STRUCTRE OF A COMPLETE CTRL FILE

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HEADER   Si2, cubic face-centred    <COMMENT LINE >
VERS     LMASA-47  <COMMENT LINE : VERSION>
IO       VERBOS=50 HELP=F WKP=F IACTIV=F ERRTOL=2 OUTPUT=LM ERR=ERR
                <SETS VERBOSITY & ALSO OUTPUT FILENAMES>
SYMGRP   NGEN=3 GENGRP=I:(.25,.25,.25) R4X:(.25,.25,.25) R3D
         SPCGRP=Fd-3m USESYM=F  <SYMMETRY INFORMATION>
STRUC    ALAT=10.246
         PLAT=0.0 0.5 0.5
                0.5 0.0 0.5
                0.5 0.5 0.0 FIXLAT=T <LATTICE CONSTANTS & TRANSLATIONS>
DIM       NBAS=4 NCLASS=2 NL=3 LDIM=10 IDIM=26 NSYMOP=48 NKP=29
                 <NO. OF ATOMS IN UNIT CELL, NO. OF CATEGORIES OF ATOMS>
OPTIONS  NSPIN=1 REL=T CCOR=T NONLOC=F NRXC=1 NRMIX=2 CORDRD=F
         NITATOM=30 CHARGE=T FATBAND=F AFM=F SEWALD=F FS=F
         CARTESIAN=T WRIBAS=F Q=---
              <SPIN-POL OR NOT, CONTROL FOR CHARGE PLOT, FATBAND PLOT>
CLASS    ATOM=Si Z=14 R=2.52242437 LMX=2 CONF=3 3 3 4 IDXDN=1 1 2
                 IDMOD=0 0 0
         ATOM=E  Z= 0 R=2.52242437 LMX=2 CONF=1 2 3 4 IDXDN=1 2 2
                 IDMOD=0 0 0
 <INFO ABOUT ATOMS, CLASSES OF ATOMS, ATOMIC NO., MT RADIUS, DOWNFOLDING>
SITE      ATOM=Si POS=0.00 0.00 0.00
          ATOM=Si POS=0.25 0.25 0.25
          ATOM=E  POS=-.25 -.25 -.25
          ATOM=E  POS=0.50 0.50 0.50 <ATOMIC POSITIONS>
SCALE     SCLWSR=T OMMAX1=.16 .18 .20 OMMAX2=.40 .45 .50
                <CONTROL FOR OVERLAP>
STR       KAPPA2=0 RMAXS=3.2 NDIMIN=350 NOCALC=F IALPHA=0
                <CONTROL FOR STRUCTURE MATRIX>
          DOWATS=F DELTR=.1 LMAXW=8
          ATOM=Si SIGMA=.7 .7 .7
          ATOM=E  SIGMA=.7 .7 .7
                <CONTROL FOR SCREENING>
START     NIT=30 BROY=T WC=-1 NMIX=1 BETA=.5 <SCF CYCLE, CONTROL FORMIXING>
          FREE=F CNVG=.00001 CNVGET=.00001 BEGMOM=T CNTROL=T
          EFERMI=-.05420343 VMTZ=-.72429873
          ATOM=Si  P=3.83698167 3.70953041 3.25041054
                   Q=1.16917314 -.05480112 0.05014661
                     1.88163872 0.04222314 0.06004022
                     0.17585824 0.00000001 0.00694699
        enu   =-.65011799 -.30212436 -.33637219
        c     =-.86577353 0.09002402 1.50210437
        sqrdel=0.39928750 -.36357278 0.37629523
        p     =0.08840331 0.05612691 0.02497862
        gamma =0.40270844 0.09614703 0.05193821
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        ATOM=E   P=1.43080343 2.24441192 3.15346004
              Q=0.30413028 0.00142483 0.01955739
                0.33049045 -.00000002 0.01741343
                0.13870916 -.00000003 0.00592533
           enu   =-.50098649 -.46305908 -.36388582
           c     =0.04055896 1.27780032 3.12071828
           sqrdel=0.42486705 0.44943572 0.47994056
           p     =0.05736880 0.01631235 0.00636293
           gamma =0.42378471 0.11799037 0.06428706 <INFO ABOUT POT PARAM & CHARGES>
CHARGE    LMTODAT=T ELF=F ADDCOR=F SPINDENS=F CHARWIN=F EMIN=-2 EMAX=2
PLOT      ORIGIN=-.5 -.5 -.5
          R1=0.0 0.0 1.0 NDELR1=71
          R2=1.0 1.0 0.0 NDELR2=71
          R3=0.0 0.0 0.5 NDELR3= 0
          FORMAT=1  <CONTROL FOR CHOSING BOX OR PLANS FOR RS PLOTTING>
BZ        NKABC=8 8 8 TETRA=T METAL=T TOL=.000001
          N=0 W=.005 RANGE=5 NPTS=1001
EWALD     NKDMX=250 AS=2 TOL=.000001
RHOFIT    FIT=F KAPPA2=0 RMAXS=3.5 OUTPUT=5
             ATOM=Si LMXRHO=2 SIGMA=.7 .7 .7
             ATOM=E  LMXRHO=2 SIGMA=.7 .7 .7
SCELL     PLAT=0.0 0.5 0.5
                   0.5 0.0 0.5
                   0.5 0.5 0.0 EQUIV=T <CONTROL FOR CREATING SUPERCELLS>
HARTREE   BEGATOM=T LT1=2 LT2=2 LT3=2
DOS       NOPTS=801 EMIN=-1 EMAX=1.2  <CONTROL FOR DOS PLOTS>
SYML      NQ=35 Q1=0.50 0.50 0.50 LAB1=L
                   Q2=0.00 0.00 0.00 LAB2=G
             NQ=40 Q1=0.00 0.00 0.00 LAB1=G
                   Q2=0.00 1.00 0.00 LAB2=X
<CONTROL FOR BAND STRUCTURE PLOT: INFO ABOUT HIGH-SYMM POINTS>
FINDES    RMINES=.9 RMAXES=4 NRXYZ=48 48 48  <CONTROL FOR ES's>
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