# 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"