```
!234567890
!      Written by In-Ho Lee, KRISS, September 11, 2013.
       module eigenvalues
       implicit none
       private
       save
       integer ne,nk,nbandi
       real*8 ef,temper
       logical ldirect
       real*8, allocatable :: rkpt(:,:),eiv(:,:),wgt(:),cblowest(:),vbhighest(:)

       public :: ne,nk,nbandi,rkpt,eiv,wgt,ef,temper,cblowest,vbhighest,ldirect
       end module eigenvalues
!234567890
!      Written by In-Ho Lee, KRISS, September 11, 2013.
       subroutine egp_test(otname,einame,egp1,egp2,lfault)
       USE eigenvalues, ONLY : ldirect
       implicit none
       logical lfault
       character*280 otname,einame,cname1
       character*80 string0
       integer islc
       real*8 egp1,egp2
       logical lfault1,lfault2,lfault3,lfault7

       lfault=.false.
       lfault1=.false.
       lfault2=.false.
       lfault3=.false.
       egp1=-1.d0
       egp2=-1.d0
       call read_outcar1(otname,lfault1)
       if(lfault1) goto 911
       call read_eigenval(einame,lfault2)
       if(lfault2) goto 911
       call check_gap(egp1,egp2,lfault3)
       if(.not. lfault3)then
       if(ldirect)then
       islc=len_trim(otname) ; islc=islc-6 ; cname1=otname(1:islc) ; cname1=trim
(cname1)//'CONTCAR'
       lfault7=.false.
       open(71,file=trim(cname1),form='formatted')
       do
       read(71,'(a80)',err=711,end=799) string0
       if(len_trim(string0) == 0) goto 799
       if(len_trim(string0) > 0) write(6,*) trim(string0)
       enddo
  711  continue
       lfault7=.true.
  799  continue
       close(71)
                  endif
                        endif
  911  continue
       if(lfault1 .or. lfault2 .or. lfault3) lfault=.true.
       if(lfault)then
       egp1=0.d0
       egp2=0.d0
                  endif
       if(egp1 <= -1.d0) egp1=0.d0
       if(egp2 <= -1.d0) egp2=0.d0
       end
!234567890
!      Written by In-Ho Lee, KRISS, July 3, 2014.
       subroutine eds_test(otname,einame,test,lfault)
       implicit none
       logical lfault
       character*280 otname,einame
       real*8 test
```



```
       logical lfault1,lfault2,lfault3
       real*8 test0,test1

       lfault=.false.
       lfault1=.false.
       lfault2=.false.
       lfault3=.false.
       test0=0.d0
       test1=0.d0
       call read_outcar1(otname,lfault1)
       if(lfault1) goto 911
       call read_eigenval(einame,lfault2)
       if(lfault2) goto 911
       call check_dos(test0,test1,lfault3)
  911  continue
       test=test0
       if(lfault1 .or. lfault2 .or. lfault3) lfault=.true.
       end
!234567890
!      Written by In-Ho Lee, KRISS, July 3, 2014.
       subroutine eds_test1(otname,einame,test,lfault)
       implicit none
       logical lfault
       character*280 otname,einame
       real*8 test
       logical lfault1,lfault2,lfault3
       real*8 test0,test1

       lfault=.false.
       lfault1=.false.
       lfault2=.false.
       lfault3=.false.
       test0=0.d0
       test1=0.d0
       call read_outcar1(otname,lfault1)
       if(lfault1) goto 911
       call read_eigenval(einame,lfault2)
       if(lfault2) goto 911
       call check_dos(test0,test1,lfault3)
  911  continue
       test=test1
       if(lfault1 .or. lfault2 .or. lfault3) lfault=.true.
       end
!234567890
!      Written by In-Ho Lee, KRISS, December 2, 2014.
       subroutine eds_test2(otname,einame,test,lfault)
       implicit none
       logical lfault
       character*280 otname,einame
       real*8 test
       logical lfault1,lfault2,lfault3
       real*8 test0,test1

       lfault=.false.
       lfault1=.false.
       lfault2=.false.
       lfault3=.false.
       test0=0.d0
       test1=0.d0
       call read_outcar1(otname,lfault1)
       if(lfault1) goto 911
       call read_eigenval(einame,lfault2)
       if(lfault2) goto 911
       call check_emass(test0,test1,lfault3)
  911  continue
       test=test1 ; if(test > test0) test=test0
       if(lfault1 .or. lfault2 .or. lfault3) lfault=.true.
       end
!234567890
```

```
!       Written by In-Ho Lee, KRISS, September 11, 2013.
        subroutine emass_test(otname,einame,tstm1,tstm2,gapsize,lfault)
        USE strings, ONLY : parse,value
        implicit none
        character*280 otname,einame
        real*8 tstm1,tstm2,gapsize
        logical lfault,lexist
        character*280 cemcout
        character*80 string0
        integer islc,kount
        logical lfault1,lfault2
        integer ios,nargs
        character*200 str1
        character*200 args(40)
        character*20 delims

        lfault=.false.
        lfault1=.false. ; lfault2=.false.
        gapsize=-1.d22
        call read_outcar1(otname,lfault1)
        if(lfault1) goto 911
        islc=len_trim(otname) ; islc=islc-6 ; cemcout=otname(1:islc) ; cemcout=tr
im(cemcout)//'EMCOUT'
        kount=0
        inquire(file=trim(cemcout),exist=lexist)
        if(.not. lexist)then
        lfault1=.true.
        goto 911
                        endif
        open(72,file=trim(cemcout),form='formatted')
        do
        kount=kount+1
        read(72,'(a80)',err=711,end=799) string0
        delims=' '
        call parse(string0,delims,args,nargs)
        if(nargs >= 2)then
        if(args(1) == 'serious')then
        if(args(2) == 'problem')then
        tstm1=1.d6 ; tstm2=1.d6
        goto 711
                                endif
                                endif
                        endif
        if(nargs > 0)then
        if(kount == 1)then
        call value(args(1),tstm1,ios)
        if(ios /= 0) tstm1=1.d6
                        endif
        if(kount == 2)then
        call value(args(1),tstm2,ios)
        if(ios /= 0) tstm2=1.d6
                        endif
                       endif
        if(len_trim(string0) == 0) goto 799
        if(len_trim(string0) > 0) write(6,*) trim(string0)
        if(kount == 2) goto 799
        enddo
  711   continue
        lfault2=.true.
  799   continue
        read(72,*) gapsize
        write(6,*) gapsize,' gapsize'
        close(72)
  911   continue
        if(lfault1) lfault=.true.
        if(lfault2) lfault=.true.
        end
!234567890
!       Written by In-Ho Lee, KRISS, September 11, 2013.
```



```
        subroutine read_outcar1(otname,lfault1)
        USE eigenvalues, ONLY : ef
        implicit none
        character*280 otname
        logical lfault1
        character*7 ctest7
        logical lfault

        lfault=.false.
        ef=1.d19
        open(81,file=trim(otname),form='formatted')
        do
        read(81,*,err=911,end=999) ctest7
        if(ctest7 == 'E-fermi')then
        backspace(81)
        read(81,101,err=911,end=999) ef
                                endif
  101   format(10x,f9.4)
        enddo
  911   continue
        lfault=.true.
  999   continue
        close(81)
!       write(6,*) ef,' ef from OUTCAR'
!
        if(lfault)then
        ef=1.d19
        write(6,*) 'there is a falut with OUTCAR'
                endif
        lfault1=lfault
        end
!234567890
!       Written by In-Ho Lee, KRISS, September 11, 2013.
        subroutine read_eigenval(einame,lfault1)
        USE eigenvalues, ONLY : ef,rkpt,wgt,eiv,ne,nk,nbandi,temper
        implicit none
        character*280 einame
        logical lfault1
        integer j,i,ik
        real*8 tmpx,tmpy,tmpz,sol1,sol2,tol
        logical lfault
        real*8, external ::  fdft,zeroin

        lfault=.false.
        ne=0
        nk=0
        nbandi=0
        open(81,file=trim(einame),form='formatted')
        read(81,*,err=911,end=999)
        read(81,*,err=911,end=999)
        read(81,*,err=911,end=999)
        read(81,*,err=911,end=999)
        read(81,*,err=911,end=999)
!       read(81,'(i5,i5,i5)',err=911,end=999) ne,nk,nbandi
! version 5.4.1
        read(81,'(i7,i7,i7)',err=911,end=999) ne,nk,nbandi
        if(nk > 100000   .or. nk <= 0) goto 911
        if(nbandi > 2000 .or. nbandi <= 0) goto 911
        if(ne > 4000     .or. ne <= 0) goto 911
        allocate(eiv(nbandi,nk))
        allocate(wgt(nk))
        allocate(rkpt(3,nk))
        do ik=1,nk
!       write(6,*) ik
        read(81,*,err=911,end=999)
        read(81,*,err=911,end=999) tmpx,tmpy,tmpz,wgt(ik)
        rkpt(1,ik)=tmpx
        rkpt(2,ik)=tmpy
        rkpt(3,ik)=tmpz
```

```
      do i=1,nbandi
      read(81,*,err=911,end=999) j,eiv(i,ik)
      enddo
      enddo
      goto 999
  911 continue
      lfault=.true.
  999 continue
      close(81)
!     just skip new calculation, just use the ef value from OUTCAR
!     write(6,*) sum(wgt)
!     1.d-5 eV = 3.1577464d0 / (2.d0*13.6058d0)  K
!     au2kelvin= 3.1577464d5
      temper=1.d-4
      sol1=ef-1.d0
      sol2=ef+1.d0
!     write(6,*) sol1,fdft(sol1)
!     write(6,*) sol2,fdft(sol2)
!     tol=1.d-16 ; ef=zeroin(sol1,sol2,fdft,tol)
!     write(6,*) ef,' ef from calculaton, EIGENVAL'
      lfault1=lfault
!     write(6,*) 'in eigenval',nk
      end
!234567890
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      real*8 function fdft(x)
      USE eigenvalues, ONLY : ne,wgt,eiv,temper,nbandi,nk
      implicit none
      real*8 x
      integer ik,i
      real*8 xxr

      fdft=float(ne)
      do ik=1,nk
      do i=1,nbandi
      xxr=(eiv(i,ik)-x)/temper ; if(xxr >  50.d0) xxr=50.d0 ; if(xxr < -50.d0)
xxr=-50.d0
      fdft=fdft-(2.d0*wgt(ik))/(1.d0+exp(xxr))
      enddo
      enddo
      return
      end
!234567890
!     Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine check_gap(egp1,egp2,lfault1)
      USE eigenvalues, ONLY : temper,ef,rkpt,wgt,eiv,nbandi,nk,cblowest,vbighe
st,ldirect
      implicit none
      logical lfault1
      real*8 egp1,egp2
      integer ik,i,i1,i2
      real*8 t1,t2,test,obj,tst1,tst2,occtol,smallest,dgap,xxr
      logical lfault
      real*8, allocatable :: wrk7(:),wrk8(:)
      integer, allocatable :: iwrk7(:),iwrk8(:)

      lfault=.false.
      occtol=1.d-10
!     write(6,*) ef,' ef'
      dgap=1.d19
      if(nk <= 0)then
      lfault=.true.
                endif
      if(nbandi <= 0)then
      lfault=.true.
                     endif
      if(lfault) goto 119
      allocate(cblowest(nk),vbighest(nk))
      do ik=1,nk
```



```
      i2=nbandi
      do i=nbandi,1,-1
      if(eiv(i,ik) >= ef)then
      xxr=(eiv(i,ik)-ef)/temper ; if(xxr >  50.d0) xxr=50.d0 ; if(xxr < -50.d0)
 xxr=-50.d0
      t2=(2.d0*wgt(ik))/(1.d0+exp(xxr))
      if(t2 < occtol) i2=i
                      endif
      enddo
      i1=1
      do i=1,nbandi
      if(eiv(i,ik) <= ef)then
      xxr=(eiv(i,ik)-ef)/temper ; if(xxr >  50.d0) xxr=50.d0 ; if(xxr < -50.d0)
 xxr=-50.d0
      t1=(2.d0*wgt(ik))/(1.d0+exp(xxr))
      if(t1 > occtol) i1=i
                      endif
      enddo
!
      if(i1 <1 .or. i1 > nbandi)then
      i1=1
      lfault=.true.
      write(6,*) 'something went wrong in egap.f90'
                                endif
      if(i2 <1 .or. i2 > nbandi)then
      i2=1
      lfault=.true.
      write(6,*) 'something went wrong in egap.f90'
                                endif
      if(lfault) goto 119
!
      cblowest(ik)=eiv(i2,ik)
      vbighest(ik)=eiv(i1,ik)
!     t1=(2.d0        )/(1.d0+exp((cblowest(ik)-ef)/temper))
!     t2=(2.d0        )/(1.d0+exp((vbighest(ik)-ef)/temper))
!     write(6,*) t1,t2
!     write(6,*) cblowest(ik)-vbighest(ik)
      test=cblowest(ik)-vbighest(ik)
      if(dgap > test)then
      dgap=test
                  endif
      enddo
      allocate(wrk7(nk),wrk8(nk)) ; allocate(iwrk7(nk),iwrk8(nk))
      wrk7=cblowest
      wrk8=vbighest
      call sortnr(nk,wrk7,iwrk7)
      call sortnr(nk,wrk8,iwrk8)
      write(6,*) 'cb minimum'
      write(6,'(20f12.6)') (wrk7(iwrk7(i)),i=1,min(10,nk))
      write(6,*) 'vb maximum'
      write(6,'(20f12.6)') (wrk8(iwrk8(nk-i+1)),i=1,min(10,nk))
      if(nk >= 8)then
      write(6,'(20f12.6)') wrk7(iwrk7(1))-wrk8(iwrk8(nk)), wrk7(iwrk7(2))-wrk8(iw
rk8(nk)), wrk7(iwrk7(3))-wrk8(iwrk8(nk)), &
      wrk7(iwrk7(4))-wrk8(iwrk8(nk)), wrk7(iwrk7(5))-wrk8(iwrk8(nk)),&
      wrk7(iwrk7(6))-wrk8(iwrk8(nk)), wrk7(iwrk7(7))-wrk8(iwrk8(nk)), wrk7(iwrk
7(8))-wrk8(iwrk8(nk))
                endif
      smallest=minval(cblowest)-maxval(vbighest)

      tst1=wrk7(iwrk7(1))-wrk8(iwrk8(nk))
      tst2=wrk7(iwrk7(2))-wrk8(iwrk8(nk))
      if(abs(tst1-dgap) <1.d-8)then
      write(6,*) 'direct gap',tst1,'indirect gap',tst2
      egp1=tst2
      egp2=tst1
      smallest=tst2
                                endif
      if(smallest < dgap )then
```

```
      write(6,*) 'indirect gap, direct gap ', smallest,dgap
      egp1=smallest
      egp2=dgap
                        endif
      if(smallest <  dgap)then
      ldirect=.false.
      write(6,'(a17,2x,2f16.8,2x,i6,1x,a7)') 'indirect band gap',dgap,smallest,nk,'nk fine'
                        else
      write(6,'(a15,2x,2f16.8,2x,i6,1x,a11,1x,a7)') 'direct band gap',dgap,smallest,nk,'+++++++
++++','nk fine'
      ldirect=.true.
                        endif
  119 continue
      if(allocated(wrk7)) deallocate(wrk7)
      if(allocated(wrk8)) deallocate(wrk8)
      if(allocated(iwrk7)) deallocate(iwrk7)
      if(allocated(iwrk8)) deallocate(iwrk8)
      if(allocated(cblowest)) deallocate(cblowest)
      if(allocated(vbhighest)) deallocate(vbhighest)
      if(allocated(eiv)) deallocate(eiv)
      if(allocated(wgt)) deallocate(wgt)
      if(allocated(rkpt)) deallocate(rkpt)
      if(lfault)then
      egp1=0.d0
      egp2=0.d0
                endif
      call flush(6)
      lfault1=lfault
      end
!234567890
!     Written by In-Ho Lee, KRISS, July 3, 2014.
      subroutine check_dos(test0,test1,lfault1)
      USE eigenvalues, ONLY : temper,ef,rkpt,wgt,eiv,nbandi,nk,cblowest,vbhighe
st
      implicit none
      logical lfault1
      real*8 test0,test1
      logical lfault
      logical linsulator
      real*8 tmq,tmr,pi,dee,epl,yyr,se,sf,ds,ddss(4000)
      real*8 cbm,vbm,rqpt(3,2)
      integer ic,ig,ng,ik,i

      lfault=.false.
      linsulator=.false.
      if(nk <= 0)then
      lfault=.true.
                endif
      if(nbandi <= 0)then
      lfault=.true.
                      endif
      if(lfault) goto 119
      pi=4.d0*atan(1.d0)
      epl=0.005d0
      ng=4000
      ddss=0.d0
      sf=maxval(eiv)+1.0d0
      se=minval(eiv)-1.0d0
      ds=(sf-se)/float(ng-1)
      dee=5.0d0*ds
      do ik=1,nk
      do i=1,nbandi
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      yyr=(yyr-eiv(i,ik))/sqrt(2.d0*epl)
      if(yyr < -12.d0) yyr=-12.d0
      if(yyr >  12.d0) yyr= 12.d0
      ddss(ig)=ddss(ig)+2.d0*wgt(ik)/sqrt(2.d0*pi*epl)*exp(-yyr**2)
      enddo
```



```
      enddo
      enddo
!
      cbm=1.d19 ; vbm=-1.d19
      do ik=1,nk
      do i=1,nbandi
      if(eiv(i,ik) >= ef .and. eiv(i,ik) <= cbm)then
      cbm=eiv(i,ik)
      rqpt(:,2)=rkpt(:,ik)
                                                endif
      if(eiv(i,ik) <  ef .and. eiv(i,ik) >= vbm)then
      vbm=eiv(i,ik)
      rqpt(:,1)=rkpt(:,ik)
                                                endif
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      yyr=(yyr-eiv(i,ik))/sqrt(2.d0*epl)
      if(yyr < -12.d0) yyr=-12.d0
      if(yyr >  12.d0) yyr= 12.d0
      ddss(ig)=ddss(ig)+2.d0*wgt(ik)/sqrt(2.d0*pi*epl)*exp(-yyr**2)
      enddo
      enddo
      enddo
      if(abs(cbm-vbm) > 5.0d0*ds)then
      linsulator=.true.
      goto 119
                                    endif
!
      tmr=0.d0
      tmq=0.d0
      test0=0.d0
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      if(yyr >= ef-dee/2.0 .and. yyr  <= ef+dee/2.0d0)then
      test0=test0+ddss(ig)
      tmq=tmq+1.d0
                                                      endif
      if(yyr <= ef) tmr=tmr+ddss(ig)
      enddo
      tmr=tmr*ds
      test0=test0/tmq
      test0=-abs(test0/tmr)
!
      ic=1
      tmq=1.d19
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      if(tmq > abs(yyr-ef))then
      tmq=abs(yyr-ef)
      ic=ig
                            endif
      enddo
      if(ic+2 <= 4000 .and. ic-2 >= 1)then
      test1=(-ddss(ic+2)+8.d0*ddss(ic+1)-8.d0*ddss(ic-1)+ddss(ic-2))/(12.d0*ds)
      test1=test1/tmr
      test1=-abs(test1)
                                        else
      test1=0.d0
                                        endif
!
  119 continue
      if(allocated(eiv)) deallocate(eiv)
      if(allocated(wgt)) deallocate(wgt)
      if(allocated(rkpt)) deallocate(rkpt)
      if(allocated(cblowest)) deallocate(cblowest)
      if(allocated(vbhighest)) deallocate(vbhighest)
      if(lfault)then
      test0=0.d0
      test1=0.d0
```

```
                endif
      if(linsulator)then
      test0=0.d0
      test1=0.d0
                  endif
!     call flush(6)
      lfault1=lfault
      end
!234567890
!     Written by In-Ho Lee, KRISS, December 2, 2014.
      subroutine check_emass(test0,test1,lfault1)
      USE eigenvalues, ONLY : temper,ef,rkpt,wgt,eiv,nbandi,nk,cblowest,vbhighe
st
      implicit none
      logical lfault1
      real*8 test0,test1
      logical lfault
      logical lmetal
      real*8 tmp,tmq,tmr,xxr,pi,dee,epl,yyr,se,sf,ds,ddss(4000)
      real*8 cbm,vbm,zzz(2),rqpt(3,2)
      integer ic,iv,ig,ng,ik,i,ide

      lmetal=.false.
      lfault=.false.
      if(nk <= 0)then
      lfault=.true.
                endif
      if(nbandi <= 0)then
      lfault=.true.
                  endif
      if(lfault) goto 119
      pi=4.d0*atan(1.d0)
      epl=0.005d0
      ng=4000
      ddss=0.d0
      sf=maxval(eiv)+1.0d0
      se=minval(eiv)-1.0d0
      ds=(sf-se)/float(ng-1)
      cbm=1.d19 ; vbm=-1.d19
      do ik=1,nk
      do i=1,nbandi
      if(eiv(i,ik) >= ef .and. eiv(i,ik) <= cbm)then
      cbm=eiv(i,ik)
      rqpt(:,2)=rkpt(:,ik)
                                          endif
      if(eiv(i,ik) <  ef .and. eiv(i,ik) >= vbm)then
      vbm=eiv(i,ik)
      rqpt(:,1)=rkpt(:,ik)
                                          endif
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      yyr=(yyr-eiv(i,ik))/sqrt(2.d0*epl)
      if(yyr < -12.d0) yyr=-12.d0
      if(yyr >  12.d0) yyr= 12.d0
      ddss(ig)=ddss(ig)+2.d0*wgt(ik)/sqrt(2.d0*pi*epl)*exp(-yyr**2)
      enddo
      enddo
      enddo
      if(abs(cbm-vbm) < 5.0d0*ds)then
      lmetal=.true.
      goto 119
                                endif
      tmr=0.d0
      tmp=1.d19 ; ic=ng
      tmq=1.d19 ; iv=1
      do ig=1,ng
      yyr=se+ds*float(ig-1)
      if(yyr <= ef) tmr=tmr+ddss(ig)
      if(abs(yyr-cbm) <= tmp)then
```



```
      tmp=abs(yyr-cbm)
      ic=ig
                                endif
      if(abs(yyr-vbm) <= tmq)then
      tmq=abs(yyr-vbm)
      iv=ig
                                endif
      enddo
      tmr=tmr*ds
!
      dee=0.1d0
      ide=dee/ds ; if(ide <=1) ide=1       ; ig=ic+1+ide
      if(ig <= 4000 .and. ig >=1)then
      yyr=se+ds*float(ig-1) ; xxr=((ddss(ig)/tmr)/sqrt(yyr-cbm))**(2.d0/3.d0)
                                else
      xxr=0.d0
                                endif
      zzz(1)=-xxr
      ide=2.0d0*dee/ds ; if(ide <=1) ide=1 ; ig=ic+1+ide
      if(ig <= 4000 .and. ig >=1)then
      yyr=se+ds*float(ig-1) ; xxr=((ddss(ig)/tmr)/sqrt(yyr-cbm))**(2.d0/3.d0)
                                else
      xxr=0.d0
                                endif
      zzz(2)=-xxr
      test1=(zzz(1)+zzz(2))/2.d0
      if(abs(zzz(1)) < 1.d-8 .or. abs(zzz(2)) < 1.d-8 ) test1=0.d0
      ide=dee/ds ; if(ide <=1) ide=1       ; ig=iv-1-ide
      if(ig <= 4000 .and. ig >=1)then
      yyr=se+ds*float(ig-1) ; xxr=((ddss(ig)/tmr)/sqrt(vbm-yyr))**(2.d0/3.d0)
                                else
      xxr=0.d0
                                endif
      zzz(1)=-xxr
      ide=2.0d0*dee/ds ; if(ide <=1) ide=1 ; ig=iv-1-ide
      if(ig <= 4000 .and. ig >=1)then
      yyr=se+ds*float(ig-1) ; xxr=((ddss(ig)/tmr)/sqrt(vbm-yyr))**(2.d0/3.d0)
                                else
      xxr=0.d0
                                endif
      zzz(2)=-xxr
      test0=(zzz(1)+zzz(2))/2.d0
      if(abs(zzz(1)) < 1.d-8 .or. abs(zzz(2)) < 1.d-8 ) test0=0.d0
!     write(6,'(3f18.10)') vbm,ef,cbm
!     write(6,'(3f20.12)') rqpt(1,1),rqpt(2,1),rqpt(3,1)
!     write(6,'(3f20.12)') rqpt(1,2),rqpt(2,2),rqpt(3,2)
!
 119  continue
      if(allocated(eiv)) deallocate(eiv)
      if(allocated(wgt)) deallocate(wgt)
      if(allocated(rkpt)) deallocate(rkpt)
      if(allocated(cblowest)) deallocate(cblowest)
      if(allocated(vbhighest)) deallocate(vbhighest)
      if(lfault)then
      test0=0.d0
      test1=0.d0
                endif
      if(lmetal)then
      test0=0.d0
      test1=0.d0
                endif
!     call flush(6)
      lfault1=lfault
      end
!
```