O 0.7500 0.4435 0.0565

 O 0.0565 0.7500 0.4435

K\_POINTS

21

 -0.5 1.0 0.0 1

 -0.4 0.8 0.0 2

 -0.3 0.6 0.0 3

 -0.2 0.4 0.0 4

 -0.1 0.2 0.0 5

 0.0 0.0 0.0 6

 0.0 0.2 0.1 7

 0.0 0.4 0.2 8

 0.0 0.6 0.3 9

 0.0 0.8 0.4 10

 0.0 1.0 0.5 11

 -0.1 0.9 0.5 12

 -0.2 0.8 0.5 13

 -0.3 0.7 0.5 14

 -0.4 0.6 0.5 15

 -0.5 0.5 0.5 16

 -0.4 0.4 0.4 17

 -0.3 0.3 0.3 18

 -0.2 0.2 0.2 19

 -0.1 0.1 0.1 20

 0.0 0.0 0.0 21

/

EOF

$ECHO " running the band-structure calculation for fe2o3...\c"

$PW\_COMMAND < fe2o3.band.in > fe2o3.band.out

check\_failure $?

$ECHO " done"

# post-processing for band structure

cat > fe2o3.bands.in << EOF

 &bands

 prefix = 'fe2o3'

 outdir = '$TMP\_DIR/'

 filband = 'fe2o3bands.dat'

/

EOF

$ECHO " running the post-processing for band structure...\c"

$BANDS\_COMMAND < fe2o3.bands.in > fe2o3.bands.out

check\_failure $?

$ECHO " done"

# plotband.x

cat > fe2o3.plotband.in << EOF

fe2o3bands.dat

-20.0 40

fe2o3bands.xmgr

fe2o3bands.ps

5.4685

1.0 5.4685

EOF

$ECHO " running plotband.x to generate fe2o3bands.ps...\c"

$PLOTBAND\_COMMAND < fe2o3.plotband.in > fe2o3.plotband.out

check\_failure $?

$ECHO " done"

$ECHO

$ECHO "$EXAMPLE\_DIR: done"