Instructions for COMDECK Files for LAPW Code

```
*COMDECK P1
      PARAMETER (NATD=1,NTYPD=1)
```

NATD MAXIMUM NUMBER OF ATOMS IN UNIT CELL
NTYPD MAXIMUM NUMBER OF ATOM TYPES IN UNIT CELL
NATD = number of atoms in the unit-cell
NTYPD = number of inequivalent atoms

```
*COMDECK P2
      PARAMETER (N3D=100,N2D=1,NIS2D=1,NIZMD=1)
      PARAMETER (MMSTRD=48,NTSTRD=5000,LOOS1D=8,LOOS2D=8,LOOS3D=8)
      PARAMETER (MMAXD1=5,MMAXD2=5,MMAXD3=5,MAXYZD=32*32*32)
      PARAMETER (LL1D=16,LL2D=16,LL3D=16,NCFFTD=LL3D/2+1)
      PARAMETER (NXYZD=LL1D*LL2D*LL3D)
```

N3D MAXIMUM NUMBER OF 3-D STARS
N2D MAXIMUM NUMBER OF 2-D STARS (USED ONLY IF LSURF.EQ .T.)
NIS2D INDEX FOR PERPENDICULAR G-VECTORS (LSURF.EQ .T.)
NIZMD INDEX FOR PERPENDICULAR G-VECTORS (LSURF.EQ .T.)
MMSTRD MAXIMUM MEMBERS IN A PLANE-WAVE STAR
NTSTRD MAXIMUM NUMBER OF PLANE-WAVES IN STAR-LIST
LOOS1D MAXIMUM VALUE OF N1 IN G=N1*B1+N2*B2+N3*B3, WHERE G IS A RECIP VECTOR APPEARING IN THE BASIS FUNCTION LAPW-LIST, AND B1,B2,B3 ARE THE PRIMITIVE VECTORS OF THE RECIP. LATTICE.
LOOS2D MAXIMUM VALUE OF N2 ABOVE
LOOS3D MAXIMUM VALUE OF N3 ABOVE
NXYZD MAXIMUM NUMBER OF POINT USED IN REAL AND/OR RECIPROCAL SPACE FOR FAST-FOURIER-TRANSFORM (CFFT). NXYZD MUST BE .GE. 2**(M1+M2+M3).
NCFFTD MAX(2**M1,2**M2,2**M3)/2 M1,M2,M3 ARE INPUT IN PTIOE1
MMAXD1 OPTIMALLY, SHOULD BE EQUAL TO M1+1 (M1,M2,M2 ARE INPUT)
MMAXD2 OPTIMALLY, SHOULD BE EQUAL TO M2+1
MMAXD3 OPTIMALLY, SHOULD BE EQUAL TO M3+1
MAXYZD MIN(8*NXYZD,2**(MMAXD1+MMAXD2+MMAXD3))

NOTE THE ONLY RESTRICTION TO MMAXD1,MMAXD2,MMAXD3 IS THE STORAGE ROOM THE SYSTEM COULD HAVE.

N3D is the number of stars for the charge density and potential.
MMSTRD = number of space groups
NTSTRD = number of plane waves for charge density
LOOS1D, etc = Box for FFT – even number and fit inside box
very expensive for memory – program will tell you what this value could have been – run with 0 iters to test
MMAXD1, etc = number of FFT's + 1
MAXYZD = 32*32*32 = $2^5*2^5*2^5$
Note: be sure to change all FFT dimensions consistently.

```
*COMDECK P3
      PARAMETER (JMTD=350,NMZD=1,NMZXYD=1,NXYM1D=1,JNMTD=100)
```

JMTD RADIAL MESH
NMZD MESH FOR VACUUM (LSURF.EQ .T.)
NMZXYD MESH FOR VACUUM WARPING TERMS (LSURF.EQ .T.)
NXYM1D MAXIMUM NUMBER OF 2-D STARS FOR VACUUM (LSURF.EQ .T.)
JNMTD RADIAL MESH FOR NMT TERMS
JMTD = biggest number of mesh points in sphere for biggest atom
JNMTD = biggest atom in non-spherical mesh

```
*COMDECK P4  (Lattice Harmonics)
      PARAMETER (MEMD=9,NLHD=9,NTYPSD=1,LMLTHD=81)
```

MEMD MAXIMUM NUMBER OF LATT. HARM. MEMBERS
NLHD MAXIMUM NUMBER OF LATT. HARM. PER SYMMETRY KIND
NTYPSD MAXIMUM NUMBER OF SYMMETRY KINDS
LMLTHD MAXIMUM (LM) INDEX FOR LATT. HARM.
MEMD = largest number in a lattice harmonic (≤ 17)
NLHD = number of sets of lattice harmonics
NTYPSD = number of atoms with different sets of lattice harmonics
(symmetry types); this should be less than or equal to the number of inequivalent atoms – look up (code will print out)

```
*COMDECK P5
      PARAMETER (NVD=200,NTWFD=9,LMWFD=81,NOBD=20,NTBD=NOBD)
      PARAMETER (NHERVD=1)
```

NVD MAXIMUM NUMBER OF LAPW BASIS FUNCTIONS
NTWFD MAXIMUM L+1 IN BASIS FUNCTIONS USED IN EVALUATING THE SPHERICAL MUFFIN-TIN OVERLAP AND HAMILTONIAN MATRIX ELEMENTS.
LMWFD MAXIMUM (LM) INDEX IN WAVE FUNCTIONS
NOBD MAXIMUM NUMBER OF OCCUPIED BANDS
NTBD MAXIMUM NUMBER OF BANDS
NHERVD EQUAL TO NVD FOR A HERMITIAN HAMITONIAN BUT SET TO 1 FOR A REAL HAMITONIAN.
NVD = number of basis functions = number of LAPW's + local orbitals
NOBD = maximum number of bands (double for spin-orbit)
NHERVD =1 for inversion symmetry
hardwire to NHERVD=NVD for no inversion symmetry

NOTE: code will automatically readjust (reduce) RKMAX to fit the number of basis functions – be careful!

For spin-orbit, increase NOBD because spin-orbit doubles the number of bands.

If you get the error message that RKMAX was truncated, then you need to increase NVD.

Note: I discovered that I had problems with calculating the eigenvalues when the number of bands (NOBD) was set to too small a value. I got an error message:

ERROR IN SECSY2 IER1, IER2, No. OF BANDS = 2471 0 20

This went away when I increased the number of bands.

It looks as though you need NOBD to be at least as big as the number of bands in your energy window.

```
*COMDECK P6
      PARAMETER (N2VD=1,NUVACD=1)
```

N2VD MAX. NUMBER OF 2-D VECTORS IN LAPW BASIS (LSURF.EQ .T.)

NUVACD MAX.NUM. OF UNIQUE ABS(K+G) IN LAPW BASIS (LSURF.EQ. .T.)

```
*COMDECK P7
      PARAMETER (NTNMTD=9)
      PARAMETER (LLNMTD=NTNMTD*(NTNMTD+1)/2)
```

NTNMTD MAXIMUM L+1 IN BASIS FUNCTIONS USED IN EVALUATING THE NON-SPHERICAL MUFFIN-TIN HAMILTONIAN MATRIX ELEMENTS. THIS IS ALSO USED TO DETERMINE THE MAXIMUM L+1 IN THE WAVE FUNCTIONS USED IN SYNTHESIZING THE NON-SPHERICAL CHARGE DENSITY IN RHONMT.

LLNMTD NTNMTD*(NTNMTD+1)/2 L'L INDEX IN RHONMT

```
*COMDECK P8
      PARAMETER (NKPTD=300,NWDD=1,NWDDV=1,NTETD=200)
```

NKPTD MAXIMUM NUMBER OF K-POINTS IN IRREDUCIBLE BZ

NWDD MAXIMUM NUMBER OF ENERGY WINDOWS

NWDDV MAXIMUM NUMBER OF VALENCE ENERGY WINDOWS

NTETD MAXIMUM NUMBER OF TETRAHEDRA (FOR DIMENSION, SEE DIMENSION CHECK IN SUBR. PTIOE2)

NKPTD = number of k-points (sometimes slightly bigger)

NTETD = number of tetrahedrons in full zone

```
*COMDECK P9 (Spin-Orbit)
      PARAMETER (NTSPND=5,NSOBND=1,JSPND=1)
      PARAMETER (LMSPND=NTSPND*NTSPND,NSOD=2*NSOBND)
```

NTSPND MAXIMUM L+1 IN WAVEFUNCTION USED IN THE SPIN-ORBIT SECOND VARIATIONAL STEP.

NSOBND MAXIMUM NUMBER OF BANDS USED IN THE TRIAL WAVE FUNCTION IN THE SPIN-ORBIT STEP.

JSPND FOR NON-SPIN POLARIZED CALCULATION = 1
FOR SPIN POLARIZED CALCULATION = 2

LMSPND NTSPND*NTSPND

NSOD 2*NSOBND

NSOBND = number of bands for 2nd variation
(maximum number of non-relativistic bands)

JSPND = number of spins (even if not using spin-orbit)

```
*COMDECK P10
      PARAMETER (NCMSH=499,NCSTD=24)
```

NCMSH EXTENDED RADIAL MESH FOR CORE RADIAL FUNCTIONS

NCSTD MAXIMUM NUMBER OF CORE STATES

NCMSH = mesh for core states (499 or 600 for forces)

```
*COMDECK P11
      PARAMETER (LAYD=1)
```

LAYD MAXIMUM NUMBER OF LAYERS IN SLAB (LSURF.EQ. .T.)

```
*COMDECK P12
      PARAMETER (MXLSD=10,NCVD=11)
```

MXLSD MAXIMUM L-VALUE OF ANY LATTICE HARMONIC

NCVD MAXIMUM N-VALUE USED IN CONSTRUCTION OF THE PSEUDO-CHARGE DENSITY

```
*COMDECK P13
      PARAMETER (NPD=25)
```

NPD NUMBER OF RANDOM PLOTTING POINTS USED ON MUFFIN-TIN SPHERE SURFACES

```
*COMDECK P14
      PARAMETER (NPLTD=200,NCOND=30)
```

Use for plotting programs.

```
*COMDECK P15
      PARAMETER (NSPFD=121,NSTD=30)
```

NSPFD NUMBER OF RANDOM POINTS ON SPHERICAL SHELL USED TO OBTAIN EXCHANGE-CORRELATION TERMS IN LEAST SQUARES FIT

NSTD NUMBER OF RANDOM POINTS ON SPHERICAL SHELL USED TO TEST THE QUALITY OF THE LEAST SQUARES FIT (THESE POINTS ARE DISTINCT FROM THE NSPFD POINTS ABOVE)

```
*COMDECK P16
      PARAMETER (LMAX1D=9)
      PARAMETER (NGNTD=(3*LMAX1D+1)/2)
```

LMAX1D MAXIMUM L+1 VALUE FOR ANY SPHERICAL HARMONIC
NGNTD (3*LMAX1D+1)/2

```
*COMDECK P17
      PARAMETER (NOPD=48)
      PARAMETER (NEMAXD=501,IDFAC=600,NSPIND=1,KREAD=1000)
```

NOPD NUMBER OF SPACE GROUP OPERATIONS (E.G. 48 FOR CUBIC)
NEMAXD FOR D.O.S CALCULATION. EQUAL MAX NUMBER OF E-MESH PTS.
IDFAC " NUMBER OF PROJECTIONS
NSPIND " NUMBER OF SPINS

NOPD = number of space group operations
NEMAXD and IDFAC for DOS
NSPIND = number of spins
KREAD for DOS