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!      Written by In-Ho Lee, KRISS, September 11, 2013.
!
!      Conformational Space Annealing (CSA) with First-Principles Electronic Str
!      ucture Calculations
!      Atomic positions and six lattice parameters (a,b,c,alpha,beta,gamma) are
!      dynamical variables for the CSA.
!      References: Phys. Rev. Lett. 91, 080201 (2003); Phys. Rev. B 90, 115209
!      (2014).
!
!      #####          ###          ##          ##          ##          #####          #####
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!
!      Ab initio MATerials DEsign Using cSa
!
!      Written by In-Ho Lee, KRISS, September 11, 2013.
module csa_application
implicit none
private
save
integer natom,nft,nlopt
integer iobj
integer nspecies
real*8 refal(3),refa2(3),refa3(3),refvol,voltol,extpress,au2ev,au2mbar,au
2ang
real*8 rc1,rc2,shift
logical lvcs,lpbc
integer, allocatable :: nelelements(:),itype(:),ncoord(:)
character*2, allocatable :: symb1(:)
real*8, allocatable :: sigmamatrix(:, :)
real*8, allocatable :: wrk2(:),wrk4(:)
integer, allocatable :: iwrk2(:),iwrk4(:)
public :: iobj
public :: natom,nft,nlopt,rc1,rc2,shift,ncoord
public :: iwrk2,wrk2,iwrk4,wrk4,refvol,voltol
public :: lvcs,lpbc,nspecies,symb1,nelements,sigmamatrix,itype
public :: au2mbar,au2ev,au2ang,refal,refa2,refa3,extpress
end module csa_application
!
!      Written by In-Ho Lee, KRISS, September 11, 2013.
module csa
implicit none
private
save
integer ndeg,npop,npopl,nmate,npert,nevol,idiff,jdiff,nfrac,ndirectory
integer iseed1,iseed2,ndeg_r,npop_r,npopl_r
real*8 dcut,davg,amp,drate,energy_best
real*8, allocatable :: posi(:, :),posil(:, :),energy_sorted(:, :),energy_sorte
dl(:, :),posi_best(:)
real*8, allocatable :: qosi(:, :),qosil(:, :),wrk1(:),qosi0(:),qosi00(:),pr
ev(:)
real*8, allocatable :: posi_r(:, :),posil_r(:, :),energy_sorted_r(:, :),energy
_sortedl_r(:, :),posi_best_r(:)
integer, allocatable :: iwrk1(:)
real*8 energy0,energy_best_r,davg_r
logical iterative

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logical lquit
character*280 cwd
public :: csa_initial,csa_first_bank,csa_evolution,csa_final,lquit

contains

!      Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_initial()
USE csa_application, ONLY : iobj
USE csa_application, ONLY : nft,nlopt,natom,rc1,rc2,shift,refvol,voltol
USE csa_application, ONLY : iwrk2,wrk2,iwrk4,wrk4,ncoord,lpbc,lvcs
USE csa_application, ONLY : nspecies,nelements,symb1,itype,sigmamatrix
USE csa_application, ONLY : refal,refa2,refa3,extpress,au2ev,au2mbar,au2a
ng
implicit none
integer idiff0,npop0,npopl0,nmate0,npert0,nfrac0,nevol0,iseed10,iseed20
real*8 amp0,drate0,factor
real*8 cmatrix(3,3),s6(6),cellvol0,extpress0,vtest
real*8 covlaentr
integer i,j,na,ish
logical lexist,lnewjob

read(5,*) nspecies
allocate(symb1(nspecies),nelements(nspecies))
allocate(sigmamatrix(nspecies,nspecies))
read(5,*) (symb1(i),i=1,nspecies)
read(5,*) (nelements(i),i=1,nspecies)
read(5,*) cellvol0,extpress0,voltol
read(5,*) cmatrix(1,1),cmatrix(1,2),cmatrix(1,3)
read(5,*) cmatrix(2,1),cmatrix(2,2),cmatrix(2,3)
read(5,*) cmatrix(3,1),cmatrix(3,2),cmatrix(3,3)
do i=1,nspecies
symb1(i)=adjustl(symb1(i))
read(5,*) (sigmamatrix(i,j),j=1,nspecies)
enddo
read(5,*) lvcs,lpbc,iobj
read(5,*) ndirectory
read(5,*) cwd
cwd=adjustl(cwd)
!
!      read(5, '(a280)') cwd
!      cwd=adjustl(cwd)
do i=1,280
if(cwd(i:i) == ' ')then
j=i
exit
endif
enddo
do i=j,280
cwd(i:i)=' '
enddo
cwd=trim(cwd)
i=len_trim(cwd) ; if(cwd(i:i) /= '/') cwd=trim(cwd)//'/' ; cwd=trim(cwd)
read(5,*) idiff0,nevol0
read(5,*) npop0,npopl0
read(5,*) nmate0,npert0,nfrac0
read(5,*) amp0,drate0
read(5,*) iseed10,iseed20,lnewjob
jdiff=1
if(idiff0 < 0)then
idiff0=iabs(idiff0)
jdiff=-1
endif
if(ndirectory <= 0) ndirectory=npop0
call init_seed()
if(iseed10 <= 0 .or. iseed20 <= 0)then
call random_number(vtest)
iseed10=vtest*31328.d0+1.d0
call random_number(vtest)
iseed20=vtest*30081.d0+1.d0

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endif

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!
inquire(file='POTCAR',exist=lexist)
if(.not. lexist)then
write(6,*) 'POTCAR is not present.'
stop
endif
inquire(file='INCAR_rlx',exist=lexist)
if(.not. lexist)then
write(6,*) 'INCAR_rlx is not present.'
stop
endif
inquire(file='INCAR_rlxall',exist=lexist)
if(.not. lexist)then
write(6,*) 'INCAR_rlxall is not present.'
stop
endif
inquire(file='INCAR_bs',exist=lexist)
if(.not. lexist)then
write(6,*) 'INCAR_bs is not present.'
stop
endif
inquire(file='CSA_SOLDIER.pbs',exist=lexist)
if(.not. lexist)then
write(6,*) 'CSA_SOLDIER.pbs is not present.'
stop
endif

factor=1.0d0
na=0
do i=1,nspecies
do j=1,nspecies
if(sigmamatrix(i,j) <= 0.0d0)then
na=1
factor=min(factor,abs(sigmamatrix(i,j)))
sigmamatrix(i,j)=abs(sigmamatrix(i,j))
endif
enddo
enddo
do i=1,nspecies
do j=1,nspecies
if(abs(sigmamatrix(i,j)) < 1.d-1)then
sigmamatrix(i,j)=covlaentrr(symbl(i))+covlaentrr(symbl(j))
sigmamatrix(i,j)=sigmamatrix(i,j)*0.4d0
endif
enddo
enddo
if(na > 0)then
if(factor > 1.0d0) factor=1.0d0
if(factor < 0.1d0) factor=0.1d0
do i=1,nspecies
do j=1,nspecies
sigmamatrix(i,j)=covlaentrr(symbl(i))+covlaentrr(symbl(j))
enddo
enddo
sigmamatrix=abs(factor)*sigmamatrix
endif
do i=1,nspecies
do j=1,nspecies
if(sigmamatrix(i,j) < 0.11d0) sigmamatrix(i,j)=0.11d0
enddo
enddo
sigmamatrix=(sigmamatrix+transpose(sigmamatrix))/2.0d0

i=0
i=1
if(i==1)then
write(6,*) nspecies
write(6,*(20(2x,a2,1x))) (symbl(i),i=1,nspecies)

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write(6,*(20(i4,1x))) (nelements(i),i=1,nspecies)
write(6,*(3f18.8)) cellvol0,extpress0,voltol
write(6,*(3f22.12)) cmatrix(1,1),cmatrix(1,2),cmatrix(1,3)
write(6,*(3f22.12)) cmatrix(2,1),cmatrix(2,2),cmatrix(2,3)
write(6,*(3f22.12)) cmatrix(3,1),cmatrix(3,2),cmatrix(3,3)
do i=1,nspecies
write(6,*(20f10.4)) (sigmamatrix(i,j),j=1,nspecies)
enddo
write(6,*) 'sigmamatrix in Angstrom'
do i=1,nspecies
do j=1,nspecies
write(6,*(2x,a2,2x,a2,f12.4)) symbl(i),symbl(j),sigmamatrix(i,j)
enddo
enddo
if(iobj == 0) write(6,*) 'enthalpy minimization (See INCAR)'
if(iobj == 1) write(6,*) 'direct band gap optimization (See objective funtion)'
if(iobj == 2) write(6,*) 'electronic DOS at Fermi level maximization (See objective funtion)'
if(iobj == 3) write(6,*) 'electronic DOS slope at Fermi level maximization (See objective funtion)'
if(iobj == 4) write(6,*) 'electronic DOS derived effective mass maximization (See objective funtion)'

write(6,*) lvcs,lpbc,iobj
write(6,*) ndirectory
write(6,*) trim(cwd)
write(6,*) idiff0,nevol0
write(6,*) npop0,npop10
write(6,*) nmate0,npert0,nfrac0
write(6,*) amp0,drate0
write(6,*) lseed10,lseed20,lnewjob
endif

!
if(lnewjob)then
inquire(file='fort.l',exist=lexist)
if(lexist)then
open(1,file='fort.l',form='formatted')
close(1,status='delete')
write(6,*) 'fort.l is deleted.'
endif
else
inquire(file='fort.l',exist=lexist)
if(.not. lexist)then
write(6,*) 'fort.l is not present. Thus, this is a new job.'
lnewjob=.true.
else
write(6,*) 'fort.l is present. This is an iterative job.'
endif
endif

!
na=0
do j=1,nspecies
na=na+nelements(j)
enddo
allocate(itype(na))
na=0
do i=1,nspecies
do j=1,nelements(i)
na=na+1
itype(na)=i
enddo
enddo
natom=na

!
if(.not. lpbc) lvcs=.false.
if(lvcs) lpbc=.true.
call latmat(s6,cmatrix,0)
call latmatvol(s6,cmatrix,cellvol0)
call latmat(s6,cmatrix,0)
vtest=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,1)
&

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      +(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,2)
&
      +(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,3)
vtest=abs(vtest)
print*, vtest, 'vtest, cellvol0', cellvol0
print*, cmatrix(1,1), cmatrix(1,2), cmatrix(1,3)
print*, cmatrix(2,1), cmatrix(2,2), cmatrix(2,3)
print*, cmatrix(3,1), cmatrix(3,2), cmatrix(3,3)
if(abs(vtest-cellvol0) > 1.d-8) then
write(6,*) 'something went wrong'
      stop
endif

!
au2mbar=2.9421912d2 ; au2ev=13.6058d0*2.d0 ; au2ang=0.529177d0
extpress=extpress0/au2mbar ! extpress0 is in units of Mbar

!
refal(:)=cmatrix(1,:) ; refa2(:)=cmatrix(2,:) ; refa3(:)=cmatrix(3,:) ; r
efvol=cellvol0
if(voltol < 0.d0) then
voltol=abs(voltol)
endif
print*, voltol, 'voltol (%)', voltol*100.d0

!
iseed1=iseed10 ; iseed2=iseed20
iseed1=mod(iseed1,31328+1) ; iseed2=mod(iseed2,30081+1)
call rmarin(iseed1,iseed2)
rc1=0.d0 ; rc2=0.d0
do i=1,nspecies
do j=1,nspecies
rc1=rc1+sigmamatrix(i,j)
rc2=rc2+1.d0
enddo
enddo
rc1=rc1/rc2
!! rc1=sigmamatrix(1,1)*1.45d0
rc1=rc1*1.45d0
rc2=rc1*(1.70d0/1.35d0)
shift=0.0d0

!
ndeg=3*natom+6
npop=npop0
npopl=npopl0
if(npop <= 0) npop=20
if(npopl <= 0) npopl=npop
nmate=nmate0*npop
npert=npert0*npop
if(nmate <= 0) nmate=80*npop
if(npert <= 0) npert=20*npop
nevol=nevol0
if(nevol <= 0) nevol=30
amp=amp0
nfrac=nfrac0
if(nfrac <= 0) nfrac=4
if(natom <= 4) then
nfrac=2
write(6,*) 'natom,nfrac', natom,nfrac
endif
drate=drate0

!
idiff=idiff0
! write(6,*) nspecies, 'nspecies, na', na
write(6, '(20(2x,a2.1x))') (syml(j), j=1,nspecies)
write(6, '(20(i4))') (nelements(j), j=1,nspecies)
write(6,*) lvecs, 'lvecs,lpbc', lpbc
write(6, '(2i5,2x,a24,2x,2i5)') npop,npopl, 'npop,npopl,iseed1,iseed2', iseed1,iseed2
write(6, '(2x,a5,2x,i5)') 'idiff', idiff
! write(6, '(2f10.5,2x,3i7,1x,a33,1x,i7)') amp,drate,nmate,npert,nfrac, 'amp,
drate,nmate,npert,nfrac,nevol', nevol
write(6, '(f6.3,f15.9,1x,3i7,1x,a33,1x,i7)') amp,drate,nmate,npert,nfrac, 'amp,drate,nmat

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e,npert,nfrac,nevol', nevol
write(6, '(3f13.6,2x,a13)') rc1,rc2,shift, 'rc1,rc2,shift'

!
allocate(posi(ndeg,npop)) ; allocate(posil(ndeg,npopl))
allocate(energy_sorted(npop)) ; allocate(energy_sorted1(npopl))
allocate(qosi(ndeg,npop), qosil(ndeg,npopl))
allocate(posi_best(ndeg))
allocate(qosi0(ndeg), qosi00(ndeg))
allocate(iwrk1(max(npop,npopl,3))) ; allocate(wrk1(max(npop,npopl,3)))
allocate(prev(npop))
allocate(ncoord(natom))
allocate(wrk2(natom)) ; allocate(iwrk2(natom))
allocate(wrk4(natom*natom)) ; allocate(iwrk4(natom*natom))
energy_sorted=1.d20 ; energy_sorted1=1.d20
ish=ndeg-6
do i=1,6
posi(ish+i,:)=s6(i)
posil(ish+i,:)=s6(i)
enddo
litative=.false.
inquire(file='fort.1', exist=lexist)
if(lexist) then
call csa_bank_dump(1)
if(ndeg_r == ndeg) litative=.true.
write(6,*) 'iterative, npopl_r,npopl', npopl_r,npopl
write(6,*) 'iterative, npop_r,npop', npop_r,npop
write(6,*) 'iterative, energy_best_r', energy_best_r
j=min(npopl,npopl_r)
posil(:,1:j)=posil_r(:,1:j)
energy_sorted1(1:j)=energy_sorted1_r(1:j)
j=min(npop,npop_r)
posi(:,1:j)=posi_r(:,1:j)
energy_sorted(1:j)=energy_sorted_r(1:j)
posi_best=posi_best_r
energy_best=energy_best_r
endif
nft=0 ; nlopt=0 ; energy_best=1.d23
open(7,file='fort.7',form='formatted')
open(8,file='fort.8',form='formatted')
call flush(6)
end subroutine csa_initial

!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_final()
USE csa_application, ONLY : iwrk2,wrk2,iwrk4,wrk4
USE csa_application, ONLY : nft,nlopt,nspecies,nelements,syml,natom,sign
amatrx,itype,ncoord
implicit none

call onedprint10(energy_sorted,npop)
write(6,*) nft,nlopt, 'nft,nlopt', energy_best,natom
write(7,*) nft,nlopt, 'nft,nlopt', energy_best,natom
write(8, '(i5,2x,f19.9,2x,2i9)') natom,energy_best,nft,nlopt
call flush(8)
call csa_bank_dump(0)

!
if(allocated(posi_r)) deallocate(posi_r)
if(allocated(posil_r)) deallocate(posil_r)
if(allocated(energy_sorted_r)) deallocate(energy_sorted_r)
if(allocated(energy_sorted1_r)) deallocate(energy_sorted1_r)
if(allocated(posi_best_r)) deallocate(posi_best_r)
deallocate(posi,posil) ; deallocate(qosi,qosil)
deallocate(posi_best)
deallocate(qosi0,qosi00)
deallocate(energy_sorted) ; deallocate(energy_sorted1)
deallocate(prev)
deallocate(ncoord)
deallocate(sigmamatrix)
deallocate(syml,nelements,itype)

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deallocate(iwrk1,iwrk2,iwrk4)
deallocate(wrk1,wrk2,wrk4)
close(7)
close(8)
end subroutine csa_final

!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_first_bank()
USE csa_application, ONLY : natom,lvcs,lpbc,refa1,refa2,refa3,voltol
USE csa_application, ONLY : refvol,nspecies,nelements,symbl,sigmamatrix
implicit none
integer i,j,k,ish,ispgrp
real*8 tmq,tmr,tmp,dista,amatrx(3,3),s6(6),cellvol0,vtest,s60(6)
logical lflagls
real*8, allocatable :: sigmamatrix0(:,:)
real ranmar

ish=ndeg-6
if(lpbc)then
amatrx(1,:)=refa1(:) ; amatrx(2,:)=refa2(:) ; amatrx(3,:)=refa3(:)
cellvol0=(amatrx(1,2)*amatrx(2,3)-amatrx(1,3)*amatrx(2,2))*amatrx(3,
1) &      +(amatrx(1,3)*amatrx(2,1)-amatrx(1,1)*amatrx(2,3))*amatrx(3,
2) &      +(amatrx(1,1)*amatrx(2,2)-amatrx(1,2)*amatrx(2,1))*amatrx(3,
3)      cellvol0=abs(cellvol0)
call latmat(s6,amatrx,0)
s60=s6
do i=1,6
posi(ish+i,:)=s6(i)
posil(ish+i,:)=s6(i)
enddo
endif

! dynamic variables in a random initialization mode
if(lpbc) then
do j=1,npop
if(lvcs)then
vtest=cellvol0*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call gen_lattice_matrix(amatrx,s6,vtest)
do i=1,6
qosi0(ish+i)=s6(i)
enddo
else
do i=1,6
qosi0(ish+i)=s60(i)
enddo
endif
do i=1,ndeg-6
qosi0(i)=ranmar()
enddo
call danglingbond_care()

!
if(ranmar() < 1.10)then
if(lpbc)then
qosi00(:)=qosi0(:)
ispgrp=0
allocate(sigmamatrix0(nspecies,nspecies))
sigmamatrix0=sigmamatrix*0.5d0
call gen_latt_site(ispgrp,ndeg,nspecies,nelements,symbl,sigmamatrix0,voltol,refvol,qosi0,lpbc,lvcs,lflagls)
deallocate(sigmamatrix0)
if(.not. lflagls) qosi0(:)=qosi00(:)
endif
endif

!
posi(:,j)=qosi0(:)
enddo

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do j=1,npop1
if(lvcs)then
vtest=cellvol0*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call gen_lattice_matrix(amatrx,s6,vtest)
do i=1,6
qosi0(ish+i)=s6(i)
enddo
else
do i=1,6
qosi0(ish+i)=s60(i)
enddo
endif
do i=1,ndeg-6
qosi0(i)=ranmar()
enddo
call danglingbond_care()

!
if(ranmar() < 1.10)then
if(lpbc)then
qosi00(:)=qosi0(:)
ispgrp=0
allocate(sigmamatrix0(nspecies,nspecies))
sigmamatrix0=sigmamatrix*0.5d0
call gen_latt_site(ispgrp,ndeg,nspecies,nelements,symbl,sigmamatrix0,voltol,refvol,qosi0,lpbc,lvcs,lflagls)
deallocate(sigmamatrix0)
if(.not. lflagls) qosi0(:)=qosi00(:)
endif
endif

!
posil(:,j)=qosi0(:)
enddo
endif

if(.not. lpbc)then
tmp=amp
do j=1,npop
do i=1,natom*3
qosi0(i)=(ranmar()-0.5)*tmp
enddo
call danglingbond_care()
posi(:,j)=qosi0(:)
enddo
do j=1,npop1
do i=1,natom*3
qosi0(i)=(ranmar()-0.5)*tmp
enddo
call danglingbond_care()
posil(:,j)=qosi0(:)
enddo
endif

!
if(.not. lvcs)then
amatrx(1,:)=refa1(:) ; amatrx(2,:)=refa2(:) ; amatrx(3,:)=refa3(:)
call latmat(s6,amatrx,0)
do i=1,6
posi(ish+i,:)=s6(i)
posil(ish+i,:)=s6(i)
enddo
if(lpbc) write(6,*) 'reference lattice vectors are used, lvcs',lvcs
endif
if(.not. lpbc)then
amatrx(1,:)=refa1(:) ; amatrx(2,:)=refa2(:) ; amatrx(3,:)=refa3(:)
call latmat(s6,amatrx,0)
do i=1,6
posi(ish+i,:)=s6(i)
posil(ish+i,:)=s6(i)
enddo
write(6,*) 'reference lattice vectors are never used, lpbc',lpbc
write(6,*) 'it is a nominal one'

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endif
!
if(npop <= npopl)then
if(.not. iterative)then
call master_slave(npopl,ndirectory,-1)
j=min(npop,npopl)
posi(:,1:j)=posil(:,1:j) ; energy_sorted(1:j)=energy_sortedl(1:j)
else
call master_slave(npopl-npopl_r,ndirectory,-1)
do j=1,npopl_r
if(npopl-j+1 <1) exit
posil(:,npopl-j+1)=posil_r(:,j)
energy_sortedl(npopl-j+1)=energy_sortedl_r(j)
enddo
do j=1,npop_r
if(npop-j+1 <1) exit
posi(:,npop-j+1)=posi_r(:,j)
energy_sorted(npop-j+1)=energy_sorted_r(j)
enddo
do j=1,npopl-npopl_r
if(j <= npop)then
posi(:,j)=posil(:,j)
energy_sorted(j)=energy_sortedl(j)
endif
enddo
endif
call csa_bank_sort(1)
call csa_bank_sort(0)
endif
!
if(npop > npopl)then
if(.not. iterative)then
call master_slave(npop,ndirectory,1)
j=min(npop,npopl)
posil(:,1:j)=posi(:,1:j) ; energy_sortedl(1:j)=energy_sorted(1:j)
else
call master_slave(npop-npop_r,ndirectory,1)
do j=1,npopl_r
if(npopl-j+1 <1) exit
posil(:,npopl-j+1)=posil_r(:,j)
energy_sortedl(npopl-j+1)=energy_sortedl_r(j)
enddo
do j=1,npop_r
if(npop-j+1 <1) exit
posi(:,npop-j+1)=posi_r(:,j)
energy_sorted(npop-j+1)=energy_sorted_r(j)
enddo
do j=1,npop-npop_r
if(j <= npopl)then
posil(:,j)=posi(:,j)
energy_sortedl(j)=energy_sorted(j)
endif
enddo
endif
call csa_bank_sort(0)
call csa_bank_sort(1)
endif
!
call csa_difference(1,0,davg,tmq,tmr)
write(6,'(f18.8,2x,a4)') davg,'davg'
dcut=davg/2.0d0
if(iterative)then
if(davg_r > 0.0d0) dcut=davg_r/2.0d0
write(6,*) 'iterative,davg_r,davg',davg_r,davg
endif
!
call csa_update_best(0)
write(6,'(1x,e22.12,2x,a37)') energy_best,'objective functions in the first bank'
call onedprint10(energy_sorted,npop)

```

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```

end subroutine csa_first_bank
!234567890
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_difference(imode,jctl,davg,dsig,dista)
USE csa_application, ONLY : nspecies,nelements,symbl,sigmamatrix,rc1,rc2,
lpbc
USE prdf, ONLY : prdf_init,prdf_final,get_prdf,prdf_cmp
USE bldist, ONLY : bldist_init,bldist_final,get_blsrtd,bldist_cmp
USE qlabmod, ONLY : qlab_init,qlab_final,get_qlab,qlab_cmp
USE elemdist, ONLY : elemdist_init,elemdist_final,get_hist,elemdist_cmp
implicit none
integer imode,jctl
real*8 davg,dsig,dista
real*8 rmax0,tmp,tmq
integer j,i222,ktmp

rmax0=6.d0
if(imode == 1 .or. imode == 2)then
do j=1,npop
if(idiff == 1)then
if(j == 1) call elemdist_init(rmax0,nspecies,nelements,rc1,rc2,npop,lpbc)
call get_hist(j,posi(1,j))
endif
if(idiff == 2)then
i222=1
if(j == 1) call bldist_init(rmax0,jdiff,i222,nelements,nspecies,npop,lpbc)
)
call get_blsrtd(j,posi(1,j))
endif
if(idiff == 3)then
i222=2
if(j == 1) call bldist_init(rmax0,jdiff,i222,nelements,nspecies,npop,lpbc)
)
call get_blsrtd(j,posi(1,j))
endif
if(idiff == 4)then
if(j == 1) call qlab_init(rmax0,nspecies,nelements,sigmamatrix,npop,lpbc)
call get_qlab(j,posi(1,j))
endif
if(idiff == 5)then
if(j == 1) call prdf_init(rmax0,nspecies,nelements,symbl,npop,lpbc)
call get_prdf(j,posi(1,j))
endif
if(idiff == 6)then
ktmp=npop
if(j == 1) call prdf_init(rmax0,nspecies,nelements,symbl,ktmp,lpbc)
call get_prdf(j,posi(1,j))
endif
enddo
endif

if(imode == 1)then
if(idiff == 1) call elemdist_final(1,davg,dsig)
if(idiff == 2) call bldist_final(1,davg,dsig)
if(idiff == 3) call bldist_final(1,davg,dsig)
if(idiff == 4) call qlab_final(1,davg,dsig)
if(idiff == 5) call prdf_final(1,davg,dsig)
if(idiff == 6) call prdf_final(1,davg,dsig)
endif
if(imode == 2)then
if(jctl == 0)then
if(idiff == 1) call get_hist(0,qosi0)
if(idiff == 2) call get_blsrtd(0,qosi0)
if(idiff == 3) call get_blsrtd(0,qosi0)
if(idiff == 4) call get_qlab(0,qosi0)
if(idiff == 5) call get_prdf(0,qosi0)
if(idiff == 6) call get_prdf(0,qosi0)
endif
endif
endif
if(imode == 3)then

```

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```

nwork=npert+nmate
call master_slave(nwork,ndirectory,2)
end subroutine csa_perturbation_mate

!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_rnd_lattice_basis(icm,nwork,iseq)
  use csa_application, ONLY : iobj
  use csa_application, ONLY : natom,shift,wrk2,iwrk2,lvcs,lpbc,nspecies,nel
  use csa_application, ONLY : symbl,sigmamatrix
  implicit none
  integer icm,nwork,iseq(nwork)
  real*8 vec(3),uec(3),rx(3,3),ry(3,3),rz(3,3),ss(3,3),tt(3,3),ddv1,ddv2,dd
v3,shift00,dv1,dv2,dv3
  real*8 a1(3),a2(3),a3(3),cmatrix(3,3),amatrix(3,3),r6(6),s6(6),t6(6),tmp,
tmq,xxmix
  real*8 sig0,xl0,xl,cellvol0,xxr,xxi,vtest,wec(3,2)
  integer ish,i,il,i2,nb,jfrac,j,ii,jj,kk,ll,lslice,jslice,kslice,lslice,jt
r,ity
  integer icase,nptsize,jcase,jmutation,jparents(2)
  integer ispggrp
  logical llattice,lcate,lflags
  real*8, allocatable :: sigmamatrix0(:,:)
  real ranmar

  icase=1
  icase=2
  tmp=amp*2.d0
  nptsize=5
  jcase=3
  jcase=2
  jcase=1

!
! ish=ndeg-6 ; lcate=.false.

!
! if(iseq(icm)==1)then
!   il=dbl(ranmar())*nptsize+1 ; tmq=tmp/dbl(il)
!   xxi=ranmar()+0.3
!   either from first bank or from bank
!   if(ranmar() < 0.10)then
!     j=dbl(ranmar())*npopl+1 ; qosi(:,1)=posi(:,j)
!     jmutation=-j
!   else
!     j=dbl(ranmar())*npop+1 ; qosi(:,1)=posi(:,j)
!     jmutation=j
!   endif
!   qosi0(:)=qosi(:,1)
!   if(ranmar() < 0.05)then
!     qosi0(:)=qosi(:,1)
!     do i=1,natom
!       qosi0(3*(i-1)+1)=qosi(3*(i-1)+1,1)+(ranmar()-0.5)
!       qosi0(3*(i-1)+2)=qosi(3*(i-1)+2,1)+(ranmar()-0.5)
!       qosi0(3*(i-1)+3)=qosi(3*(i-1)+3,1)+(ranmar()-0.5)
!     enddo
!   else
!     il=dbl(ranmar())*nptsize+1 ; tmq=tmp/dbl(il)
!     if(.not. lpbc)then
!       do i=1,natom
!         qosi0(3*(i-1)+1)=qosi(3*(i-1)+1,1)+(ranmar()-0.5)*tmq
!         qosi0(3*(i-1)+2)=qosi(3*(i-1)+2,1)+(ranmar()-0.5)*tmq
!         qosi0(3*(i-1)+3)=qosi(3*(i-1)+3,1)+(ranmar()-0.5)*tmq
!       enddo
!       if(ranmar() < 0.05)then
!         j=dbl(ranmar())*3+1
!         vtest=1.d19
!         do i=1,natom
!           if(vtest > qosi0(3*(i-1)+j)) vtest=qosi0(3*(i-1)+j)

```

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```

enddo
xxr=vtest
vtest=-1.d19
do i=1,natom
  if(vtest < qosi0(3*(i-1)+j)) vtest=qosi0(3*(i-1)+j)
enddo
xxr=vtest-xxr
xxr=xxr*(1.d0+ranmar()-0.5)
do i=1,natom
  qosi0(3*(i-1)+j)=qosi(3*(i-1)+j,1)+(tmq)*sin(xxi*3.141592d0*qosi(3*(i-1)+
j,1)/xxr)
enddo
endif
endif

if(lpbc)then
  do i=1,6
    t6(i)=qosi0(ish+i)
  enddo
  call latmat(t6,cmatrix,1)
  a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
  cellvol0=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,
1) &
  + (cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,
2) &
  + (cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,
3)
  cellvol0=abs(cellvol0)
  endif
  if(lpbc)then
    dv1=sqrt(dot_product(a1,a1)) ; dv2=sqrt(dot_product(a2,a2)) ; dv3=sqrt(do
t_product(a3,a3))
    ddv1=dv1/(1.d-2) ; ddv2=dv2/(1.d-2) ; ddv3=dv3/(1.d-2)
    shift00=1.d-3/(max(dv1,dv2,dv3))
    else
    shift00=shift
    dv1=1.d0 ; dv2=1.d0 ; dv3=1.d0
    ddv1=1.d0/(1.d-2) ; ddv2=1.d0/(1.d-2) ; ddv3=1.d0/(1.d-2)
  endif
  if(lpbc)then
    do i=1,natom
      qosi0(3*(i-1)+1)=qosi(3*(i-1)+1,1)+(ranmar()-0.5)*(tmq/dv1)
      qosi0(3*(i-1)+2)=qosi(3*(i-1)+2,1)+(ranmar()-0.5)*(tmq/dv2)
      qosi0(3*(i-1)+3)=qosi(3*(i-1)+3,1)+(ranmar()-0.5)*(tmq/dv3)
    enddo
    if(ranmar() < 0.05)then
      j=dbl(ranmar())*3+1
      if(j ==1) xxr=dv1
      if(j ==2) xxr=dv2
      if(j ==3) xxr=dv3
      do i=1,natom
        qosi0(3*(i-1)+j)=qosi(3*(i-1)+j,1)+(tmq/xxr)*sin(xxi*3.141592653589793238
d0*qosi(3*(i-1)+j,1))
      enddo
    endif
  endif
endif

!
if(nspecies >= 2)then
  if(natom > 2)then
    do i2=1,1+3*dbl(ranmar())+int(natom/3)
      continue
    410 i=dbl(ranmar())*natom+1
        j=dbl(ranmar())*natom+1
        if(itype(i) == itype(j)) goto 410
        wec(1,1)=qosi0(3*(i-1)+1)
        wec(2,1)=qosi0(3*(i-1)+2)
        wec(3,1)=qosi0(3*(i-1)+3)
        wec(1,2)=qosi0(3*(j-1)+1)
        wec(2,2)=qosi0(3*(j-1)+2)

```



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```

wec(3,2)=qosi0(3*(j-1)+3)
qosi0(3*(i-1)+1)=wec(1,2)
qosi0(3*(i-1)+2)=wec(2,2)
qosi0(3*(i-1)+3)=wec(3,2)
qosi0(3*(j-1)+1)=wec(1,1)
qosi0(3*(j-1)+2)=wec(2,1)
qosi0(3*(j-1)+3)=wec(3,1)
enddo
endif
endif

!
if(ranmar() < 0.10)then
if(nspecies > 1)then
do i=1,natom
wrk2(i)=ranmar()
enddo
call sortnr(natom,wrk2,iwrk2)
qosi(:,1)=qosi0(:)
do i=1,natom
j=iwrk2(i)
qosi0(3*(i-1)+1)=qosi(3*(j-1)+1,1)
qosi0(3*(i-1)+2)=qosi(3*(j-1)+2,1)
qosi0(3*(i-1)+3)=qosi(3*(j-1)+3,1)
enddo
endif
endif

!
if(lvcs)then
do i=1,6
r6(i)=qosi0(ish+i)
enddo
jtr=0
do
jtr=jtr+1
if(jcase ==1)then
sig0=1.d0 ; x10=0.d0
do i=1,6
call gauss(sig0,x10,x1)
t6(i)=r6(i)+(0.04d0*r6(i))*x1
enddo
endif

!
if(ranmar() > 0.7)then
i=dbl(ranmar())*3+1
331 continue
vtest=(0.80d0+ranmar())*0.40d0
if(vtest < 0.95 .or. vtest > 1.05)then
t6(i)=r6(i)*vtest
else
goto 331
endif
endif

!
if(jtr >200)then
vtest=refvol*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call latmatvol(t6,cmatrix,vtest)
call latmat(t6,cmatrix,0)
endif
endif

!
if(jcase ==2)then
do i=1,6
t6(i)=r6(i)+(0.25d0*r6(i))*(ranmar()-0.5)
enddo
endif

!
if(jcase ==3)then
vtest=cellvol*(1.d0+voltol*(ranmar()-0.5)*2.d0)
vtest=refvol*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call gen_lattice_matrix(amatrix,s6,vtest)
islice=dbl(ranmar())*5+1

```

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```

xmix=0.1d0*dble(islice)
do i=1,6
t6(i)=r6(i)*(1.d0-xmix)+s6(i)*xmix
enddo
endif
if(jcase ==4)then
call latmat(r6,cmatrix,1)
call lat_mutation(cmatrix)
call latmat(t6,cmatrix,0)
vtest=refvol*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call latmatvol(t6,cmatrix,vtest)
call latmat(t6,cmatrix,0)
endif
call latmat(t6,cmatrix,1)

!
&
vtest=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,1)
&
+(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,2)
&
+(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,3)
vtest=abs(vtest)
if(vtest > refvol*(1.d0-voltol) .and. vtest < refvol*(1.d0+voltol))then
call check_lat(llattice,lcate,cmatrix)
else
endif

llattice=.false.
endif

if(llattice) goto 555
if(jtr > 300)then
do i=1,6
t6(i)=r6(i)
enddo
write(6,*) 'we have trouble with lattice variations 300'
goto 555
endif
enddo
555 continue
if(jtr > 100) write(6,'(i5,2x,a13)') jtr,'jtr- code=1'
do i=1,6
qosi0(ish+i)=t6(i)
enddo
endif

!
differential evolution type : mutation and crossover for position vectors
if(ranmar() < -0.1)then
if(icm > npop)then
call onedffvltm(ndeg,npop,posit,qosi0)
do i=1,6
qosi0(ish+i)=t6(i)
enddo
if(lpbc)then
do i=1,natom*3
qosi0(i)=qosi0(i)-anint(qosi0(i))
if(qosi0(i) <= 0.d0) qosi0(i)=qosi0(i)+1.d0
enddo
endif
endif

!
soft mutation : assumption : already optimized fixed lattice parameters
if(ranmar() < 0.7 .and. iobj == 0)then
if(icm > npop)then
j=dbl(ranmar())*npop+1
do i=1,1
j=min(dble(j),dble(ranmar())*npop+1)
enddo

!
jmutation=j
qosi(:,1)=posit(:,j)
qosi0(:,1)=qosi(:,1)
if(lpbc)then
call softmutation(ndeg,qosi0,j,amp,t6)

```



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```

        else
        call softmutation1(ndeg,qosi0,j,amp)
        endif
        if(ranmar() < 0.10)then
        if(lpbc)then
        if(lvcs)then
!      qosi(:,1)=qosi0(:)
        ispgpr=0
        allocate(sigmamatrix0(nspecies,nspecies))
        sigmamatrix0=sigmamatrix*0.5d0
        call gen_latt_site(ispgpr,ndeg,nspecies,nelements,symb1,sigmamatrix0,volt
ol,refvol,qosi0,lpbc,lvcs,lflagls)
        deallocate(sigmamatrix0)
        if(.not. lflagls) qosi0(:)=qosi(:,1)
!      endif
        endif

        endif

        if(jmutation <0)then
        xmix=energy_sorted1(-jmutation)
        else
        xmix=energy_sorted(jmutation)
        endif
        write(6,'(i5,lx,e22,l2,lx,a18,lx,i6)') jmutation,xmix,'jmutation,jparents',icm
!      endif

!      if(iseq(icm)==2)then
!      if(icas == 1)then
!      ii=dbl(ranmar())*npop+1
11      continue
!      jj=dbl(ranmar())*npop+1
!      if( ii == jj) goto 11
!      endif
!      if(icas == 2)then
!      ii=npop/2 ; ii=-dbl(ii)*log(ranmar()) ; if(ii <= 0 .or. ii > npop) ii=np
op*dbl(ranmar())+1
22      continue
!      jj=npop/2 ; jj=-dbl(jj)*log(ranmar()) ; if(jj <= 0 .or. jj > npop) jj=np
op*dbl(ranmar())+1
!      if( ii == jj) goto 22
!      endif
!      if(icas == 3)then
!      ii=min(dbl(ranmar())*npop+1,dbl(ranmar())*npop+1)
33      continue
!      jj=min(dbl(ranmar())*npop+1,dbl(ranmar())*npop+1)
!      if( ii == jj) goto 33
!      endif
        qosi(:,ii)=posi(:,ii)
        qosi(:,jj)=posi(:,jj)
        jparents(1)=ii
        jparents(2)=jj
!      either from first bank or from bank
!      if(ranmar() < 0.10)then
!      j=dbl(ranmar())*npop+1
!      qosi(:,jj)=posil(:,j)
!      jparents(2)=-jj
!      jparents(2)=-j
!      endif

!      if(lpbc)then
!      call tocarx(qosi(1,ii))
!      call tocarx(qosi(1,jj))
!      endif
!      call centering(qosi(1,ii))
!      call centering(qosi(1,jj))

!      if(natom > 20)then
!      call gen_randrot(rx,ry,rz)
!      tt=matmul(ry,rz) ; ss=matmul(rx,tt)

```

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```

        do i=1,natom
        vec(1)=qosi(3*(i-1)+1,ii)
        vec(2)=qosi(3*(i-1)+2,ii)
        vec(3)=qosi(3*(i-1)+3,ii)
        uec=matmul(ss,vec)
        qosi(3*(i-1)+1,ii)=uec(1)
        qosi(3*(i-1)+2,ii)=uec(2)
        qosi(3*(i-1)+3,ii)=uec(3)
        enddo
        endif

!      call gen_randrot(rx,ry,rz)
!      tt=matmul(ry,rz) ; ss=matmul(rx,tt)
!      do i=1,natom
!      vec(1)=qosi(3*(i-1)+1,jj)
!      vec(2)=qosi(3*(i-1)+2,jj)
!      vec(3)=qosi(3*(i-1)+3,jj)
!      uec=matmul(ss,vec)
!      qosi(3*(i-1)+1,jj)=uec(1)
!      qosi(3*(i-1)+2,jj)=uec(2)
!      qosi(3*(i-1)+3,jj)=uec(3)
!      enddo

!      qosi0(:)=qosi(:,ii)
!      do i=1,natom
!      wrk2(i)=qosi0(3*(i-1)+1)
!      enddo
!      call sortnr(natom,wrk2,iwrk2)
!      nb=0
!      do i1=1,nspecies
!      do i=1,natom
!      i2=iwrk2(i)
!      if(itype(i2) == i1)then
!      nb=nb+1
!      qosi(3*(nb-1)+1,ii)=qosi0(3*(i2-1)+1)
!      qosi(3*(nb-1)+2,ii)=qosi0(3*(i2-1)+2)
!      qosi(3*(nb-1)+3,ii)=qosi0(3*(i2-1)+3)
!      endif
!      enddo
!      enddo
!      if(lpbc)then
!      do i=1,6
!      t6(i)=qosi0(ish+i)
!      enddo
!      call latmat(t6,cmatrix,1)
!      a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
!      cellvol0=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,
1) &
!      +(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,
2) &
!      +(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,
3)
!      cellvol0=abs(cellvol0)
!      endif
!      if(lpbc)then
!      dvl=sqrt(dot_product(a1,a1)) ; dv2=sqrt(dot_product(a2,a2)) ; dv3=sqrt(do
t_product(a3,a3))
!      ddv1=dvl/(1.d-2) ; ddv2=dv2/(1.d-2) ; ddv3=dv3/(1.d-2)
!      shift00=1.d-3/(max(dv1,dv2,dv3))
!      else
!      shift00=shift
!      dvl=1.d0 ; dv2=1.d0 ; dv3=1.d0
!      ddv1=1.d0/(1.d-2) ; ddv2=1.d0/(1.d-2) ; ddv3=1.d0/(1.d-2)
!      endif

!      qosi0(:)=qosi(:,jj)
!      do i=1,natom
!      wrk2(i)=qosi0(3*(i-1)+1)
!      enddo

```

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```

call sortnr(natom,wrk2,iwrk2)
nb=0
do il=1,nspecies
do i=1,natom
i2=iwrk2(i)
if(itype(i2) == i1)then
nb=nb+1
qosi(3*(nb-1)+1,jj)=qosi0(3*(i2-1)+1)
qosi(3*(nb-1)+2,jj)=qosi0(3*(i2-1)+2)
qosi(3*(nb-1)+3,jj)=qosi0(3*(i2-1)+3)
endif
enddo
enddo
! additional rotation around x axis
call gen_randrot(rx,ry,rz)
do i=1,natom
vec(1)=qosi(3*(i-1)+1,jj)
vec(2)=qosi(3*(i-1)+2,jj)
vec(3)=qosi(3*(i-1)+3,jj)
uec=matmul(rx,vec)
qosi(3*(i-1)+1,jj)=uec(1)
qosi(3*(i-1)+2,jj)=uec(2)
qosi(3*(i-1)+3,jj)=uec(3)
enddo
!
nb=0
do ity=1,nspecies
jfrac=dbl(ranmar())*(nfrac-1)+1
islice=(dbl(jfrac)/dbl(nfrac)) *dbl(nelements(ity))
if(islice <= 1) islice=1 ; if(islice >= nelements(ity)-1) islice=nelement
s(ity)-1
i2=0
do i=1,islice
nb=nb+1
i2=i2+1
qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,ii)+(ranmar()-0.5)/ddv1-shift00*0.5d0
qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,ii)+(ranmar()-0.5)/ddv2
qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,ii)+(ranmar()-0.5)/ddv3
enddo
do i=islice+1,nelements(ity)
nb=nb+1
i2=i2+1
qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,jj)+(ranmar()-0.5)/ddv1+shift00*0.5d0
qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,jj)+(ranmar()-0.5)/ddv2
qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,jj)+(ranmar()-0.5)/ddv3
enddo
if(i2 /= nelements(ity))then
write(6,*) 'something went wrong 2-1'
stop
endif
enddo
if(nb /= natom)then
write(6,*) 'something went wrong 2'
stop
endif
!
if(lvcs)then
jtr=0
do
jtr=jtr+1
islice=dbl(ranmar())*5+1
if(islice <= 1) islice=1 ; if(islice >= 5) islice=5
nb=0
do i=1,islice
nb=nb+1
qosi0(ish+i)=qosi(ish+i,ii)
enddo
do i=islice+1,6
nb=nb+1

```

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```

qosi0(ish+i)=qosi(ish+i,jj)
enddo
if(nb /= 6)then
write(6,*) 'something went wrong 2-vcs'
stop
endif
if(jtr > 100)then
sig0=1.d0 ; x10=0.d0
do i=1,6
call gauss(sig0,x10,x1)
if(ranmar() > 0.5)then
qosi0(ish+i)=qosi(ish+i,ii)+(0.04d0*qosi(ish+i,ii))*x1
else
qosi0(ish+i)=qosi(ish+i,jj)+(0.04d0*qosi(ish+i,jj))*x1
endif
enddo
endif
if(jtr > 200)then
sig0=1.d0 ; x10=0.d0
do i=1,6
call gauss(sig0,x10,x1)
qosi0(ish+i)=qosi(ish+i,ii)+(0.04d0*qosi(ish+i,ii))*x1
enddo
endif
if(jtr > 300)then
sig0=1.d0 ; x10=0.d0
do i=1,6
call gauss(sig0,x10,x1)
qosi0(ish+i)=qosi(ish+i,jj)+(0.01d0*qosi(ish+i,jj))*x1
if(ranmar() > 0.5) qosi0(ish+i)=qosi(ish+i,ii)+(0.01d0*qosi(ish+i,ii))*x1
enddo
endif
do i=1,6
t6(i)=qosi0(ish+i)
enddo
call latmat(t6,cmatrix,1)
vtest=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,1)
&
&
+ (cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,2)
+ (cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,3)
vtest=abs(vtest)
if(vtest > refvol*(1.d0-voltol) .and. vtest < refvol*(1.d0+voltol))then
call check_lat(llattice,lcate,cmatrix)
else
endif
llattice=.false.
if(llattice) goto 666
if(jtr > 400)then
do i=1,6
t6(i)=qosi(ish+i,ii)
enddo
vtest=refvol*(1.d0+voltol*(ranmar()-0.5)*2.d0)
call gen_lattice_matrix(cmatrix,t6,vtest)
goto 666
endif
enddo
continue
666 if(jtr > 400) write(6,*) 'we have trouble with ii,jj 400 : new lattice vector'
if(jtr > 100) write(6,*(i5,2x,a13')) jtr,'jtr code=2'
do i=1,6
qosi0(ish+i)=t6(i)
enddo
endif
if(lpbc) call tolatx(qosi0)
!
tmp=energy_sorted(jparents(1))
if(jparents(2) < 0)then
xmix=energy_sorted1(-jparents(2))

```

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```

        else
          xmix=energy_sorted(jparents(2))
        endif
        write(6,'(2i5,1x,2e22.12,1x,a8,1x,i6)' jparents(1),jparents(2),tmp,xmix,'jparents',
icm
        endif
!
      if(iseq(icm)==3)then
        ii=dbl(ranmar())*npop+1
        jj=dbl(ranmar())*npop+1
        kk=dbl(ranmar())*npop+1
        qosi(:,ii)=posi(:,ii)
        qosi(:,jj)=posi(:,jj)
        qosi(:,kk)=posi(:,kk)
!      either from first bank or from bank
        if(ranmar() < 0.10)then
          j=dbl(ranmar())*npop+1
          qosi(:,jj)=posi(:,j)
        endif
!      either from first bank or from bank
        if(ranmar() < 0.10)then
          j=dbl(ranmar())*npop+1
          qosi(:,kk)=posi(:,j)
        endif
        if(lpbc)then
          call tocarx(qosi(1,ii))
          call tocarx(qosi(1,jj))
          call tocarx(qosi(1,kk))
        endif
        call centering(qosi(1,ii))
        call centering(qosi(1,jj))
        call centering(qosi(1,kk))
!
        call gen_randrot(rx,ry,rz)
        do i=1,natom
          vec(1)=qosi(3*(i-1)+1,jj)
          vec(2)=qosi(3*(i-1)+2,jj)
          vec(3)=qosi(3*(i-1)+3,jj)
          uec=matmul(rz,vec)
          vec=matmul(ry,vec)
          uec=matmul(rx,vec)
          qosi(3*(i-1)+1,jj)=vec(1)
          qosi(3*(i-1)+2,jj)=vec(2)
          qosi(3*(i-1)+3,jj)=vec(3)
        enddo
!
        call gen_randrot(rx,ry,rz)
        do i=1,natom
          vec(1)=qosi(3*(i-1)+1,kk)
          vec(2)=qosi(3*(i-1)+2,kk)
          vec(3)=qosi(3*(i-1)+3,kk)
          uec=matmul(rz,vec)
          vec=matmul(ry,vec)
          uec=matmul(rx,vec)
          qosi(3*(i-1)+1,kk)=vec(1)
          qosi(3*(i-1)+2,kk)=vec(2)
          qosi(3*(i-1)+3,kk)=vec(3)
        enddo
!
        qosi(:)=qosi(:,ii)
        do i=1,natom
          wrk2(i)=qosi(3*(i-1)+1)
        enddo
        call sortnr(natom,wrk2,iwrk2)
        nb=0
        do il=1,nspecies
          do i=1,natom
            i2=iwrk2(i)
            if(itype(i2) == il)then

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```

          nb=nb+1
          qosi(3*(nb-1)+1,ii)=qosi0(3*(i2-1)+1)
          qosi(3*(nb-1)+2,ii)=qosi0(3*(i2-1)+2)
          qosi(3*(nb-1)+3,ii)=qosi0(3*(i2-1)+3)
        endif
      enddo
    enddo
    if(lpbc)then
      do i=1,6
        t6(i)=qosi0(ish+i)
      enddo
      call latmat(t6,cmatrix,1)
      a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
      cellvol0=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,
1) &
          +(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,
2) &
          +(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,
3)
      cellvol0=abs(cellvol0)
    endif
    if(lpbc)then
      dv1=sqrt(dot_product(a1,a1)) ; dv2=sqrt(dot_product(a2,a2)) ; dv3=sqrt(do
t_product(a3,a3))
      ddv1=dv1/(1.d-2) ; ddv2=dv2/(1.d-2) ; ddv3=dv3/(1.d-2)
      shift00=1.d-3/(max(dv1,dv2,dv3))
    else
      shift00=shift
      dv1=1.d0 ; dv2=1.d0 ; dv3=1.d0
      ddv1=1.d0/(1.d-2) ; ddv2=1.d0/(1.d-2) ; ddv3=1.d0/(1.d-2)
    endif
!
    qosi(:)=qosi(:,jj)
    do i=1,natom
      wrk2(i)=qosi0(3*(i-1)+1)
    enddo
    call sortnr(natom,wrk2,iwrk2)
    nb=0
    do il=1,nspecies
      do i=1,natom
        i2=iwrk2(i)
        if(itype(i2) == il)then
          nb=nb+1
          qosi(3*(nb-1)+1,jj)=qosi0(3*(i2-1)+1)
          qosi(3*(nb-1)+2,jj)=qosi0(3*(i2-1)+2)
          qosi(3*(nb-1)+3,jj)=qosi0(3*(i2-1)+3)
        endif
      enddo
    enddo
!
    qosi(:)=qosi(:,kk)
    do i=1,natom
      wrk2(i)=qosi0(3*(i-1)+1)
    enddo
    call sortnr(natom,wrk2,iwrk2)
!
    do i=1,natom
      i1=iwrk2(i)
      qosi(3*(i-1)+1,kk)=qosi0(3*(i1-1)+1)
      qosi(3*(i-1)+2,kk)=qosi0(3*(i1-1)+2)
      qosi(3*(i-1)+3,kk)=qosi0(3*(i1-1)+3)
    enddo
    nb=0
    do il=1,nspecies
      do i=1,natom
        i2=iwrk2(i)
        if(itype(i2) == il)then
          nb=nb+1
          qosi(3*(nb-1)+1,kk)=qosi0(3*(i2-1)+1)
          qosi(3*(nb-1)+2,kk)=qosi0(3*(i2-1)+2)

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```

qosi(3*(nb-1)+3,kk)=qosi0(3*(i2-1)+3)
endif
enddo
enddo
! additional rotation around x axis
call gen_randrot(rx,ry,rz)
do i=1,natom
vec(1)=qosi(3*(i-1)+1,jj)
vec(2)=qosi(3*(i-1)+2,jj)
vec(3)=qosi(3*(i-1)+3,jj)
uec=matmul(rx,vec)
qosi(3*(i-1)+1,jj)=uec(1)
qosi(3*(i-1)+2,jj)=uec(2)
qosi(3*(i-1)+3,jj)=uec(3)
enddo
!
nb=0
do ity=1,nspecies
il=dbl(ranmar())*(nfrac-1)+1
i=dbl(ranmar())*(nfrac-1)+1
jslice=(dbl(il)/dbl(nfrac)) *dbl(nelements(ity))
kslice=(dbl(i)/dbl(nfrac)) *dbl(nelements(ity))
if(jslice <= 1) jslice=1 ; if(jslice >= nelements(ity)-1) jslice=nelement
s(ity)-1
if(kslice <= 1) kslice=1 ; if(kslice >= nelements(ity)-1) kslice=nelement
s(ity)-1
i=jslice
il=kslice
jslice=min(il,i)
kslice=max(il,i)
i2=0
do i=1,jslice
nb=nb+1
i2=i2+1
qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,ii)+(ranmar()-0.5)/ddv1-shift00*0.5d0
qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,ii)+(ranmar()-0.5)/ddv2
qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,ii)+(ranmar()-0.5)/ddv3
enddo
do i=jslice+1,kslice
nb=nb+1
i2=i2+1
qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,jj)+(ranmar()-0.5)/ddv1
qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,jj)+(ranmar()-0.5)/ddv2
qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,jj)+(ranmar()-0.5)/ddv3
enddo
do i=kslice+1,nelements(ity)
nb=nb+1
i2=i2+1
qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,kk)+(ranmar()-0.5)/ddv1-shift00*0.5d0
qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,kk)+(ranmar()-0.5)/ddv2
qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,kk)+(ranmar()-0.5)/ddv3
enddo
if(i2 /= nelements(ity))then
write(6,*) 'something went wrong 3-1'
stop
endif
enddo
if(nb /= natom)then
write(6,*) 'something went wrong 3'
stop
endif
!
if(lvcs)then
jtr=0
do
jtr=jtr+1
jslice=dbl(ranmar())*5+1
kslice=dbl(ranmar())*5+1
if(jslice <= 1) jslice=1 ; if(jslice >= 5) jslice=5

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```

if(kslice <= 1) kslice=1 ; if(kslice >= 5) kslice=5
i=jslice
il=kslice
jslice=min(il,i)
kslice=max(il,i)
nb=0
do i=1,jslice
nb=nb+1
qosi0(ish+i)=qosi(ish+i,ii)
enddo
do i=jslice+1,kslice
nb=nb+1
qosi0(ish+i)=qosi(ish+i,jj)
enddo
do i=kslice+1,6
nb=nb+1
qosi0(ish+i)=qosi(ish+i,kk)
enddo
if(nb /= 6)then
write(6,*) 'something went wrong 3-vcs'
stop
endif
!
if(jtr > 100)then
sig0=1.d0 ; xl0=0.d0
do i=1,6
call gauss(sig0,xl0,xl)
vtest=ranmar()
if(vtest < 0.33333) qosi0(ish+i)=qosi(ish+i,ii)+(0.
04d0*qosi(ish+i,ii))*xl
if(vtest > 0.33333 .and. vtest < 0.66666) qosi0(ish+i)=qosi(ish+i,jj)+(0.
04d0*qosi(ish+i,jj))*xl
if(vtest > 0.66666) qosi0(ish+i)=qosi(ish+i,kk)+(0.
04d0*qosi(ish+i,kk))*xl
enddo
endif
!
if(jtr > 200)then
sig0=1.d0 ; xl0=0.d0
do i=1,6
call gauss(sig0,xl0,xl)
qosi0(ish+i)=qosi(ish+i,ii)+(0.04d0*qosi(ish+i,ii))*xl
enddo
endif
do i=1,6
t6(i)=qosi0(ish+i)
enddo
call latmat(t6,cmatrix,1)
vtest=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,1)
&
+(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,2)
&
+(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,3)
vtest=abs(vtest)
if(vtest > refvol*(1.d0-voltol) .and. vtest < refvol*(1.d0+voltol))then
call check_lat(llattice,lcate,cmatrix)
else
endif
llattice=.false.
endif
if(llattice) goto 777
if(jtr > 400)then
do i=1,6
t6(i)=qosi(ish+i,ii)
enddo
! write(6,*) 'we have trouble with ii,jj,kk'
goto 777
endif
enddo
continue
777

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```

if(jtr > 400) write(6,*) 'we have trouble with ii,jj,kk, 400'
if(jtr > 100) write(6,'(i5,2x,a13)') jtr,'jtr code=3'
do i=1,6
  qosi0(ish+i)=t6(i)
enddo
endif
if(lpbc) call tolatx(qosi0)
endif

!
if(iseq(icm)==4)then
  ii=dbl(ranmar())*npop+1
  jj=dbl(ranmar())*npop+1
  kk=dbl(ranmar())*npop+1
  ll=dbl(ranmar())*npop+1
  qosi(:,ii)=posi(:,ii)
  qosi(:,jj)=posi(:,jj)
  qosi(:,kk)=posi(:,kk)
  qosi(:,ll)=posi(:,ll)
!
  either from first bank or from bank
  if(ranmar() < 0.10)then
    j=dbl(ranmar())*npop+1
    qosi(:,jj)=posi(:,j)
  endif
!
  either from first bank or from bank
  if(ranmar() < 0.10)then
    j=dbl(ranmar())*npop+1
    qosi(:,kk)=posi(:,j)
  endif
!
  either from first bank or from bank
  if(ranmar() < 0.10)then
    j=dbl(ranmar())*npop+1
    qosi(:,ll)=posi(:,j)
  endif

  if(lpbc)then
    call tocarx(qosi(1,ii))
    call tocarx(qosi(1,jj))
    call tocarx(qosi(1,kk))
    call tocarx(qosi(1,ll))
  endif
  call centering(qosi(1,ii))
  call centering(qosi(1,jj))
  call centering(qosi(1,kk))
  call centering(qosi(1,ll))
!
  call gen_randrot(rx,ry,rz)
  do i=1,natom
    vec(1)=qosi(3*(i-1)+1,jj)
    vec(2)=qosi(3*(i-1)+2,jj)
    vec(3)=qosi(3*(i-1)+3,jj)
    uec=matmul(rz,vec)
    vec=matmul(ry,vec)
    uec=matmul(rx,vec)
    qosi(3*(i-1)+1,jj)=uec(1)
    qosi(3*(i-1)+2,jj)=uec(2)
    qosi(3*(i-1)+3,jj)=uec(3)
  enddo
!
  call gen_randrot(rx,ry,rz)
  do i=1,natom
    vec(1)=qosi(3*(i-1)+1,kk)
    vec(2)=qosi(3*(i-1)+2,kk)
    vec(3)=qosi(3*(i-1)+3,kk)
    uec=matmul(rz,vec)
    vec=matmul(ry,vec)
    uec=matmul(rx,vec)
    qosi(3*(i-1)+1,kk)=uec(1)
    qosi(3*(i-1)+2,kk)=uec(2)
    qosi(3*(i-1)+3,kk)=uec(3)
  enddo

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```

!
call gen_randrot(rx,ry,rz)
do i=1,natom
  vec(1)=qosi(3*(i-1)+1,ll)
  vec(2)=qosi(3*(i-1)+2,ll)
  vec(3)=qosi(3*(i-1)+3,ll)
  uec=matmul(rz,vec)
  vec=matmul(ry,vec)
  uec=matmul(rx,vec)
  qosi(3*(i-1)+1,ll)=uec(1)
  qosi(3*(i-1)+2,ll)=uec(2)
  qosi(3*(i-1)+3,ll)=uec(3)
enddo
!
qosi0(:)=qosi(:,ii)
do i=1,natom
  wrk2(i)=qosi0(3*(i-1)+1)
enddo
call sortnr(natom,wrk2,iwrk2)
nb=0
do il=1,nspecies
  do i=1,natom
    i2=iwrk2(i)
    if(itype(i2) == il)then
      nb=nb+1
      qosi(3*(nb-1)+1,ii)=qosi0(3*(i2-1)+1)
      qosi(3*(nb-1)+2,ii)=qosi0(3*(i2-1)+2)
      qosi(3*(nb-1)+3,ii)=qosi0(3*(i2-1)+3)
    endif
  enddo
enddo
if(lpbc)then
  do i=1,6
    t6(i)=qosi0(ish+i)
  enddo
  call latmat(t6,cmatrix,1)
  a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
  cellvol0=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,
1) &
      +(cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,
2) &
      +(cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,
3)
  cellvol0=abs(cellvol0)
  endif
  if(lpbc)then
    dv1=sqrt(dot_product(a1,a1)) ; dv2=sqrt(dot_product(a2,a2)) ; dv3=sqrt(dot
t_product(a3,a3))
    ddv1=dv1/(1.d-2) ; ddv2=dv2/(1.d-2) ; ddv3=dv3/(1.d-2)
    shift00=1.d-3/(max(dv1,dv2,dv3))
    else
    shift00=shift
    dv1=1.d0 ; dv2=1.d0 ; dv3=1.d0
    ddv1=1.d0/(1.d-2) ; ddv2=1.d0/(1.d-2) ; ddv3=1.d0/(1.d-2)
  endif
!
  qosi0(:)=qosi(:,jj)
  do i=1,natom
    wrk2(i)=qosi0(3*(i-1)+1)
  enddo
  call sortnr(natom,wrk2,iwrk2)
  nb=0
  do il=1,nspecies
    do i=1,natom
      i2=iwrk2(i)
      if(itype(i2) == il)then
        nb=nb+1
        qosi(3*(nb-1)+1,jj)=qosi0(3*(i2-1)+1)
        qosi(3*(nb-1)+2,jj)=qosi0(3*(i2-1)+2)

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```

qosi(3*(nb-1)+3,jj)=qosi0(3*(i2-1)+3)
      endif
    enddo
    enddo

!
qosi0(:)=qosi(:,kk)
do i=1,natom
  wrk2(i)=qosi0(3*(i-1)+1)
enddo
call sortnr(natom,wrk2,iwrk2)
nb=0
do il=1,nspecies
  do i=1,natom
    i2=iwrk2(i)
    if(itype(i2) == il)then
      nb=nb+1
      qosi(3*(nb-1)+1,kk)=qosi0(3*(i2-1)+1)
      qosi(3*(nb-1)+2,kk)=qosi0(3*(i2-1)+2)
      qosi(3*(nb-1)+3,kk)=qosi0(3*(i2-1)+3)
    endif
  enddo
enddo

!
qosi0(:)=qosi(:,ll)
do i=1,natom
  wrk2(i)=qosi0(3*(i-1)+1)
enddo
call sortnr(natom,wrk2,iwrk2)
nb=0
do il=1,nspecies
  do i=1,natom
    i2=iwrk2(i)
    if(itype(i2) == il)then
      nb=nb+1
      qosi(3*(nb-1)+1,ll)=qosi0(3*(i2-1)+1)
      qosi(3*(nb-1)+2,ll)=qosi0(3*(i2-1)+2)
      qosi(3*(nb-1)+3,ll)=qosi0(3*(i2-1)+3)
    endif
  enddo
enddo

!
additional rotation around x axis
call gen_randrot(rx,ry,rz)
do i=1,natom
  vec(1)=qosi(3*(i-1)+1,jj)
  vec(2)=qosi(3*(i-1)+2,jj)
  vec(3)=qosi(3*(i-1)+3,jj)
  uec=matmul(rx,vec)
  qosi(3*(i-1)+1,jj)=vec(1)
  qosi(3*(i-1)+2,jj)=vec(2)
  qosi(3*(i-1)+3,jj)=vec(3)
enddo

!
nb=0
do ity=1,nspecies
  i=dbl(ranmar())*(nfrac-1)+1
  jslice=(dbl(i)/dbl(nfrac)) *dbl(nelements(ity))
  i=dbl(ranmar())*(nfrac-1)+1
  kslice=(dbl(i)/dbl(nfrac)) *dbl(nelements(ity))
  i=dbl(ranmar())*(nfrac-1)+1
  lslice=(dbl(i)/dbl(nfrac)) *dbl(nelements(ity))
  if(jslice <= 1) jslice=1 ; if(jslice >= nelements(ity)-1) jslice=nelement
s(ity)-1
  if(kslice <= 1) kslice=1 ; if(kslice >= nelements(ity)-1) kslice=nelement
s(ity)-1
  if(lslice <= 1) lslice=1 ; if(lslice >= nelements(ity)-1) lslice=nelement
s(ity)-1
  wrk1(1)=dbl(jslice)
  wrk1(2)=dbl(kslice)
  wrk1(3)=dbl(lslice)

```

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```

call sortnr(3,wrk1,iwrk1)
jslice=wrk1(iwrk1(1))
kslice=wrk1(iwrk1(2))
lslice=wrk1(iwrk1(3))
i2=0
do i=1,jslice
  nb=nb+1
  i2=i2+1
  qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,ii)+(ranmar()-0.5)/ddv1-shift00*0.5d0
  qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,ii)+(ranmar()-0.5)/ddv2
  qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,ii)+(ranmar()-0.5)/ddv3
enddo
do i=jslice+1,kslice
  nb=nb+1
  i2=i2+1
  qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,jj)+(ranmar()-0.5)/ddv1
  qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,jj)+(ranmar()-0.5)/ddv2
  qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,jj)+(ranmar()-0.5)/ddv3
enddo
do i=kslice+1,lslice
  nb=nb+1
  i2=i2+1
  qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,kk)+(ranmar()-0.5)/ddv1
  qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,kk)+(ranmar()-0.5)/ddv2
  qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,kk)+(ranmar()-0.5)/ddv3
enddo
do i=lslice+1,nelements(ity)
  nb=nb+1
  i2=i2+1
  qosi0(3*(nb-1)+1)=qosi(3*(nb-1)+1,ll)+(ranmar()-0.5)/ddv1+shift00*0.5d0
  qosi0(3*(nb-1)+2)=qosi(3*(nb-1)+2,ll)+(ranmar()-0.5)/ddv2
  qosi0(3*(nb-1)+3)=qosi(3*(nb-1)+3,ll)+(ranmar()-0.5)/ddv3
enddo
if(i2 /= nelements(ity))then
  write(6,*) 'something went wrong 4-1'
  stop
endif

enddo
if(nb /= natom)then
  write(6,*) 'something went wrong 4'
  stop
endif

!
if(lvcs)then
  jtr=0
  do
    jtr=jtr+1
    jslice=dbl(ranmar())*5+1
    kslice=dbl(ranmar())*5+1
    lslice=dbl(ranmar())*5+1
    if(jslice <= 1) jslice=1 ; if(jslice >= 5) jslice=5
    if(kslice <= 1) kslice=1 ; if(kslice >= 5) kslice=5
    if(lslice <= 1) lslice=1 ; if(lslice >= 5) lslice=5
    wrk1(1)=dbl(jslice)
    wrk1(2)=dbl(kslice)
    wrk1(3)=dbl(lslice)
    call sortnr(3,wrk1,iwrk1)
    jslice=wrk1(iwrk1(1))
    kslice=wrk1(iwrk1(2))
    lslice=wrk1(iwrk1(3))
    nb=0
    do i=1,jslice
      nb=nb+1
      qosi0(ish+i)=qosi(ish+i,ii)
    enddo
    do i=jslice+1,kslice
      nb=nb+1
      qosi0(ish+i)=qosi(ish+i,jj)
    enddo

```

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```

do i=kslice+1,lslice
  nb=nb+1
  qosi0(ish+i)=qosi(ish+i,kk)
enddo
do i=lslice+1,6
  nb=nb+1
  qosi0(ish+i)=qosi(ish+i,ll)
enddo
if(nb /= 6)then
  write(6,*) 'something went wrong 4-vcs'
  stop
endif

!
  if(jtr > 100)then
    sig0=1.d0 ; x10=0.d0
    do i=1,6
      call gauss(sig0,x10,x1)
      vtest=rammar()
      if(vtest < 0.2500)
        qosi0(ish+i)=qosi(ish+i,ii)+(0.04
d0*qosi(ish+i,ii))*x1
      if(vtest > 0.2500 .and. vtest < 0.5000) qosi0(ish+i)=qosi(ish+i,jj)+(0.04
d0*qosi(ish+i,jj))*x1
      if(vtest > 0.5000 .and. vtest < 0.7500) qosi0(ish+i)=qosi(ish+i,kk)+(0.04
d0*qosi(ish+i,kk))*x1
      if(vtest > 0.7500)
        qosi0(ish+i)=qosi(ish+i,ll)+(0.04
d0*qosi(ish+i,ll))*x1
      enddo
    endif

!
    if(jtr > 200)then
      sig0=1.d0 ; x10=0.d0
      do i=1,6
        call gauss(sig0,x10,x1)
        qosi0(ish+i)=qosi(ish+i,ii)+(0.04d0*qosi(ish+i,ii))*x1
      enddo
    endif

    do i=1,6
      t6(i)=qosi0(ish+i)
    enddo
    call latmat(t6,cmatrix,1)
    vtest=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,1)
&
    + (cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,2)
&
    + (cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,3)
    vtest=abs(vtest)
    if(vtest > refvol*(1.d0-voltol) .and. vtest < refvol*(1.d0+voltol))then
      call check_lat(llattice,locate,cmatrix)
    else
      llattice=.false.
    endif

    if(llattice) goto 888
    if(jtr > 400)then
      do i=1,6
        t6(i)=qosi(ish+i,ii)
      enddo
!
      write(6,*) 'we have trouble with ii,jj,kk,ll'
      goto 888
    endif

    enddo
888 continue
    if(jtr > 400) write(6,*) 'we have trouble with ii,jj,kk,ll 400'
    if(jtr > 100) write(6,*(i5,2x,a13')) jtr,'jtr code=4'
    do i=1,6
      qosi0(ish+i)=t6(i)
    enddo
  endif
  if(lpbc) call tolatx(qosi0)
endif

```

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```

!
special process for low coordinated atoms and contacts
call danglingbond_care()

end subroutine csa_rnd_lattice_basis

!
!
Written by In-Ho Lee, KRISS, January 28, 2013.
subroutine tocaxx(qqq)
USE csa_application, ONLY : natom
implicit none
real*8 qqq(ndeg)
integer j,i,ish
real*8 t6(6),cmatrix(3,3),a1(3),a2(3),a3(3),x,y,z

ish=ndeg-6
do i=1,6
  t6(i)=qqq(ish+i)
enddo
call latmat(t6,cmatrix,1)
a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)

!
do j=1,natom
  x=a1(1)*qqq(3*(j-1)+1)+a2(1)*qqq(3*(j-1)+2)+a3(1)*qqq(3*(j-1)+3)
  y=a1(2)*qqq(3*(j-1)+1)+a2(2)*qqq(3*(j-1)+2)+a3(2)*qqq(3*(j-1)+3)
  z=a1(3)*qqq(3*(j-1)+1)+a2(3)*qqq(3*(j-1)+2)+a3(3)*qqq(3*(j-1)+3)
  qqq(3*(j-1)+1)=x
  qqq(3*(j-1)+2)=y
  qqq(3*(j-1)+3)=z
enddo
end subroutine tocaxx

!
!
Written by In-Ho Lee, KRISS, January 28, 2013.
subroutine tolatx(qqq)
USE csa_application, ONLY : natom
implicit none
real*8 qqq(ndeg)
real*8 b(3,3),devid
integer j,i,ish
real*8 t6(6),cmatrix(3,3),a1(3),a2(3),a3(3),d1,d2,d3

ish=ndeg-6
do i=1,6
  t6(i)=qqq(ish+i)
enddo
call latmat(t6,cmatrix,1)
a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)

!
devid=a1(1)*a2(2)*a3(3)-a1(2)*a2(1)*a3(3)-a1(1)*a2(3)*a3(2) &
+ a1(3)*a2(1)*a3(2)+a1(2)*a2(3)*a3(1)-a1(3)*a2(2)*a3(1)
b(1,1)=-a2(3)*a3(2)+a2(2)*a3(3)
b(2,1)= a1(3)*a3(2)-a1(2)*a3(3)
b(3,1)=-a1(3)*a2(2)+a1(2)*a2(3)
b(1,2)= a2(3)*a3(1)-a2(1)*a3(3)
b(2,2)=-a1(3)*a3(1)+a1(1)*a3(3)
b(3,2)= a1(3)*a2(1)-a1(1)*a2(3)
b(1,3)=-a2(2)*a3(1)+a2(1)*a3(2)
b(2,3)= a1(2)*a3(1)-a1(1)*a3(2)
b(3,3)=-a1(2)*a2(1)+a1(1)*a2(2)
b(:, :)=b(:, :)/devid

!
do j=1,natom
  d1=b(1,1)*qqq(3*(j-1)+1)+b(1,2)*qqq(3*(j-1)+2)+b(1,3)*qqq(3*(j-1)+3)
  d2=b(2,1)*qqq(3*(j-1)+1)+b(2,2)*qqq(3*(j-1)+2)+b(2,3)*qqq(3*(j-1)+3)
  d3=b(3,1)*qqq(3*(j-1)+1)+b(3,2)*qqq(3*(j-1)+2)+b(3,3)*qqq(3*(j-1)+3)
  qqq(3*(j-1)+1)=d1
  qqq(3*(j-1)+2)=d2
  qqq(3*(j-1)+3)=d3
enddo
do j=1,natom
  qqq(3*(j-1)+1)=qqq(3*(j-1)+1)-anint(qqq(3*(j-1)+1))

```



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```

      qqg(3*(j-1)+2)=qqg(3*(j-1)+2)-anint(qqg(3*(j-1)+2))
      qqg(3*(j-1)+3)=qqg(3*(j-1)+3)-anint(qqg(3*(j-1)+3))
    enddo
    do j=1,natom
      if(qqg(3*(j-1)+1) < 0.d0) qqg(3*(j-1)+1)=qqg(3*(j-1)+1)+1.d0
      if(qqg(3*(j-1)+2) < 0.d0) qqg(3*(j-1)+2)=qqg(3*(j-1)+2)+1.d0
      if(qqg(3*(j-1)+3) < 0.d0) qqg(3*(j-1)+3)=qqg(3*(j-1)+3)+1.d0
    enddo
  end subroutine tolatx

```

```

!      Written by In-Ho Lee, KRISS, January 28, 2013.
      subroutine lat_mutation(cmatrix)
      implicit none
      real*8 cmatrix(3,3)
      real*8 unitm(3,3),tmpmat(3,3),gaussm(3,3),strainedm(3,3),x,y
      integer i,j
      real ranmar

```

```

      tmpmat=cmatrix
      unitm=0.d0
      do i=1,3
        unitm(i,i)=1.d0
      enddo
      do i=1,3
        do j=1,3
          x=ranmar()
          y=ranmar()
          if(y > 0.5) gaussm(i,j)=exp(-x**2)*0.25
          if(y <=0.5) gaussm(i,j)=-exp(-x**2)*0.25
          if(i == j) gaussm(i,j)=abs(gaussm(i,j))*3.0
        enddo
      enddo
      strainedm=unitm+gaussm
      cmatrix=matmul(tmpmat,strainedm)
    end subroutine lat_mutation

```

```

!      Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine csa_bank_dump(idirection)
      implicit none
      integer idirection

```

```

      if(idirection == 0)then
        open(1,file='fort.l',form='formatted')
        write(1,*) ndeg,npop,npopl
        write(1,*) posil,energy_sortedl
        write(1,*) posi,energy_sorted
        write(1,*) posi_best,energy_best,davg
        close(1)
      endif
      if(idirection == 1)then
        open(1,file='fort.l',form='formatted')
        read(1,*) ndeg_r,npop_r,npopl_r
        if(ndeg_r /= ndeg)then
          write(6,*) 'system size mismatch'
          write(6,*) 'fort.l and csa.in are different from each other'
          close(1)
          return
        endif
        allocate(posi_r(ndeg,npop_r))
        allocate(posil_r(ndeg,npopl_r))
        allocate(energy_sorted_r(npop_r))
        allocate(energy_sortedl_r(npopl_r))
        allocate(posi_best_r(ndeg))
        read(1,*) posil_r,energy_sortedl_r
        read(1,*) posi_r,energy_sorted_r
        read(1,*) posi_best_r,energy_best_r,davg_r
        close(1)
      endif
    end subroutine csa_bank_dump

```

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```

!      Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine csa_bank_sort(ibank)
      implicit none
      integer ibank
      integer j,jl

      if(ibank ==1)then
        wrkl(1:npopl)=energy_sortedl(1:npopl) ; qosil=posil ; call sortnr(npopl,w
        rk1,iwrkl)
        do j=1,npopl
          jl=iwrkl(j)
          posil(:,j)=qosil(:,jl)
          energy_sortedl(j)=wrkl(jl)
        enddo
      else
        wrkl(1:npop)=energy_sorted(1:npop) ; qosi=posi ; call sortnr(npop,wrkl,iw
        rk1)
        do j=1,npop
          jl=iwrkl(j)
          posi(:,j)=qosi(:,jl)
          energy_sorted(j)=wrkl(jl)
        enddo
      endif
    end subroutine csa_bank_sort

```

```

!      Written by In-Ho Lee, KRISS, September 11, 2013.
      subroutine danglingbond_care()
      USE csa_application, ONLY : natom,rcl,ncoord,wrk2,iwrk2,lpbc
      implicit none
      integer i,iord
      integer itgt,imvg,i3,ish
      real*8 dv1,dv2,dv3,cmatrix(3,3),t6(6),a1(3),a2(3),a3(3)
      real ranmar

      ish=ndeg-6
      if(lpbc)then
        do i=1,6
          t6(i)=qosi0(ish+i)
        enddo
        call latmat(t6,cmatrix,1)
        a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
        dv1=sqrt(dot_product(a1,a1))/1.1d0
        dv2=sqrt(dot_product(a2,a2))/1.1d0
        dv3=sqrt(dot_product(a3,a3))/1.1d0
      else
        dv1=0.5d0/rcl
        dv2=0.5d0/rcl
        dv3=0.5d0/rcl
      endif
      if(.not. lpbc)then
        call centering(qosi0)
        do iord=1,1
          call gen_coordination()
          do i=1,natom
            wrk2(i)=dble(ncoord(i))
          enddo
          call sortnr(natom,wrk2,iwrk2)
          do i=1,natom
            if(wrk2(iwrk2(i)) < 1)then
              qosi0(3*(iwrk2(i)-1)+1)=qosi0(3*(iwrk2(i)-1)+1)*0.1
              qosi0(3*(iwrk2(i)-1)+2)=qosi0(3*(iwrk2(i)-1)+2)*0.1
              qosi0(3*(iwrk2(i)-1)+3)=qosi0(3*(iwrk2(i)-1)+3)*0.1
            endif
          enddo
        enddo
        if(natom >2)then
          imvg=iwrk2(1) ; itgt=iwrk2(2) ; i3=iwrk2(3)
          qosi0(3*(imvg-1)+1)=qosi0(3*(i3-1)+1)+(ranmar()-0.5)/dv1
          qosi0(3*(imvg-1)+2)=qosi0(3*(i3-1)+2)+(ranmar()-0.5)/dv2

```

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```

qosi0(3*(imvg-1)+3)=qosi0(3*(i3-1)+3)+(ranmar()-0.5)/dv3
qosi0(3*(itgt-1)+1)=qosi0(3*(i3-1)+1)+(ranmar()-0.5)/dv1
qosi0(3*(itgt-1)+2)=qosi0(3*(i3-1)+2)+(ranmar()-0.5)/dv2
qosi0(3*(itgt-1)+3)=qosi0(3*(i3-1)+3)+(ranmar()-0.5)/dv3
    endif
call repulsion_care()
enddo

    endif
if(lpbc)then
do iord=1,1
call gen_coordination()
do i=1,natom
wrk2(i)=dble(ncoord(i))
enddo
call sortnr(natom,wrk2,iwrk2)
imvg=iwrk2(1) ; itgt=iwrk2(2)
qosi0(3*(imvg-1)+1)=qosi0(3*(itgt-1)+1)+(ranmar()-0.5)/dv1
qosi0(3*(imvg-1)+2)=qosi0(3*(itgt-1)+2)+(ranmar()-0.5)/dv2
qosi0(3*(imvg-1)+3)=qosi0(3*(itgt-1)+3)+(ranmar()-0.5)/dv3
call repulsion_care()
enddo
    endif
end subroutine danglingbond_care
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine repulsion_care()
USE csa_application, ONLY : natom,lpbc,sigmamatrix,nspecies,itype
USE csa_application, ONLY : iwrk2,iwrk4
implicit none
real*8 dv1,dv2,dv3,repul0,repul1,repul,ddxx,cmatrix(3,3),t6(6),a1(3),a2(3),a3(3),cellvol0
integer i,j,itr,ktr,ljitramax,ish
integer iswp,jswp,itr
real*8 wec(3,2)
integer nprint
integer kcase
real ranmar

do i=1,natom*3
call tonormal(qosi0(i))
enddo
nprint=0
nprint=1
repul0=0.d0
repul1=0.d0
do i=1,nspecies
do j=i,nspecies
repul0=repul0+1.d0
repul1=repul1+sigmamatrix(i,j)
enddo
enddo
repul1=repul1/repul0

kcase=2
kcase=1
kcase=3

ddxx=1.5d0 *repul1
if(kcase ==1) ddxx=1.5d0 *repul1
if(kcase ==2) ddxx=1.5d0 *sigmamatrix(1,1)

ljitrmax=100000*natom
!
ljitrmax=0

if(ljitrmax <= 0) return
iwrk2=1

```

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```

ish=ndeg-6
if(lpbc)then
do i=1,6
t6(i)=qosi0(ish+i)
enddo
call latmat(t6,cmatrix,1)
a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
cellvol0=(cmatrix(1,2)*cmatrix(2,3)-cmatrix(1,3)*cmatrix(2,2))*cmatrix(3,
1) &
+ (cmatrix(1,3)*cmatrix(2,1)-cmatrix(1,1)*cmatrix(2,3))*cmatrix(3,
2) &
+ (cmatrix(1,1)*cmatrix(2,2)-cmatrix(1,2)*cmatrix(2,1))*cmatrix(3,
3)
cellvol0=abs(cellvol0)
repul=(cellvol0/dble(natom))**(1.d0/3.d0)
ddxx=repul/2.d0

dv1=sqrt(dot_product(a1,a1))/ddxx
dv2=sqrt(dot_product(a2,a2))/ddxx
dv3=sqrt(dot_product(a3,a3))/ddxx
call direct_pbc(qosi0)
qosi00=qosi0
call cal_repulsion(qosi00,repul0)
repul=0.d0 ; itr=0
repul1=repul0
if(repul1 < 1.d-8) goto 101
do itr=1,ljitramax
!
if(nspecies >= 2)then
if(natom > 2)then
do itr=1,1+3*dble(ranmar())+int(natom/3)
510 continue
iswp=dble(ranmar())*natom+1 ; jswp=dble(ranmar())*natom+1
if(itype(iswp) == itype(jswp)) goto 510
wec(1,1)=qosi0(3*(iswp-1)+1)
wec(2,1)=qosi0(3*(iswp-1)+2)
wec(3,1)=qosi0(3*(iswp-1)+3)
wec(1,2)=qosi0(3*(jswp-1)+1)
wec(2,2)=qosi0(3*(jswp-1)+2)
wec(3,2)=qosi0(3*(jswp-1)+3)
qosi0(3*(iswp-1)+1)=wec(1,2)
qosi0(3*(iswp-1)+2)=wec(2,2)
qosi0(3*(iswp-1)+3)=wec(3,2)
qosi0(3*(jswp-1)+1)=wec(1,1)
qosi0(3*(jswp-1)+2)=wec(2,1)
qosi0(3*(jswp-1)+3)=wec(3,1)
enddo
    endif
endif
!
! do ktr=1,1000

do i=1,natom
if(iwrk2(i) ==1)then
qosi0(3*(i-1)+1)=qosi00(3*(i-1)+1)+(ranmar()-0.5)/dv1
qosi0(3*(i-1)+2)=qosi00(3*(i-1)+2)+(ranmar()-0.5)/dv2
qosi0(3*(i-1)+3)=qosi00(3*(i-1)+3)+(ranmar()-0.5)/dv3
j=iwrk4(i)
qosi0(3*(j-1)+1)=qosi00(3*(j-1)+1)+(ranmar()-0.5)/dv1
qosi0(3*(j-1)+2)=qosi00(3*(j-1)+2)+(ranmar()-0.5)/dv2
qosi0(3*(j-1)+3)=qosi00(3*(j-1)+3)+(ranmar()-0.5)/dv3
    endif
enddo
if(ranmar() < 0.05)then
do i=1,natom
qosi0(3*(i-1)+1)=qosi00(3*(i-1)+1)+(ranmar()-0.5)/dv1
qosi0(3*(i-1)+2)=qosi00(3*(i-1)+2)+(ranmar()-0.5)/dv2
qosi0(3*(i-1)+3)=qosi00(3*(i-1)+3)+(ranmar()-0.5)/dv3
enddo

```

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```

        endif
        call direct_pbc(qosi0)
        call cal_repulsion(qosi0,repul)
        if(repul0 > repul)then
!       write(6,'(a7,2x,2e18.8)') 'updated', repul,repul0
        qosi00(:)=qosi0(:)
        repul0=repul
!       if(repul0 <1.d-8) exit
        if(repul0 <1.d-8) goto 101
        endif
!
        enddo
        enddo
101      continue
        if(nprint ==1)then
          write(6,'(i8,lx,a9,lx,2f16.1,2x,f18.8)') itr,'itr,repul',repul0,repul1,cellvol0
          if(repul > 1.d-8) write(6,'(i8,lx,a9,lx,4f18.8)') itr,'itr,repul',repul,repul0,repu
!1,cellvol0
        endif
!       do i=1,natom
!       write(6,'(3f18.8)') qosi00(3*(i-1)+1),qosi00(3*(i-1)+2),qosi00(3*(i-1)+3)
!       enddo
        qosi0=qosi00
        call direct_pbc(qosi0)
        else
        call centering(qosi0)
        qosi00=qosi0
        call cal_repulsion(qosi00,repul0)
        repul=0.d0 ; itr=0
        repul1=repul0
        if(repul1 < 1.d-8) goto 102
        do itr=1,ljitramax
!
        if(nspecies >= 2)then
          if(natom > 2)then
            do itr=1,1+3*dble(ranmar())+int(natom/3)
              continue
610          iswp=dble(ranmar())*natom+1 ; jswp=dble(ranmar())*natom+1
          if(itype(iswp) == itype(jswp)) goto 610
          wec(1,1)=qosi0(3*(iswp-1)+1)
          wec(2,1)=qosi0(3*(iswp-1)+2)
          wec(3,1)=qosi0(3*(iswp-1)+3)
          wec(1,2)=qosi0(3*(jswp-1)+1)
          wec(2,2)=qosi0(3*(jswp-1)+2)
          wec(3,2)=qosi0(3*(jswp-1)+3)
          qosi0(3*(iswp-1)+1)=wec(1,2)
          qosi0(3*(iswp-1)+2)=wec(2,2)
          qosi0(3*(iswp-1)+3)=wec(3,2)
          qosi0(3*(jswp-1)+1)=wec(1,1)
          qosi0(3*(jswp-1)+2)=wec(2,1)
          qosi0(3*(jswp-1)+3)=wec(3,1)
          enddo
        endif
        endif
!
        do ktr=1,1000
!
        do i=1,natom
          if(iwrk2(i) == 1) then
            qosi0(3*(i-1)+1)=qosi00(3*(i-1)+1)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
            qosi0(3*(i-1)+2)=qosi00(3*(i-1)+2)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
            qosi0(3*(i-1)+3)=qosi00(3*(i-1)+3)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
          )
          j=iwrk4(i)
          qosi0(3*(j-1)+1)=qosi00(3*(j-1)+1)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
          qosi0(3*(j-1)+2)=qosi00(3*(j-1)+2)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5

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```

        qosi0(3*(j-1)+3)=qosi00(3*(j-1)+3)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
        )
        endif
        enddo
        if(ranmar() < 0.05)then
          do i=1,natom
            qosi0(3*(i-1)+1)=qosi00(3*(i-1)+1)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
            qosi0(3*(i-1)+2)=qosi00(3*(i-1)+2)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
            qosi0(3*(i-1)+3)=qosi00(3*(i-1)+3)+(ranmar()-0.5)*ddxx*(1.d0+ranmar()-0.5
          )
        enddo
        endif
        call centering(qosi0)
        call cal_repulsion(qosi0,repul)
        if(repul0 > repul)then
!       write(6,'(a7,2x,2e18.8)') 'updated', repul,repul0
        qosi00(:)=qosi0(:)
        repul0=repul
!       if(repul0 <1.d-8) exit
        if(repul0 <1.d-8) goto 102
        endif
!
        enddo
        enddo
102      continue
        if(nprint ==1)then
          write(6,'(i8,lx,a9,lx,2f16.1)') itr,'itr,repul',repul0,repul1
          if(repul > 1.d-8) write(6,'(i8,lx,a9,lx,3f18.8)') itr,'itr,repul',repul,repul0,repu
!1
        endif
!       do i=1,natom
!       write(6,'(3f18.8)') qosi00(3*(i-1)+1),qosi00(3*(i-1)+2),qosi00(3*(i-1)+3)
!       enddo
        qosi0=qosi00
        call centering(qosi0)
        endif
        end subroutine repulsion_care
!
!       Written by In-Ho Lee, KRISS, September 11, 2013.
        subroutine cal_repulsion(qqq,repul)
          USE csa_application, ONLY : natom,itype,sigmatrix,lpbc
          USE csa_application, ONLY : iwrk2,iwrk4
          implicit none
          real*8 repul,qqq(ndeg)
          integer i,j,ish
          real*8 x,y,z,r,d1,d2,d3,ctest,sig,rho,rs,pi,a1(3),a2(3),a3(3),cmatrix(3,3
        ),t6(6)

          iwrk2=0
          if(lpbc)then
            ish=ndeg-6
            do i=1,6
              t6(i)=qqq(ish+i)
            enddo
            call latmat(t6,cmatrix,1)
            a1(:)=cmatrix(1,:) ; a2(:)=cmatrix(2,:) ; a3(:)=cmatrix(3,:)
          endif
          sig=1.5d0
          if(lpbc)then
            ctest=a1(1)*a2(2)*a3(3)-a1(2)*a2(1)*a3(3)-a1(1)*a2(3)*a3(2) &
              +a1(3)*a2(1)*a3(2)+a1(2)*a2(3)*a3(1)-a1(3)*a2(2)*a3(1)
            ctest=abs(ctest)
            pi=4.d0*atan(1.d0)
            rho=dble(natom)/ctest
            rs=(3.d0/(rho*4.d0*pi))**(1.d0/3.d0)
            sig=(rs*2.d0)*(2.d0)**(-1.d0/6.d0)

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```

        endif
        repul=0.d0
        do i=1,natom-1
        do j=i+1,natom
        if(lpbc)then
        d1=qqq(3*(i-1)+1)-qqq(3*(j-1)+1)
        d2=qqq(3*(i-1)+2)-qqq(3*(j-1)+2)
        d3=qqq(3*(i-1)+3)-qqq(3*(j-1)+3)
        d1=d1-anint(d1)
        d2=d2-anint(d2)
        d3=d3-anint(d3)
        x=d1*a1(1)+d2*a2(1)+d3*a3(1)
        y=d1*a1(2)+d2*a2(2)+d3*a3(2)
        z=d1*a1(3)+d2*a2(3)+d3*a3(3)
        else
        x=qqq(3*(j-1)+1)-qqq(3*(i-1)+1)
        y=qqq(3*(j-1)+2)-qqq(3*(i-1)+2)
        z=qqq(3*(j-1)+3)-qqq(3*(i-1)+3)
        endif
        r=sqrt(x*x+y*y+z*z)
        if(r < 1.d-8) r=1.d-8
        sig=sigmamatrix(itype(i),itype(j))
        if( r < sig)then
        repul=repul+1.d0
        iwrk2(i)=1
        iwrk2(j)=1
        iwrk4(i)=j
        iwrk4(j)=i
        endif

        enddo
        enddo
        end subroutine cal_repulsion
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_coordination()
USE csa_application, ONLY : natom,rcl,ncoord,lpbc
implicit none
integer i,j,kkl,ish
real*8 x,y,z,r,d1,d2,d3,t6(6),cmatrix(3,3),a1(3),a2(3),a3(3)

if(lpbc)then
ish=ndeg-6
do i=1,6
t6(i)=qosi0(ish+i)
enddo
call latmat(t6,cmatrix,1)
a1(:)=cmatrix(1,:); a2(:)=cmatrix(2,:); a3(:)=cmatrix(3,:)
endif
do i=1,natom
kkl=0
do j=1,natom
if(j == i) cycle
if(lpbc)then
d1=qosi0(3*(i-1)+1)-qosi0(3*(j-1)+1)
d2=qosi0(3*(i-1)+2)-qosi0(3*(j-1)+2)
d3=qosi0(3*(i-1)+3)-qosi0(3*(j-1)+3)
d1=d1-anint(d1)
d2=d2-anint(d2)
d3=d3-anint(d3)
x=d1*a1(1)+d2*a2(1)+d3*a3(1)
y=d1*a1(2)+d2*a2(2)+d3*a3(2)
z=d1*a1(3)+d2*a2(3)+d3*a3(3)
else
x=qosi0(3*(i-1)+1)-qosi0(3*(j-1)+1)
y=qosi0(3*(i-1)+2)-qosi0(3*(j-1)+2)
z=qosi0(3*(i-1)+3)-qosi0(3*(j-1)+3)
endif
r=sqrt(x*x+y*y+z*z)
if( r <= rcl)then

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```

        kkl=kkl+1
        endif
        enddo
        ncoord(i)=kkl
        enddo
        end subroutine gen_coordination
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_lattice_matrix(amatrix,s6,cellvol0)
implicit none
real*8 amatrix(3,3),s6(6),cellvol0
integer isgindex,jtr
logical llattice,lcate
real ranmar

lcate=.false.
jtr=0
do
111 continue
jtr=jtr+1
isgindex=dble(ranmar())*230+1
call gen_sg_lat(isgindex,cellvol0,amatrix)
if(jtr > 400)then
write(6,*) ' problem in gen_lattice_matrix '
call gen_latnosym(amatrix,cellvol0)
endif
call check_lat(llattice,lcate,amatrix)
if(.not. llattice)then
write(6,*) 'not a lattice'
goto 111
else
goto 222
endif
enddo
222 continue
call latmat(s6,amatrix,0)
end subroutine gen_lattice_matrix
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_latnosym(wmat,volume)
implicit none
real*8 volume,wmat(3,3)
real*8 randomlat(6),rmat(3,3),tmq,tmr,slat(6),pi
integer i
real ranmar

wmat=0.0d0
do i=1,6
randomlat(i)=ranmar()
enddo
pi=4.0d0*atan(1.0d0)
do i=4,6
randomlat(i)=randomlat(i)*pi/2.d0
enddo
call latmat(randomlat,rmat,1)
tmr=(rmat(1,2)*rmat(2,3)-rmat(1,3)*rmat(2,2))*rmat(3,1) &
+ (rmat(1,3)*rmat(2,1)-rmat(1,1)*rmat(2,3))*rmat(3,2) &
+ (rmat(1,1)*rmat(2,2)-rmat(1,2)*rmat(2,1))*rmat(3,3)
tmq=volume/tmr ; tmq=tmq*(1.0d0/3.0d0)
slat(1)=randomlat(1)*tmq
slat(2)=randomlat(2)*tmq
slat(3)=randomlat(3)*tmq
slat(4)=randomlat(4) ; slat(5)=randomlat(5) ; slat(6)=randomlat(6)
call latmat(slat,wmat,1)
end subroutine gen_latnosym
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine check_lat_cyc(t6,cellvol0,llattice)
USE, INTRINSIC :: IEEE_ARITHMETIC, ONLY : IEEE_IS_FINITE,IEEE_IS_NAN

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```

implicit none
logical llattice
real*8 t6(6),cellvol0
real*8 cmatrix(3,3),bmatrix(3,3),s6(6)
integer i,j

llattice=.false.
call latmatvol(t6,cmatrix,cellvol0)
!---{
!
do i=1,3
do j=1,3
if(ieee_is_nan(cmatrix(i,j)))then
llattice=.false.
return
endif
if(.not. ieee_is_finite(cmatrix(i,j)))then
llattice=.false.
return
endif
endif
enddo
enddo
!---}
call latmat(t6,bmatrix,1)
call latmat(s6,bmatrix,0)
!
write(6,'(6f20.10)') ((s6(i)-t6(i)),i=1,6)
if(sum(abs(s6-t6)) < 1.d-10) llattice=.true.
!
write(6,'(6f20.10,2x,11)') ((s6(i)-t6(i)),i=1,6), llattice
end subroutine check_lat_cyc
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine check_lat(lflag,l2d,cmatrix)
USE, INTRINSIC :: IEEE_ARITHMETIC, ONLY : IEEE_IS_FINITE,IEEE_IS_NAN
implicit none
logical lflag,l2d
real*8 cmatrix(3,3)
real*8 altm(3,3),ra,rb,rc,alpha,beta,gama,cosinea,cosineb,cosinec,pi,tmp
real*8 uec(3),vec(3),wec(3),uu,vv,ww
real*8 cosinel,cosine2,cosine3
integer i,j

altm=cmatrix
pi=4.0d0*atan(1.0d0)
!---{
!
do i=1,3
do j=1,3
if(ieee_is_nan(altm(i,j)))then
lflag=.false.
return
endif
if(.not. ieee_is_finite(altm(i,j)))then
lflag=.false.
return
endif
endif
enddo
enddo
!---}
ra=sqrt(altm(1,1)**2+altm(1,2)**2+altm(1,3)**2)
rb=sqrt(altm(2,1)**2+altm(2,2)**2+altm(2,3)**2)
rc=sqrt(altm(3,1)**2+altm(3,2)**2+altm(3,3)**2)
cosinea=(altm(2,1)*altm(3,1)+altm(2,2)*altm(3,2)+altm(2,3)*altm(3,3))/rb/
rc
cosineb=(altm(1,1)*altm(3,1)+altm(1,2)*altm(3,2)+altm(1,3)*altm(3,3))/rc/
ra
cosinec=(altm(1,1)*altm(2,1)+altm(1,2)*altm(2,2)+altm(1,3)*altm(2,3))/ra/
rb

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```

tmp=180.0d0/pi
alpha=tmp*acos(cosinea) ; beta=tmp*acos(cosineb) ; gama=tmp*acos(cosinec)
lflag=.true.
if(.not. l2d)then
if(ra < 1.2d0 .or. rb < 1.2d0 .or. rc < 1.2d0) lflag=.false.
if(alpha < 20.0d0 .or. alpha > 160.0d0) lflag=.false.
if(beta < 20.0d0 .or. beta > 160.0d0) lflag=.false.
if(gama < 20.0d0 .or. gama > 160.0d0) lflag=.false.
if(ra/rb > 6.0d0 .or. ra/rb < 0.3d0) lflag=.false.
if(ra/rc > 6.0d0 .or. ra/rc < 0.3d0) lflag=.false.
if(rb/rc > 6.0d0 .or. rb/rc < 0.3d0) lflag=.false.
else
if(ra < 1.2d0 .or. rb < 1.2d0) lflag=.false.
if(alpha < 20.0d0 .or. alpha > 160.0d0) lflag=.false.
if(beta < 20.0d0 .or. beta > 160.0d0) lflag=.false.
if(gama < 20.0d0 .or. gama > 160.0d0) lflag=.false.
if(ra/rb > 6.0d0 .or. ra/rb < 0.3d0) lflag=.false.
endif
!
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uec(:)=altm(1,:)+altm(2,:)
vec(:)=altm(2,:)+altm(3,:)
wec(:)=altm(3,:)+altm(1,:)
uu=sqrt(uec(1)**2+uec(2)**2+uec(3)**2)
vv=sqrt(vec(1)**2+vec(2)**2+vec(3)**2)
ww=sqrt(wec(1)**2+wec(2)**2+wec(3)**2)
cosinel=(uec(1)*altm(3,1)+uec(2)*altm(3,2)+uec(3)*altm(3,3))/uu/rc
cosine2=(vec(1)*altm(1,1)+vec(2)*altm(1,2)+vec(3)*altm(1,3))/vv/ra
cosine3=(wec(1)*altm(2,1)+wec(2)*altm(2,2)+wec(3)*altm(2,3))/ww/rb
tmp=180.0d0/pi
cosinel=tmp*acos(cosinel)
cosine2=tmp*acos(cosine2)
cosine3=tmp*acos(cosine3)
if(l2d)then
if(cosinel < 20.d0 .or. cosinel > 160.d0) lflag=.false.
else
if(cosinel < 20.d0 .or. cosinel > 160.d0) lflag=.false.
if(cosine2 < 20.d0 .or. cosine2 > 160.d0) lflag=.false.
if(cosine3 < 20.d0 .or. cosine3 > 160.d0) lflag=.false.
endif
end subroutine check_lat
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine master_slave(nwork,ndir,kcmd)
implicit none
integer nwork,ndir,kcmd
integer iw,mm
integer, allocatable :: iseq(:)
logical, allocatable :: loccupied(:)

if(nwork <=0) return
!
if(kcmd == 2)then
allocate(iseq(nwork))
call perturbation_seq(npert,nmate,nwork,iseq)
else
if(nwork > 0)then
allocate(iseq(nwork))
iseq=1
endif
endif
!
iw=ndir ; call gen_directories(iw)
allocate(loccupied(ndir))
loccupied=.false.
mm=0
do iw=1,min(nwork,ndir)
mm=mm+1
call send_exe(mm,ndir,loccupied,kcmd,nwork,iseq)
enddo

```

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```

if(man > npopl) man=npopl
if(man < 1) man=npopl
posil(:,man)=qosi0(:)
energy_sorted1(man)=energy0
endif
if(kcmd == 2)then
call csa_update_conformations()
endif
call flush(6)
call sleep(1)
end subroutine receive
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine send_exe(mmm,ndir,loccupied,kcmd,nwork,iseq)
USE csa_application, ONLY : natom,lpbc
implicit none
integer mmm,ndir,kcmd,nwork,iseq(nwork)
logical loccupied(ndir)
integer jd,i,ish
real*8 r6(6),cmatrix(3,3),a1(3),a2(3),a3(3),ddg,pi
character*280 file_names(20),tmpname
character*280 cmd
logical lexist18
real ranmar

do jd=1,ndir
if(.not. loccupied(jd))then
call iofilearray(jd,file_names)
call csa_rnd_lattice_basis(mmm,nwork,iseq)
ish=ndeg-6
if(lpbc)then
do i=1,6
r6(i)=qosi0(ish+i)
enddo
call latmat(r6,cmatrix,1)
a1(:)=cmatrix(1,:); a2(:)=cmatrix(2,:); a3(:)=cmatrix(3,:)
endif
if(lpbc)then
call direct_pbc(qosi0)
else
call centering(qosi0)
endif
inquire(file=trim(file_names(5)),exist=lexist18)
if(lexist18)then
open(44,file=trim(file_names(5)),form='formatted')
close(44,status='delete')
endif
inquire(file=trim(file_names(18)),exist=lexist18)
if(lexist18)then
open(44,file=trim(file_names(18)),form='formatted')
close(44,status='delete')
endif
call write_poscar(mmm,file_names(3))
pi=4.0d0*atan(1.0d0)
ddg=(2.0d0*pi)*0.12d0; tmpname=trim(file_names(5))//'_012'
call write_kpoints(ddg,a1,a2,a3,tmpname)
ddg=(2.0d0*pi)*0.06d0; tmpname=trim(file_names(5))//'_006'
call write_kpoints(ddg,a1,a2,a3,tmpname)
ddg=(2.0d0*pi)*0.03d0; tmpname=trim(file_names(5))//'_003'
call write_kpoints(ddg,a1,a2,a3,tmpname)
ddg=(2.0d0*pi)*0.02d0; tmpname=trim(file_names(5))//'_002'
call write_kpoints(ddg,a1,a2,a3,tmpname)
ddg=(2.0d0*pi)*0.00d0; tmpname=trim(file_names(5))//'_000'
call write_kpoints(ddg,a1,a2,a3,tmpname)
call sleep(1)
call system('sleep 0.1')
cmd='cp '//trim(file_names(3))//'_ '//trim(file_names(3))//'_ '
cmd=trim(cmd); call system(cmd)
!
!

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```

cmd='cd '//trim(file_names(1))//'_ '//qsub /CSA_SOLDIER.pbs'
! cmd='cd '//trim(file_names(1))//'_ '//sbatch ./CSA_SOLDIER.pbs'
cmd=trim(cmd); call system(cmd)
loccupied(jd)=.true.
call system('sleep 0.1')
exit
endif

enddo
end subroutine send_exe
!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine read_stdout_log(stdname,lfault_stdout)
implicit none
character*280 stdname
logical lfault_stdout
character*6 ctest6,c6
character*2 c2
character*4 c4,c44
character*5 c5
character*7 c7
character*8 c8
character*9 c9
character*10 c10
character*11 c11
character*14 c14
logical lfault

lfault=.false.
open(18,file=trim(stdname),form='formatted')
do
read(18,*,err=911,end=999) ctest6

if(ctest6 == 'BRMIX:')then
backspace(18)
read(18,*,err=911,end=999) ctest6, c4,c7,c8
if(trim(c4) == 'very' .and. trim(c7) == 'serious' .and. trim(c8) == 'problems'
)then
print*, c4,' ',c7,' ',c8
goto 911

endif
endif

if(ctest6 == 'intern')then
backspace(18)
read(18,*,err=911,end=999) c8, c5, c14
if(trim(c8) == 'internal' .and. trim(c5) == 'ERROR' .and. trim(c14) == 'RS
PHER:running' )then
print*, c8,' ',c5,' ',c14
goto 911

endif
endif

if(ctest6 == 'APPLIC')then
backspace(18)
read(18,*,err=911,end=999) c11, c10
if(trim(c11) == 'APPLICATION' .and. trim(c10) == 'TERMINATED')then
print*, c11,' ',c10
goto 911

endif
endif

if(ctest6 == 'Ctrl-C')then
backspace(18)
read(18,*,err=911,end=999) ctest6, c9
if(trim(c9) == 'caught...')then
print*, ctest6,' ',c9
goto 911

endif
endif
endif
!
!

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    if(ctest6 == 'ERROR:')then
      backspace(18)
      read(18,*,err=911,end=999) ctest6, c5
      if(trim(c5) == 'while')then
        print*, ctest6, ' ', c5
        goto 911
      endif
      backspace(18)
      read(18,*,err=911,end=999) ctest6, c6
      if(trim(c6) == 'charge')then
        print*, ctest6, ' ', c6
        goto 911
      endif
    endif
    if(ctest6 == 'NKPT>N')then
      backspace(18)
      read(18,*,err=911,end=999) c10
      if(trim(c10) == 'NKPT>NKDIM')then
        print*, c10
        goto 911
      endif
    endif
    if(trim(ctest6) == 'exit')then
      backspace(18)
      read(18,*,err=911,end=999) c4, ctest6, c2, cc4
      if(trim(ctest6) == 'status' .and. trim(c2) == 'of' .and. trim(cc4) == 'rank'
)then
        print*, c4, ' ', ctest6, ' ', c2, ' ', cc4
        goto 911
      endif
    endif
  endif
!
  enddo
911 continue
  lfault=.true.
999 continue
  close(18)
  write(6,*) 'in stdout.log', lfault
!
! if(lfault)then
!   write(6,*) 'there is a fault sign from stdout.log'
!   call sleep(3)
!   endif
  lfault_stdout=lfault
  call read_stdout_log1(stdname, lfault_stdout)
  end subroutine read_stdout_log
!
!234567890
! http://error.wiki/VASP
! Written by In-Ho Lee, KRISS, September 11, 2013.
  subroutine read_stdout_log1(stdname, lfault_stdout)
    use strings, ONLY : parse, value
    implicit none
    character*280 stdname
    logical lfault_stdout
    integer ios, nargs
    character*200 str1
    character*200 args(40)
    character*20 delims
    logical lfault

    lfault=.false.
    open(18, file=trim(stdname), form='formatted')
    do
      read(18, '(a200)', err=911, end=999) str1
      write(6,*) len_trim(str1)
      delims=' '
      call parse(str1, delims, args, nargs)

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    if(nargs > 0)then
      if(args(1) == 'No' .and. args(2) == 'initial' .and. args(3) == 'positions') got
o 911
      if(args(1) == 'NKPT>NKDIM') goto 911
      if(args(1) == 'BRMIX' .and. args(2) == 'very' .and. args(3) == 'serious' .a
nd. args(4) == 'problems') goto 911
      if(args(1) == 'ERROR:' .and. args(2) == 'while') goto 911
      if(args(1) == 'ERROR:' .and. args(2) == 'charge') goto 911
      if(args(1) == 'ERROR:' .and. args(2) == 'there') goto 911
      if(args(1) == 'ERROR:' .and. args(2) == 'missing') goto 911
      if(args(1) == 'Error' .and. args(2) == 'EDDDAV:' .and. args(5) == 'ZHEGV
') goto 911
      if(args(1) == 'Error' .and. args(2) == 'EDDRMM:' .and. args(5) == 'ZHEG
V') goto 911
      if(args(5) == 'segmentation' .and. args(6) == 'fault') goto 911
      if(args(1) == 'ERROR' .and. args(3) == 'supplied') goto 911
      if(args(1) == 'ERROR' .and. args(2) == 'code' .and. args(3) == 'was') g
oto 911
      if(args(1) == 'ERROR' .and. args(2) == 'in' .and. args(3) == 'subspace')
goto 911
      if(args(1) == 'LAPACK:' .and. args(2) == 'Routine' .and. args(3) == 'ZPOT
RF') goto 911
      if(args(1) == 'internal' .and. args(2) == 'error') goto 911
      if(args(2) == 'internal' .and. args(3) == 'error') goto 911
      if(args(4) == 'internal' .and. args(5) == 'error') goto 911
      if(args(1) == 'internal' .and. args(2) == 'ERROR' .and. args(3) == 'RSPHER:
unning') goto 911
      if(args(1) == 'internal' .and. args(2) == 'ERROR' .and. args(3) == 'SETYLM
_AUG:') goto 911
      if(args(1) == 'Hard' .and. args(2) == 'potentials') goto 911
      if(args(1) == 'Suspicious' .and. args(2) == 'behaviour') goto 911
      if(args(1) == 'Large' .and. args(2) == 'positive' .and. args(3) == 'energies')
goto 911
      if(args(1) == 'APPLICATION' .and. args(2) == 'TERMINATED') goto 911
      if(args(1) == 'Ctrl-C' .and. args(2) == 'caught...') goto 911
      if(args(1) == 'exit' .and. args(2) == 'status' .and. args(3) == 'of' .and. ar
gs(4) == 'rank') goto 911
      if(args(1) == 'integer' .and. args(2) == 'divide' .and. args(3) == 'by') goto
911
      if(args(1) == 'Calculation' .and. args(2) == 'hangs' .and. args(3) == 'at') go
to 911
      if(args(1) == 'Fatal' .and. args(2) == 'error' .and. args(3) == 'in') goto 91
1
      if(args(4) == 'accuracy' .and. args(5) == 'cannot' .and. args(6) == 'be') got
o 911
      if(args(3) == 'accuracy' .and. args(4) == 'cannot' .and. args(5) == 'be') got
o 911
      ! October 1, 2017
      if(args(2) == 'BAD' .and. args(3) == 'TERMINATION' .and. args(4) == 'OF
') goto 911
    endif
  enddo
911 continue
  lfault=.true.
999 continue
  close(18)
  if(lfault)then
    write(6,*) 'there is a fault sign from stdout.log'
    call sleep(3)
    endif
  lfault_stdout=lfault
  end subroutine read_stdout_log1
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
  subroutine read_poscar_bac(man1, pname1)
    implicit none
    integer man1
    character*280 pname1
    logical lexist

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!

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```

qosi0(3*(i-1)+3)=z*scale1
endif
enddo
if(lpbc) call tolatx(qosi0)
goto 900

else

do i=1,na
read(81,*,err=911,end=999) d1,d2,d3
qosi0(3*(i-1)+1)=d1
qosi0(3*(i-1)+2)=d2
qosi0(3*(i-1)+3)=d3
enddo
goto 900

endif
else

if(ch9_1 == 'Cartesian' .or. ch9_1 == 'cartesian')then
do i=1,na
read(81,*,err=911,end=999) x,y,z
if(scale1 > 0.d0)then
qosi0(3*(i-1)+1)=x*scale1
qosi0(3*(i-1)+2)=y*scale1
qosi0(3*(i-1)+3)=z*scale1
endif
enddo
if(lpbc) call tolatx(qosi0)
goto 900

else

do i=1,na
read(81,*,err=911,end=999) d1,d2,d3
qosi0(3*(i-1)+1)=d1
qosi0(3*(i-1)+2)=d2
qosi0(3*(i-1)+3)=d3
enddo
goto 900

endif
endif

911 continue
999 continue
lfault2=.true.
900 continue
close(81)
if(.not. lfault2)then
cmatrix(1,:)=aa1(:) ; cmatrix(2,:)=aa2(:) ; cmatrix(3,:)=aa3(:)
call latmat(r6,cmatrix,0)
ish=ndeg-6
do i=1,6
qosi0(ish+i)=r6(i)
enddo
endif
end subroutine read_contcar

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine write_poscar(mm0,pname)
USE csa_application, ONLY : nspecies,nelements,symbl
implicit none
integer mm0
character*280 pname
integer i,j,m,na,ish,jchoice
real*8 r6(6),cmat(3,3),a1(3),a2(3),a3(3),vec(3)

jchoice=0
ish=ndeg-6
do i=1,6
r6(i)=qosi0(ish+i)
enddo
call latmat(r6,cmat,1)
a1(:)=cmat(1,:) ; a2(:)=cmat(2,:) ; a3(:)=cmat(3,:)
open(71,file=trim(pname),form='formatted')
write(71,*) mm0

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write(71,'(a3)') '1.0'
write(71,'(3f23.16)') a1(1),a1(2),a1(3)
write(71,'(3f23.16)') a2(1),a2(2),a2(3)
write(71,'(3f23.16)') a3(1),a3(2),a3(3)
write(71,'(20(2x,a2.1x))') (symbl(i),i=1,nspecies)
write(71,'(20(i4,1x))') (nelements(i),i=1,nspecies)
if(jchoice == 0) write(71,'(a6)') "Direct"
if(jchoice /= 0) write(71,'(a9)') "Cartesian"
na=0
do i=1,nspecies
do j=1,nelements(i)
na=na+1
enddo
enddo
do i=1,na*3
call tonormal(qosi0(i))
enddo
na=0
do i=1,nspecies
do j=1,nelements(i)
na=na+1
if(jchoice /= 0)then
vec(1)=qosi0(3*(na-1)+1)*a1(1)+qosi0(3*(na-1)+2)*a2(1)+qosi0(3*(na-1)+3)*
a3(1)
vec(2)=qosi0(3*(na-1)+1)*a1(2)+qosi0(3*(na-1)+2)*a2(2)+qosi0(3*(na-1)+3)*
a3(2)
vec(3)=qosi0(3*(na-1)+1)*a1(3)+qosi0(3*(na-1)+2)*a2(3)+qosi0(3*(na-1)+3)*
a3(3)
write(71,'(3f25.16)') vec(1),vec(2),vec(3)
else
write(71,'(3f20.16)') qosi0(3*(na-1)+1),qosi0(3*(na-1)+2),qosi0(3*(na-1)+3)
endif
enddo
enddo
close(71)
end subroutine write_poscar

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine write_kpoints(dk,a1,a2,a3,kname)
implicit none
character*280 kname
real*8 dk,a1(3),a2(3),a3(3)
real*8 b1(3),b2(3),b3(3),omega
real*8 dum,pi,ga,gb,gc
integer ka,kb,kc,iswitch

iswitch=0
if(dk < 0.d0) dk=0.06d0
if(dk == 0.d0)then
dk=0.015d0
iswitch=1
endif

!
call cross3(a2,a3,b1) ; call cross3(a3,a1,b2) ; call cross3(a1,a2,b3)
omega=abs(dot_product(b1,a1)) ; pi=4.0d0*atan(1.0d0)
b1=b1*(2.d0*pi/omega) ; b2=b2*(2.d0*pi/omega) ; b3=b3*(2.d0*pi/omega)
ga=sqrt(dot_product(b1,b1)) ; gb=sqrt(dot_product(b2,b2)) ; gc=sqrt(dot_p
roduct(b3,b3))
call meshijk(dk,ga,dum,ka) ; call meshijk(dk,gb,dum,kb) ; call meshijk(dk
,gc,dum,kc)
if(ka > 15) ka=15
if(kb > 15) kb=15
if(kc > 15) kc=15
if(iswitch == 1)then
ka=ka+1+ka/2
kb=kb+1+kb/2
kc=kc+1+kc/2
endif
open(71,file=trim(kname),form='formatted')

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```

write(71,"(al)") 'A'
write(71,"(il)") 0
write(71,"(al)") 'G'
write(71,"(1x,i3,2x,i3,2x,i3)") ka,kb,kc
write(71,"(1x,i2,2x,i2,2x,i2)") 0,0,0
! write(71,"(1x,3f4.2)") 0.,0.,0.
close(71)
return
end subroutine write_kpoints

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine meshijk(dk,ga,dum,ka)
implicit none
real*8 dk,ga,dum
integer ka
real*8 pi,gatmp
integer i

pi=4.0d0*atan(1.0d0)
gatmp=ga/(2.d0*pi)
gatmp=ga
ka=int(gatmp/dk) ; if(ka == 0) ka=1
dum=gatmp/dble(ka)
if(dum >= dk)then
do i=1,15
ka=ka+1 ; dum=gatmp/dble(ka)
if(dum <= dk) exit
enddo
endif
return
end subroutine meshijk

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine centering(qqq)
USE csa_application, ONLY : natom
implicit none
real*8 qqq(ndeg)
real*8 vec(3)
integer i

vec=0.d0
do i=1,natom
vec(1)=vec(1)+qqq(3*(i-1)+1)
vec(2)=vec(2)+qqq(3*(i-1)+2)
vec(3)=vec(3)+qqq(3*(i-1)+3)
enddo
vec=vec/dble(natom)
do i=1,natom
qqq(3*(i-1)+1)=qqq(3*(i-1)+1)-vec(1)
qqq(3*(i-1)+2)=qqq(3*(i-1)+2)-vec(2)
qqq(3*(i-1)+3)=qqq(3*(i-1)+3)-vec(3)
enddo
end subroutine centering

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_randrot(rx,ry,rz)
implicit none
real*8 rx(3,3),ry(3,3),rz(3,3)
real*8 pi,theta,costheta,sintheta
real ranmar

pi=4.d0*atan(1.d0)
theta=ranmar()*2.d0*pi ; costheta=cos(theta) ; sintheta=sin(theta)
rx(1,1)=1.d0
rx(1,2)=0.d0
rx(1,3)=0.d0
rx(2,1)=0.d0
rx(2,2)=costheta
rx(2,3)=-sintheta

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```

rx(3,1)=0.d0
rx(3,2)=-sintheta
rx(3,3)=costheta
theta=ranmar()*2.d0*pi ; costheta=cos(theta) ; sintheta=sin(theta)
ry(1,1)=costheta
ry(1,2)=0.d0
ry(1,3)=sintheta
ry(2,1)=0.d0
ry(2,2)=1.d0
ry(2,3)=0.d0
ry(3,1)=-sintheta
ry(3,2)=0.d0
ry(3,3)=costheta
theta=ranmar()*2.d0*pi ; costheta=cos(theta) ; sintheta=sin(theta)
rz(1,1)=costheta
rz(1,2)=-sintheta
rz(1,3)=0.d0
rz(2,1)=sintheta
rz(2,2)=costheta
rz(2,3)=0.d0
rz(3,1)=0.d0
rz(3,2)=0.d0
rz(3,3)=1.d0
end subroutine gen_randrot

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine direct_pbc(qqq)
USE csa_application, ONLY : natom
implicit none
real*8 qqq(ndeg)
real*8 vec(3)
integer i

do i=1,natom
vec(1)=qqq(3*(i-1)+1)
vec(2)=qqq(3*(i-1)+2)
vec(3)=qqq(3*(i-1)+3)
vec(1)=vec(1)-anint(vec(1))
vec(2)=vec(2)-anint(vec(2))
vec(3)=vec(3)-anint(vec(3))
if(vec(1) < 0.d0) vec(1)=vec(1)+1.d0
if(vec(2) < 0.d0) vec(2)=vec(2)+1.d0
if(vec(3) < 0.d0) vec(3)=vec(3)+1.d0
qqq(3*(i-1)+1)=vec(1)
qqq(3*(i-1)+2)=vec(2)
qqq(3*(i-1)+3)=vec(3)
enddo
end subroutine direct_pbc

!
!
end module csa

!
!
Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_directories(ndir)
implicit none
integer ndir
character*280 string
character*280 cmd
integer isize,i

isize=4
if(ndir > 0)then
do i=1,ndir
call xnumeral(i,string,isize) ; string=trim(string)
cmd='mkdir '//trim(string) ; cmd=trim(cmd) ; call system(
em(cmd)
cmd='cp ./CSA_SOLDIER.pbs '//trim(string)//'/' ; cmd=trim(cmd) ; call system(
cmd)
cmd='cp INCAR_rlx '//trim(string)//'/' ; cmd=trim(cmd) ; call system(
(cmd)

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```

cmd) cmd='cp INCAR_rlxall '//trim(string)////' ; cmd=trim(cmd) ; call system(
m(cmd) cmd='cp INCAR_bs '//trim(string)////' ; cmd=trim(cmd) ; call syste
m(cmd) cmd='cp POTCAR '//trim(string)////' ; cmd=trim(cmd) ; call syste
enddo
endif
if(ndir < 0)then
ndir=iabs(ndir)
do i=1,ndir
call xnumeral(i,string,ysize) ; string=trim(string)
cmd='rm -rf '//trim(string)////' ; cmd=trim(cmd)
call system(cmd)
call sleep(1)
enddo
endif
call sleep(1)
return
end
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine iofilearray(id,file_names)
implicit none
integer id
character*280 file_names(20)
integer ysize
character*280 string

ysize=4
call xnumeral(id,string,ysize)
string=trim(string)
file_names(1)=trim(string)////'
file_names(2)=trim(string)////'/INCAR'
file_names(3)=trim(string)////'/POSCAR'
file_names(4)=trim(string)////'/POTCAR'
file_names(5)=trim(string)////'/KPOINTS'
file_names(6)=trim(string)////'/OUTCAR'
file_names(7)=trim(string)////'/CONTCAR'
file_names(10)=trim(string)////'/STOP'
file_names(17)=trim(string)////'/OSZICAR'
file_names(18)=trim(string)////'/STOPCAR'
file_names(19)=trim(string)////'/STATUS'
file_names(11)=trim(string)////'/DOSCAR'
file_names(12)=trim(string)////'/EIGENVAL'
file_names(20)=trim(string)////'/stdout.log'
return
end
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine jobstatus(fname,i)
implicit none
character*280 fname
integer i
logical lexist
character*20 ch

i=0
inquire(file=trim(fname),exist=lexist)
if(lexist)then
open(77,file=trim(fname),form='formatted')
do
read(77,*,end=999) ch
enddo
999 continue
close(77)
if(trim(ch) == 'DONE' .or. trim(ch) == 'done') i=1
if(trim(ch) == 'Done' .or. trim(ch) == 'DOne') i=1
if(trim(ch) == 'DOnE'
) i=1

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```

endif
return
end
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine jobstatus0(fname)
implicit none
character*280 fname
character*280 cmd

! open(77,file=trim(fname),form='formatted')
! write(77,*) 'ING'
! close(77)
cmd='echo "ING">> '//trim(fname) ; cmd=trim(cmd)
call system(cmd)
call system('sleep 0.1')
return
end
!234567890
!
! Written by In-Ho Lee, KRISS, November 7, 2018.
subroutine genstopcar(incarname,outcarname,stopcarname,oszicarname)
USE strings, ONLY : parse,value,lowercase
implicit none
character*280 incarname,outcarname,stopcarname,oszicarname
integer i,j,kount,nsw,nequal
real*8 test,arr(10000)
logical lfault9,lexist9
integer ios,nargs
character*280 str1
character*280 args(40)
character*20 delims

inquire(file=trim(incarname),exist=lexist9)
if(.not. lexist9) goto 333
inquire(file=trim(outcarname),exist=lexist9)
if(.not. lexist9) goto 333
inquire(file=trim(oszicarname),exist=lexist9)
if(.not. lexist9) goto 333
lfault9=.false.
nsww=0
open(38,file=trim(incarname),form='formatted')
do
read(38,'(a280)',err=311,end=499) str1
delims=' '
call parse(str1,delims,args,nargs)
if(nargs >= 3)then
if(lowercase(args(1)) == 'nsw')then
call value(args(3),nsww,ios)
write(6,*) nsww,' nsww'
endif
endif

enddo
311 continue
lfault9=.true.
499 continue
close(38)
if(nsw == 0)then
goto 333
endif

do i=1,10000
arr(i)=dble(i)
enddo
nequal=10
kount=0
i=0
if(i == 1)then
lfault9=.false.
open(39,file=trim(outcarname),form='formatted')
do

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```

      read(39,'(a280)',err=111,end=299) str1
      delims=' '
      call parse(str1,delims,args,nargs)
      if(nargs == 7)then
        if(args(3) == 'entropy=')then
          if(args(1) == 'energy')then
            call value(args(7),test,ios)
            kount=kount+1 ; arr(kount)=test
            if(kount == 10000) kount=0
          endif
        endif
      endif
    enddo
111 continue
    lfault9=.true.
299 continue
    close(39)
      endif
    lfault9=.false.
    open(39,file=trim(oszicarname),form='formatted')
    do
      read(39,'(a280)',err=511,end=599) str1
      delims=' '
      call parse(str1,delims,args,nargs)
      if(nargs >= 7)then
        if(args(2) == 'F=')then
          if(args(4) == 'E0=')then
            call value(args(5),test,ios)
            kount=kount+1 ; arr(kount)=test
            if(kount == 10000) kount=0
          endif
        endif
      endif
    enddo
511 continue
    lfault9=.true.
599 continue
    close(39)
    write(6,*) kount,' steps'
    if(kount > 0)then
      j=0 ; test=arr(kount)
      if(kount >= nequal)then
        do i=kount,kount-nequal+1,-1
          write(6,*) test,arr(i)
          if(abs(arr(i)-test) < 1.d-7)then
            j=j+1
          endif
        enddo
      endif
    endif
    if(j >= nequal)then
      write(6,*) 'condition for stopcar generation'
      i=0
      if(iabs(nsw-kount) > 20) i=1
      if(i == 1)then
        open(44,file=trim(stopcarname),form='formatted')
        write(44,*) 'LSTOP=.TRUE.'
        close(44)
      endif
      goto 333
    endif
  endif
333 continue
end
!234567890
!   Written by In-Ho Lee, KRISS, September 18, 2007.
!   subroutine gauss (sigma,xl0,xl)
!   IMPLICIT NONE
!   real*8 sigma,xl0,xl
!   real*8 r,v1,v2

```

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```

      real ranmar

      r=2.0d0
      do while (r >= 1.d0)
        v1=2.0*ranmar()-1.0
        v2=2.0*ranmar()-1.0
        r=v1**2+v2**2
      enddo
      xl=v1*sqrt(-2.d0*log(r)/r)
      xl=xl0+sigma*xl
    end

!
!   Written by In-Ho Lee, KRISS, September 11, 2013.
!   subroutine perturbation_seq(npert1,nmatel,nnl,iseq1)
!   implicit none
!   integer npert1,nmatel,nnl,iseq1(nnl)
!   integer, allocatable :: iwrk(:),jwrk(:)
!   real*8, allocatable :: wrk(:)
!   integer n,i
!   real ranmar

      n=npert1+nmatel
      if(n /= nnl)then
        write(6,*) 'n/=nnl',n,nnl
        stop
      endif
      allocate(iwrk(n),jwrk(n)) ; allocate(wrk(n))
      do i=1,n
        wrk(i)=ranmar()
      enddo
      do i=1,npert1
        jwrk(i)=1
      enddo
      do i=1,nmatel
        jwrk(i+npert1)=2
      enddo
      call sortnr(n,wrk,iwrk)
      do i=1,n
        iseq1(i)=jwrk(iwrk(i))
      enddo
      deallocate(iwrk,jwrk) ; deallocate(wrk)
    end

!
!   Written by In-Ho Lee, KRISS, September 11, 2013.
!   subroutine onedffvltm(ndim,npop,x,y)
!   implicit none
!   integer ndim,npop
!   real*8 x(ndim,npop),y(ndim)
!   real*8, allocatable :: xnew(:, :)
!   integer j

      allocate(xnew(ndim,npop))
      call dffvltm(ndim,npop,x,xnew)
      do j=1,ndim
        y(j)=xnew(j,1)
      enddo
      deallocate(xnew)
    end

!
!   Written by In-Ho Lee, KRISS, September 11, 2013.
!   subroutine onedffvltm1(ndeg,npop,x,y)
!   implicit none
!   integer ndeg,npop
!   real*8 x(ndeg,npop),y(ndeg)
!   real*8, allocatable :: xnew(:, :)
!   real*8, allocatable :: x1(:, :),x1new(:, :),x2(:, :),x2new(:, :)
!   integer j,n1,n2,i

      allocate(xnew(ndeg,npop))

```

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```

call dffvltm(ndeg,npop,x,xnew)
do j=1,ndeg
y(j)=xnew(j,1)
enddo
deallocate(xnew)

n1=6 ; n2=npop
allocate(x1(n1,n2),x1new(n1,n2))
do i=1,n2
do j=1,n1
x1(j,i)=x(ndeg-6+j,i)
enddo
enddo
call dffvltm(n1,n2,x1,x1new)
do j=1,n1
y(ndeg-6+j)=x1new(j,1)
enddo
deallocate(x1,x1new)

n1=ndeg-6 ; n2=npop
allocate(x2(n1,n2),x2new(n1,n2))
do i=1,n2
do j=1,n1
x2(j,i)=x(j,i)
enddo
enddo
call dffvltm(n1,n2,x2,x2new)
do j=1,n1
y(j)=x2new(j,1)
enddo
deallocate(x2,x2new)
end

!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine dffvltm(ndim,npop,x,xnew)
implicit none
integer ndim,npop
real*8 x(ndim,npop),xnew(ndim,npop)
integer iarr(4),jbrn,i,j
real*8 tmt
real*8 cr,ff
real ranmar
! ff : differential weight
! cr : crossover probability
xnew=x
do i=1,npop
if(npop >=4 )then
iarr(1)=dble(ranmar())*npop+1
111 continue
iarr(2)=dble(ranmar())*npop+1
if(iarr(2) == iarr(1)) goto 111
112 continue
iarr(3)=dble(ranmar())*npop+1
if(iarr(3) == iarr(1) .or. iarr(3) == iarr(2)) goto 112
113 continue
iarr(4)=dble(ranmar())*npop+1
if(iarr(4) == iarr(3) .or. iarr(4) == iarr(2) .or. iarr(4) == iarr(1)) go
to 113
! print*, i, '--'
! print*, iarr(1),iarr(2),iarr(3),iarr(4)
jbrn=dble(ranmar())*ndim+1 ; cr=ranmar() ; ff=2.d0*dble(ranmar())+0.d0
do j=1,ndim
tmt=ranmar()
if(jbrn == j .or. tmt <= cr)then
xnew(j,i)=x(j,iarr(2))+ff*(x(j,iarr(3))-x(j,iarr(4)))
endif
if(jbrn /= j .and. tmt > cr)then
xnew(j,i)=x(j,iarr(1))
endif

```

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```

enddo
else
tmt=-1.d0
do j=1,ndim
if(tmt < abs(x(j,i))) tmt=abs(x(j,i))
enddo
tmt=tmt/10.d0
do j=1,ndim
xnew(j,i)=x(j,i)+(ranmar()-0.5)*tmt
enddo
endif
enddo
end
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine cross3(a,b,c)
implicit none
real*8 a(3),b(3),c(3)

c(1)=a(2)*b(3)-a(3)*b(2)
c(2)=a(3)*b(1)-a(1)*b(3)
c(3)=a(1)*b(2)-a(2)*b(1)
return
end
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine tonormal(xxx)
USE, INTRINSIC :: IEEE_ARITHMETIC, ONLY : IEEE_IS_FINITE,IEEE_IS_NAN
implicit none
real*8 xxx
real ranmar

! if(isnan(xxx)) xxx=ranmar()
! if(IEEE_IS_NAN(xxx)) xxx=ranmar()
! if(.not. IEEE_IS_FINITE(xxx)) xxx=ranmar()
end subroutine tonormal

!
! Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine csa_vasp_banner()
implicit none
integer i
character*93 banner(8)

banner(1)='
banner(2)='
banner(3)='
banner(4)='
banner(5)='
banner(6)='
banner(7)='
banner(8)='
do i=1,8
write(6,'(15x,a93)') banner(i)
enddo
banner(1)=' # # # # ##### # # # # # '
banner(2)=' ## ## ## ## # # # # # '
banner(3)=' # # # # # # # # # # # '
banner(4)=' # # # # # # # # # # # '
banner(5)=' ##### # # # # # # # # # '
banner(6)=' # # # # # # # # # # # '
banner(7)=' # # # # # ##### # # # # # '
banner(8)=' Ab initio MATERIALS DEsign Using cSa
do i=1,8
write(6,'(30x,a63)') banner(i)
enddo
end
!
! Written by In-Ho Lee, KRISS, September 11, 2013.
program csa_vasp5_2_12
program csa_vasp5_4_1
USE csa, ONLY : csa_initial,csa_final,csa_first_bank,csa_evolution,lquit

```

```
implicit none
character*8 fnnd ; character*10 fnnt

call date_and_time(date=fnnd,time=fnnt)
write(6,'(a10,2x,a8,2x,a10)') 'date,time ', fnnd,fnnt

call csa_vasp_banner()
call timestamp()
call csa_initial()
call csa_first_bank()
call csa_evolution()
call csa_final()
call timestamp()
end program csa_vasp5_4_1
```