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object.f90

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!234567890
!   Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine object(egp1,egp2,obj,mcmd,lfault_stdout)
implicit none
logical lfault_stdout
integer mcmd
real*8 obj,egp2,egp1,penalty
integer kcase

! default case, mcmd == 0 : enthalpy minimization
! default case, mcmd == 4 : electronic DOS derived effective mass maximization

!           mcmd == 1 : direct band gap optimization
!           mcmd == 2 : electronic DOS at Fermi level maximization
!           mcmd == 3 : electronic DOS slope at Fermi level maximization
!           mcmd == 5 : effective mass minimization
!           mcmd == 6 : special bond length preference
!

if(mcmd ==1)then
  if(egp1 >= egp2)then
    obj=-egp1
  else
    obj=abs(egp2-egp1)-egp1
  endif
kcase=0
kcase=1
if(kcase == 1)then
  penalty=0.d0
  if(egp2 < 0.5d0) penalty=0.5d0-egp2
  if(egp2 > 0.8d0) penalty=-0.8d0+egp2
  obj=obj+penalty
endif
endif
if(mcmd ==2)then
  obj=-abs(obj)
endif
if(mcmd ==3)then
  obj=-abs(obj)
endif
endif
if(mcmd ==5)then
  obj=min(egp1,egp2)
endif

if(lfault_stdout) obj=1.d19
write(6,'(e22.10,2x,a7)') obj, 'obj ftn'
return
end
!

```