WIEN2k

An Augmented Plane Wave Plus Local Orbitals Program
for Calculating Crystal Properties

User's Guide, November 2001

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Contents

List of Tables

List of Figures

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DEFINITIONS:

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1 Introduction

The Linearized Augmented Plane Wave (LAPW) method has proven to be one of the most accurate methods for the computation of the electronic structure of solids within density functional theory. A full-potential LAPW-code for crystalline solids has been developed over a period of more than twenty years. A first copyrighted version was called **WIEN** and it was published by

> P. Blaha, K. Schwarz, P. Sorantin, and S. B. Trickey, in
> Comput. Phys. Commun. 59, 399 (1990).

In the following years significantly improved and updated UNIX versions of the original **WIEN**-code were developed, which were called **WIEN93**, **WIEN95** and **WIEN97**. Now a new version, **WIEN2k**, is available, which is based on an alternative basis set. This allows a significant improvement, especially in terms of speed, universality, user-friendliness and new features.

WIEN2k is written in FORTRAN 90 and requires a UNIX operating system since the programs are linked together via C-shell scripts. It has been implemented successfully on the following computer systems: Pentium systems running under Linux, IBM RS6000, HP , SGI , Compac DEC Alpha, and SUN. It is expected to run on any modern UNIX (LINUX) system.

Hardware requirements will change from case to case (small cases with 10 atoms per unit cell can be run on any Pentium PC with 128 Mb under Linux), but generally we recommend a powerful PC or workstation with at least 256 Mb (better 512 Mb or more) memory and 1 Gb (better a few Gb) of disk space. For coarse grain parallization on the k-point level, a cluster of PCs with a 100 Mb/s network is sufficient. Faster communication is recommended for the fine grain (single k-point) parallel version.

In order to use all options and features (such as the new graphical user interface **w2web** or some of its plotting tools) the following public domain program packages in addition to a F90 compiler must be installed:

- perl 5 or higher (for **w2web** only)
- emacs or another editor of your choice
- ghostscript (with jpg support)
- gnuplot (with png support)
- www-browser
- pdf-reader (acroread,...)
- MPI+SCALAPACK (on parallel computers only)

Usually these packages should be available on modern systems. If one of these packages is not available, it can either be installed from public domain sources (see Chapt. 11) or the corresponding configuration may be changed (e.g. using vi instead of emacs). None of the principal components of **WIEN2k** requires these packages, only for advanced features or **w2web** they are needed.

WIEN2k has the following features that are new with respect to **WIEN97**:

- due to the new APW+lo basis set it is significantly faster (up to an order of magnitude). Optimizations in the most time consuming parts of LAPW1 and LAPW2 have been made.
- iterative diagonalization (for cases with large matrices and few eigenvalues)
- beside the k-point parallelization (including heterogeneous workstation clusters) a fine grain parallelization based on MPI is also available.
- A new web-based graphical user interface **w2web** has been developed. It does NOT require an X-environment and thus **WIEN2k** can be controlled from (but not run on !) any Windows-PC. This should particularly help the novice to get acquainted with **WIEN2k** but it should be useful for the regular user as well.
- support for AFM and FSM calculations
- spin-orbit coupling, including a new $p_{1/2}$-LO for higher accuracy
- wavefunction plotting
- determination of irreducible representations
- elastic constants (cubic cases only)
- Topological analysis based on Bader's "atoms in molecules" concept
- LDA+U, orbital polarization (OP), magnetic and electric fields
- new PKZB meta-GGA functional

The development of **WIEN2k** was made possible by support from many sources. We try to give credit to all who have contributed. We hope not to have forgotten anyone who made an important contribution for the development or the improvement of the **WIEN2k** code. If we did, please let us know (we apologize and will correct it). The main developers in addition to the authors are the following groups:

- C. Ambrosch-Draxl (Univ. Graz, Austria) and her group
- U. Birkenheuer (Dresden), wave function plotting
- T. Charpin (Paris), elastic constants
- R. Dohmen und J. Pichlmeier (RZG, Garching), parallelization
- C. Först (Vienna), afminput
- P. Novák and J. Kuneš (Prague), LDA+U, SO
- C. Persson (Uppsala), irreducible representations
- M. Scheffler (Fritz Haber Inst., Berlin) and his group
- E. Sjöstedt and L Nordström (Uppsala, Sweden), APW+lo
- J. Sofo and J. Fuhr (Barriloche), Bader analysis
- B. Yanchitsky and A. Timoshevskii (Kiev), sgroup

We want to thank those **WIEN97** users, who reported bugs or made suggestions and thus contributed to the new version as well as persons who have made major contributions in the development of previous versions of the code:

- R. Augustyn (Vienna), U. Birkenheuer (Munich), P. Blöchl (IBM Zürich), F. Boucher (Nantes), A. Chizmeshsya (Arizona), P. Dufek (Vienna), H. Ebert (Munich), E. Engel (Frankfurt), H. Enkisch (Dortmund), M. Fähnle (MPI Stuttgart), S. Kohlhammer (Stuttgart), T. Kokalj (Ljubljana), H. Krimmel (Stuttgart), P. Louf (Vienna), I. Mazin (Washington), M. Nelhiebel (Vienna), V. Petricek (Prague), C. Rodrigues (La Plata, Argentina), P. Schattschneider (Vienna), R. Schmid (Frankfurt), D. Singh (Washington), H. Smolinski (Dortmund), T. Soldner (Leipzig), P. Sorantin (Vienna), S. Trickey (Gainesville), S. Wilke (Exxon, USA), B. Winkler (Kiel)

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- Siemens Nixdorf (WIEN93)
- IBM (WIEN)

We take this opportunity to thank for all contributions.

For suggestions or bug reports please contact the authors by email:

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Part I

Introduction to the WIEN2k package

2 The basic concepts of the present band theory approach

2.1 The density functional theory

An efficient and accurate scheme for solving the many-electron problem of a crystal (with nuclei at fixed positions) is the local spin density approximation (LSDA) within density functional theory (Hohenberg and Kohn 64, Kohn and Sham 65). Therein the key quantities are the spin densities $\rho_\sigma(r)$ in terms of which the total energy is

$$E_{tot}(\rho_\uparrow, \rho_\downarrow) = \quad T_s(\rho_\uparrow, \rho_\downarrow) + E_{ee}(\rho_\uparrow, \rho_\downarrow) + \quad E_{Ne}(\rho_\uparrow, \rho_\downarrow) + E_{xc}(\rho_\uparrow, \rho_\downarrow) + E_{NN}$$

with E_{NN} the repulsive Coulomb energy of the fixed nuclei and the electronic contributions, labeled conventionally as, respectively, the kinetic energy (of the non-interacting particles), the electron-electron repulsion, nuclear-electron attraction, and exchange-correlation energies. Two approximations comprise the LSDA, i), the assumption that E_{xc} can be written in terms of a local exchange-correlation energy density μ_{xc} times the total (spin-up plus spin-down) electron density as

$$E_{xc} = \int \mu_{xc}(\rho_\uparrow, \rho_\downarrow) * [\rho_\uparrow + \rho \downarrow] dr \tag{2.1}$$

and ii), the particular form chosen for that μ_{xc}. Several forms exist in literature, we use the most recent and accurate fit to the Monte-Carlo simulations of Ceperly and Alder by Perdew and Wang 92. E_{tot} has a variational equivalent with the familiar Rayleigh-Ritz principle. The most effective way known to minimize E_{tot} by means of the variational principle is to introduce orbitals χ_{ik}^σ constrained to construct the spin densities as

$$\rho_\sigma(r) = \sum_{i,k} \rho_{ik}^\sigma |\chi_{ik}^\sigma(r)|^2 \tag{2.2}$$

Here, the ρ_{ik}^σ are occupation numbers such that $0 \leq \rho_{ik}^\sigma \leq 1/w_k$, where w_k is the symmetry-required weight of point k. Then variation of E_{tot} gives the Kohn-Sham equations (in Ry atomic units),

$$[-\nabla^2 + V_{Ne} + V_{ee} + V_{xc}^\sigma]\chi_{ik}^\sigma(r) = \epsilon_{ik}^\sigma(r)\chi_{ik}^\sigma(r) \tag{2.3}$$

which must be solved and thus constitute the primary computational task. This Kohn-Sham equations must be solved self-consistently in an iterative process, since finding the Kohn-Sham orbitals requires the knowledge of the potentials which themselves depend on the (spin-) density and thus on the orbitals again.

Recent progress has been made going beyond the LSDA by adding gradient terms of the electron density to the exchange-correlation energy or its corresponding potential. This has led to the generalized gradient approximation (GGA) in various parameterizations, e.g. the one by Perdew et al 92 or Perdew, Burke and Ernzerhof (PBE) 96, which is the recommended option.

A recent version called meta-GGA by Perdew et al (2000) employes for the evaluation of the exchange-correlation energy not only the gradient of the density, but also the kinetic energy density $\tau(r)$. Unfortunately, such schemes are not yet self-consistent.

2.2 The Full Potential APW methods

Recently, the development of the Augmented Plane Wave (APW) methods from Slater's APW, to LAPW and the new APW+lo was described by Schwarz et al. 2001.

2.2.1 The LAPW method

The linearized augmented plane wave (LAPW) method is among the most accurate methods for performing electronic structure calculations for crystals. It is based on the density functional theory for the treatment of exchange and correlation and uses e.g. the local spin density approximation (LSDA). Several forms of LSDA potentials exist in the literature , but recent improvements using the generalized gradient approximation (GGA) are available too (see sec. 2.1). For valence states relativistic effects can be included either in a scalar relativistic treatment (Koelling and Harmon 77) or with the second variational method including spin-orbit coupling (Macdonald 80, Novák 97). Core states are treated fully relativistically (Desclaux 69).

A description of this method to linearize Slater's old APW method (i.e. the LAPW formalism) and further programming hints are found in many references: Andersen 73, 75, Koelling 72, Koelling and Arbman 75, Wimmer et al. 81, Weinert 81, Weinert et al. 82, Blaha and Schwarz 83, Blaha et al. 85, Wei et al. 85, Mattheiss and Hamann 86, Jansen and Freeman 84, Schwarz and Blaha 96). An excellent book by D. Singh (Singh 94) describes all the details of the LAPW method and is highly recommended to the interested reader. Here only the basic ideas are summarized; details are left to those references.

Like most "energy-band methods", the LAPW method is a procedure for solving the Kohn-Sham equations for the ground state density, total energy, and (Kohn-Sham) eigenvalues (energy bands) of a many-electron system (here a crystal) by introducing a basis set which is especially adapted to the problem.

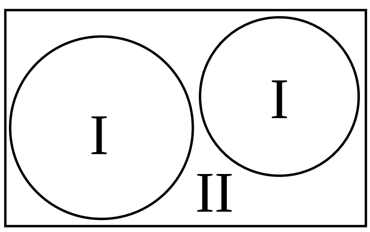

Figure 2.1: Partitioning of the unit cell into atomic spheres (I) and an interstitial region (II)

This adaptation is achieved by dividing the unit cell into (I) non-overlapping atomic spheres (centered at the atomic sites) and (II) an interstitial region. In the two types of regions different basis sets are used:

1. (I) inside atomic sphere t, of radius R_t, a linear combination of radial functions times spherical harmonics $Y_{lm}(r)$ is used (we omit the index t when it is clear from the context)
$$\phi_{\mathbf{k}_n} = \sum_{lm}[A_{lm,\mathbf{k}_n} u_l(r, E_l) + B_{lm,\mathbf{k}_n} \dot{u}_l(r, E_l)]Y_{lm}(\hat{\mathbf{r}}) \tag{2.4}$$
where $u_l(r, E_l)$ is the (at the origin) regular solution of the radial Schroedinger equation for energy E_l (chosen normally at the center of the corresponding band with l-like character) and the spherical part of the potential inside sphere t; $\dot{u}_l(r, E_l)$ is the energy derivative of u_l evaluated at the same energy E_l. A linear combination of these two functions constitute the linearization of the radial function; the coefficients A_{lm} and B_{lm} are functions of k_n (see below) determined by requiring that this basis function matches (in value and slope) each plane wave (PW) the corresponding basis function of the interstitial region; u_l and $\dot{u}_l$ are obtained by numerical integration of the radial Schroedinger equation on a radial mesh inside the sphere.

2. (II) in the interstitial region a plane wave expansion is used
$$\phi_{\mathbf{k}_n} = \frac{1}{\sqrt{\omega}} e^{i\mathbf{k}_n \cdot \mathbf{r}} \tag{2.5}$$
where $\mathbf{k}_n = \mathbf{k} + \mathbf{K}_n$; $\mathbf{K}_n$ are the reciprocal lattice vectors and $\mathbf{k}$ is the wave vector inside the first Brillouin zone. Each plane wave is augmented by an atomic-like function in every atomic sphere.

The solutions to the Kohn-Sham equations are expanded in this combined basis set of LAPW's according to the linear variation method

$$\psi_{\mathbf{k}} = \sum_n c_n \phi_{\mathbf{k}_n} \tag{2.6}$$

and the coefficients c_n are determined by the Rayleigh-Ritz variational principle. The convergence of this basis set is controlled by a cutoff parameter $R_{mt}K_{max}$ = 6 - 9, where R_{mt} is the smallest atomic sphere radius in the unit cell and K_{max} is the magnitude of the largest K vector in equation (2.6).

In order to improve upon the linearization (i.e. to increase the flexibility of the basis) and to make possible a consistent treatment of semicore and valence states in one energy window (to ensure orthogonality) additional (k_n independent) basis functions can be added. They are called "local orbitals (LO)" (Singh 91) and consist of a linear combination of 2 radial functions at 2 different energies (e.g. at the $3s$ and $4s$ energy) and one energy derivative (at one of these energies):

$$\phi_{lm}^{LO} = [A_{lm} u_l(r, E_{1,l}) + B_{lm} \dot{u}_l(r, E_{1,l}) + C_{lm} u_l(r, E_{2,l})]Y_{lm}(\hat{r}) \tag{2.7}$$

The coefficients A_{lm}, B_{lm} and C_{lm} are determined by the requirements that ϕ^{LO} should be normalized and has zero value and slope at the sphere boundary.

2.2.2 The APW+lo method

Sjöstedt, Nordström and Singh (2000) have shown that the standard LAPW method with the additional constraint on the PWs of matching in value AND slope to the solution inside the sphere is not the most efficient way to linearize Slater's APW method. It can be made much more efficient when one uses the standard APW basis, but of course with $u_l(r, E_l)$ at a fixed energy E_l in order to keep the linear eigenvalue problem. One then adds a new local orbital (lo) to have enough variational flexibility in the radial basisfunctions:

$$\phi_{\mathbf{k}_n} = \sum_{lm}[A_{lm,\mathbf{k}_n} u_l(r, E_l)]Y_{lm}(\hat{\mathbf{r}}) \tag{2.8}$$

$$\phi_{lm}^{lo} = [A_{lm}u_l(r, E_{1,l}) + B_{lm}\dot{u}_l(r, E_{1,l})]Y_{lm}(\hat{\mathbf{r}}) \tag{2.9}$$

This new lo (denoted with lower case to distinguish it from the LO given in equ. 2.7) looks almost like the old "LAPW"-basis set, but here the A_{lm} and B_{lm} do not depend on k_n and are determined by the requirement that the lo is zero at the sphere boundary and normalized.

Thus we construct basis functions that have "kinks" at the sphere boundary, which makes it necessary to include surface terms in the kinetic energy part of the Hamiltonian. Note, however, that the total wavefunction is of course smooth and differentiable.

As shown by Madsen et al. (2001) this new scheme converges practically to identical results as the LAPW method, but allows to reduce "RKmax" by about one, leading to significantly smaller basis sets (up to 50 %) and thus the corresponding computational time is drastically reduced (up to an order of magnitude). Within one calculation a mixed "LAPW and APW+lo" basis can be used for different atoms and even different l-values for the same atom (Madsen et al. 2001). In general one describes by APW+lo those orbitals which converge most slowly with the number of PWs (such as TM 3d states) or the atoms with a small sphere size, but the rest with ordinary LAPWs. One can also add a second LO at a different energy so that both, semicore and valence states, can be described simultaneously.

2.2.3 General considerations

In its general form the LAPW (APW+lo) method expands the potential in the following form

$$V(\mathbf{r}) = \begin{cases} \sum\limits_{LM} V_{LM}(r)Y_{LM}(\hat{\mathbf{r}}) & \text{inside sphere} \\ \sum\limits_{\mathbf{K}} V_{\mathbf{K}}e^{i\mathbf{K}\cdot\mathbf{r}} & \text{outside sphere} \end{cases} \tag{2.10}$$

and the charge densities analogously. Thus no shape approximations are made, a procedure frequently called a "full-potential" method.

The "muffin-tin" approximation used in early band calculations corresponds to retaining only the $l = 0$ component in the first expression of equ. 2.10 and only the $K = 0$ component in the second. This (much older) procedure corresponds to taking the spherical average inside the spheres and the volume average in the interstitial region.

The total energy is computed according to Weinert et al. 82.

Rydberg atomic units are used except internally in the atomic-like programs (LSTART and LCORE) or in subroutine outwin (LAPW1, LAPW2), where Hartree units are used. The output is always given in Rydberg units.

The forces at the atoms are calculated according to Yu et al (91). For the implementation of this formalism in WIEN see Kohler et al (96) and Madsen et al. 2001. An alternative formulation by Soler and Williams (89) has also been tested and found to be equivalent, both in computationally efficiency and numerical accuracy (Krimmel et al 94).

The Fermi energy and the weights of each band state can be calculated using a modified tetrahedron method (Blöchl et al. 94), a Gaussian or a temperature broadening scheme.

Spin-orbit interactions can be considered via a second variational step using the scalar-relativistic eigenfunctions as basis (see Macdonald 80, Singh 94 and Novák 97). In order to overcome the problems due to the missing $p_{1/2}$ radial basis function in the scalar-relativistic basis (which corresponds to $p_{3/2}$), we have recently extended the standard LAPW basis by an additional "$p_{1/2}$-local orbital", i.e. a LO with a $p_{1/2}$ basis function, which is added in the second-variational SO calculation (Kuneš et al. 2001).

It is well known that for localized electrons (like the 4f states in lanthanides or 3d states in some TM-oxides) the LDA (GGA) method is not accurate enough for a proper description. Thus we have implemented various forms of the LDA+U method as well as the "Orbital polarization method" (OP) (see Novák 2001 and references therein).

One can also consider interactions with an external magnetic (see Novák 2001) or electric field (via a supercell approach, see Stahn et al. 2000).

PROPERTIES:

The density of states (DOS) can be calculated using the modified tetrahedron method of Blöchl et al. 94.

X-ray absorption and emission spectra are determined using Fermi's golden rule and dipole matrix elements (between a core and valence or conduction band state respectively). (Neckel et al. 75, Schwarz et al 79,80)

X-ray structure factors are obtained by Fourier Transformation of the charge density.

Optical properties are obtained using the "Joint density of states" modified with the respective dipole matrix elements according to Ambrosch et al. 95, Abt et al. 94, Abt 97. A Kramers-Kronig transformation is also possible.

An analysis of the electron density according to Bader's "atoms in molecules" theory can be made using a program by J. Sofo and J. Fuhr (2001)

3 Quick Start

Contents

We assume that **WIEN2k** is properly installed and configured for your site and that you ran **userconfig_lapw** to adjust your path and environment. (For a detailed description of the installation see chapter 11.

This chapter is intended to guide the novice user in the handling of the program package. We will use the example of TiC in the sodium chloride structure to show which steps are necessary to initialize a calculation and run a self consistent field cycle. We also demonstrate how to calculate various physical properties from these SCF data. Along the way we will give all important information in a very abridged form, so that the novice user is not flooded with information, and the experienced user will be directed to more complete information.

In this chapter we will also show, how the new graphical user interface **w2web** can be utilized to setup and run the calculations.

3.1 Naming conventions

Before we begin with our introductory example, we describe the naming conventions, to which we will adhere throughout this user's guide.

On UNIX systems the files are specified by **case.type** and it is required that all files reside in a subdirectory **./case**. Here and in the following sections and in the shell scripts which run the package themselves, we follow a simple, systematic convention for file labeling.

For the general discussion (when no specific crystal is involved), we use **case**, while for a specific case, e.g. TiC, we use the following notation:

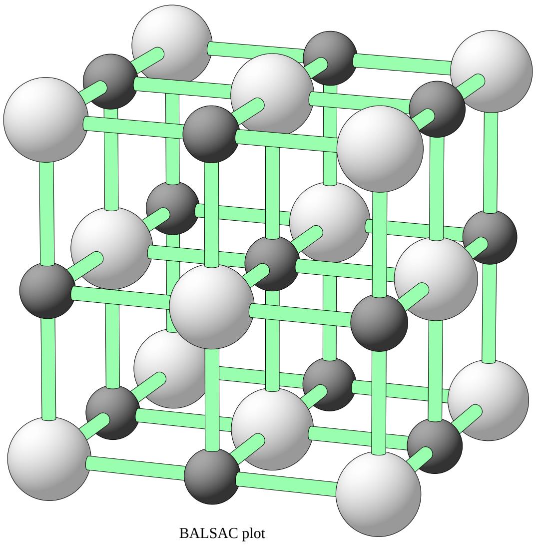

Figure 3.1: TiC in the sodium chloride structure. This plot was generated using BALSAC (see 9.11.1). Interface programs between **WIEN2k** and BALSAC are available.

`case=TiC`

The filetype "`type`" always describes the content of the file (e.g.,

`type=inm` is inPUT for mIXER).

Thus the input to MIXER for TiC is found in the file

`TiC.inm`

which should be in subdirectory `./TiC`.

3.2 Starting the w2web server

Start the user interface **w2web** on the computer where you want to execute **WIEN2k**(you may have to telnet, ssh,.. to this machine) with the command

```
w2web [-p xxxx]
```

If the default port (7890) used to serve the interface is already in use by some other process, you will get the error message `w2web failed to bind port 7890 - port already in use!`. Then you will have to choose a different port number (between 1024 and 65536) . Please remember this port number, you need it when connecting to the **w2web** server.

*Note: Only user **root** can specify port numbers below 1024!*

At the first startup of this server, you will also be asked to setup a username and password, which is required to connect to this server.

3.3 Connecting to the **w2web** server

Use your favorite WWW-browser to connect to **w2web**, specifying the correct portnumber, e.g.

```
netscape http://hostname_where_w2web_runs:7890
```

(If you do not remember the portnumber, you can find it by using "ps -ef | grep w2web" on the computer where **w2web** is running.) You should see a screen as in Fig.3.2.

3.4 Creating a new session

The user interface **w2web** uses **sessions** to distinguish between different working environments and to quickly change between different calculations. First you have to create a new session (or select an old one). Enter "TiC" and click the "*Create*" button.
Note: Creating a session does not automatically create a new directory!

You will be placed in your home directory if no working directory was designated to this session previously (or if the directory does not exist any more).

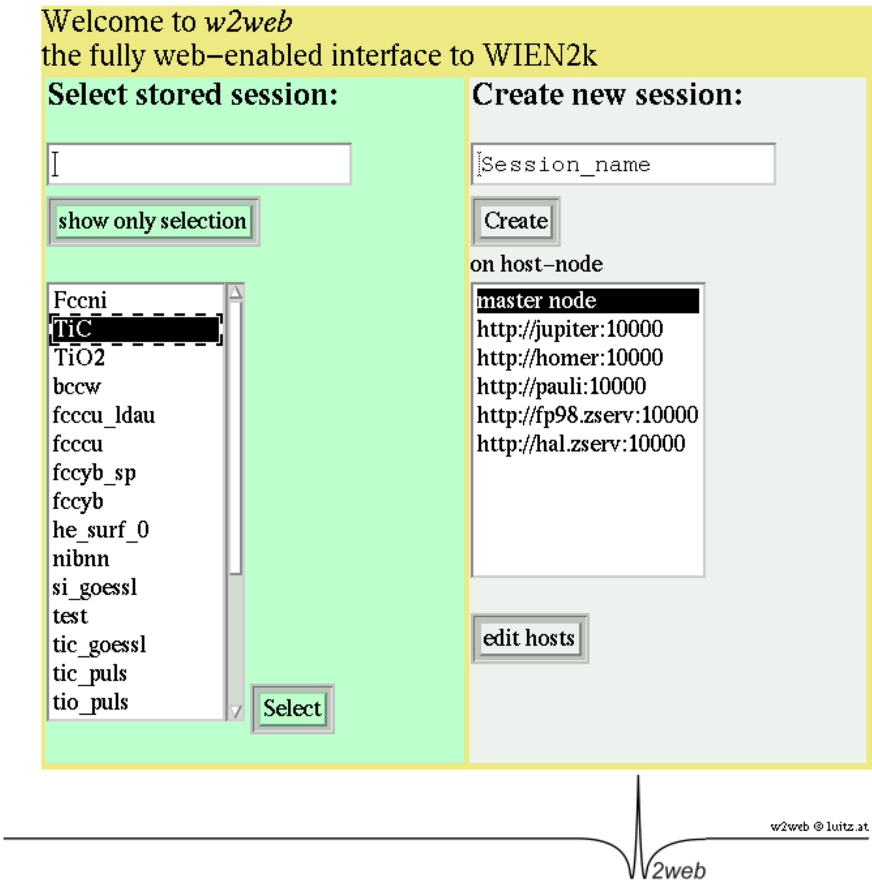

Figure 3.2: Startup screen of **w2web**

3.5 Creating a new case-directory

Using "*Session Mgmt.* □ *change directory*" you can select an existing directory or create a new one. For this example create a new directory **`lapw`** and than **`TiC`** using the "*Create*" button. After the directory has been created, you have to click on *select current directory* to assign this newly created directory to the current session.

After clicking on *Click to restart session* the main window of **w2web** will appear (Fig.3.3.

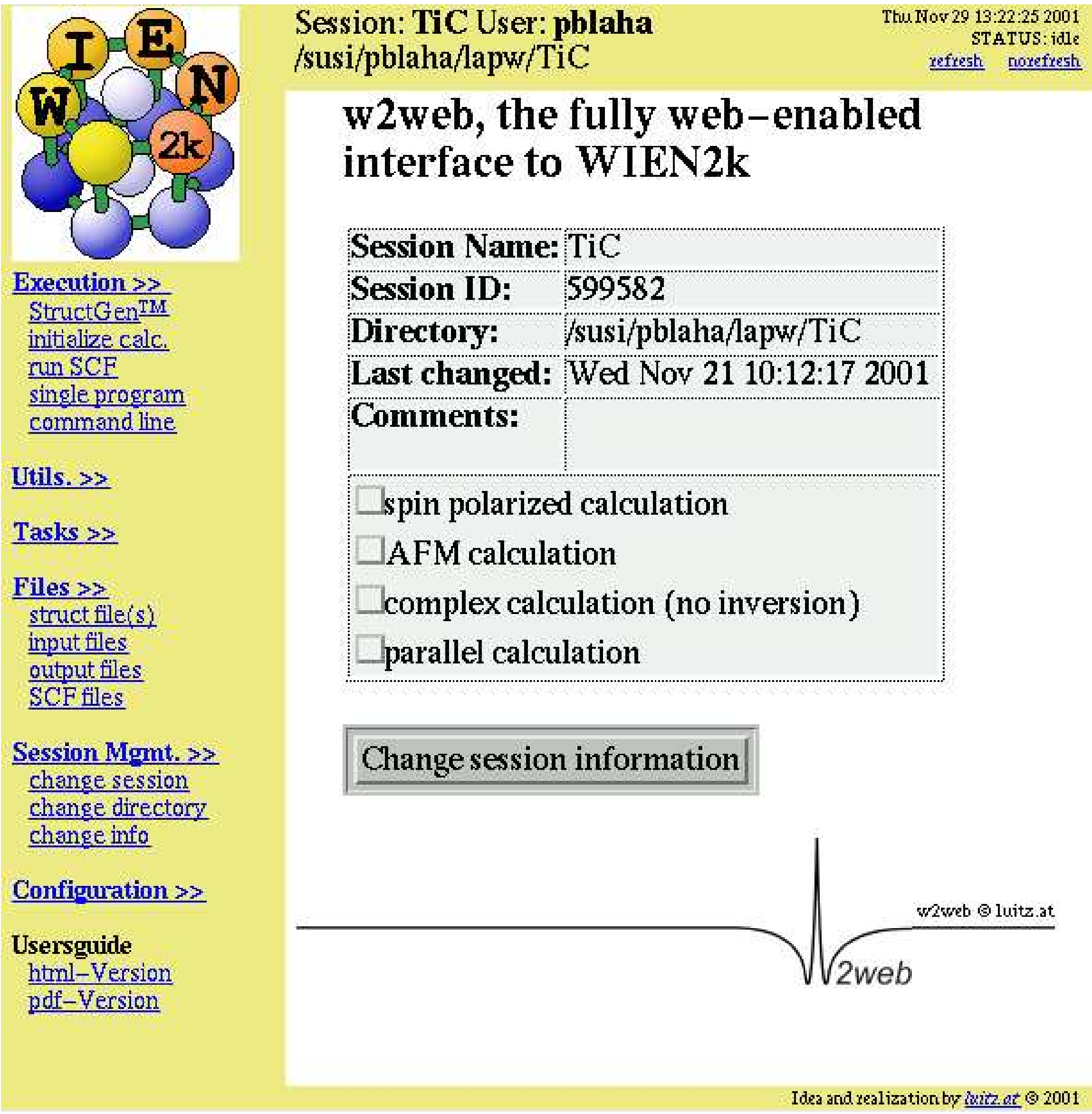

Figure 3.3: Main window of **w2web**

3.6 Creating the "master input" file case.struct

To create the file **`TiC.struct`** start the struct-file generator using "*Execution* ⇓ **StructGen^{TM}**" (see figure 3.4).

For a new case **w2web** creates an empty structure template in which you can specify structural data and calculational parameters. Later on this information is used to generate the **`TiC.struct`** file.

As a first step specify the number of atoms (2 for TiC) and fill in the data given below into the corresponding fields (white boxes):

Title	TiC
Lattice	F (for face centered)
a	4.328 Å(click on the Ang button before)
b	4.328 Å
c	4.328 Å
α, β, γ	90
Atom	Ti, enter position (0,0,0) and RMT = 2.0.
Atom	C, enter position (.5,.5,.5) and RMT = 1.9

Click **"Save Structure"** (Z and R0 will be updated automatically) and **"Continue editing"**:

*Note: You have to click on **Save Structure** after every modifications you make in the white fields. Add/remove a position/atom only if you have made no other changes before.*

Usually, the value for RMT (muffin-tin radius, sphere size) would be specified once you know the nearest neigbor distances computed in **nn**. In a face-centered (body-centered) spacegroup you have to enter just one atom (not the ones in (.5,.5,0),...).

StructGen^{TM} offers a built in calculator: Each position of equivalent atoms can be entered as a number, a fraction (e.g. $1/3$) or a simple expression (e.g. $0.21 + 1/3$). The first position defines the variables x, y and z, which can be using in expression defining the other positions (e.g. $-y$, x, $-z + 1/2$).

When you are done, exit the **StructGen^{TM}** with "*save file and clean up*". This will generate the file **`TiC.struct`** (shown now in view-only mode with a different background color), which is the master input file for all subsequent programs. This step also automatically generates the input file for the free atom program **`lstart`** (atomic configurations) **`tic.inst`**.

When you now choose "*Files* ⇓ *show all files*", you will see, that both files **`tic.struct`** and **`tic.inst`** have been created.

For a detailed description of these files consult sections 4.3 and 6.4.3.

3.7 Initialization of the calculation (init_lapw)

After the two basic input files have been created, initalization of the calculation is done by "*Execution* ⇓ *initialize calc.*". This will guide you through the steps necessary to initialite the calculation. Simply follow the steps that are highlighted in green and follow the instructions.

The initialization process is described in detail in section 5.1.2.

Alternatively you could run the script **`init_lapw`** from the command line. All actions of this script are logged in short in **`:log`** and in detail in the file **`case.dayfile`**, which can easily be accessed by *Utils.* ⇓ *show dayfile*.

Initializing the calculation will run several steps automatically, where **`x`** is the script to start **WIEN2k** programs (see section: 5.1.1).

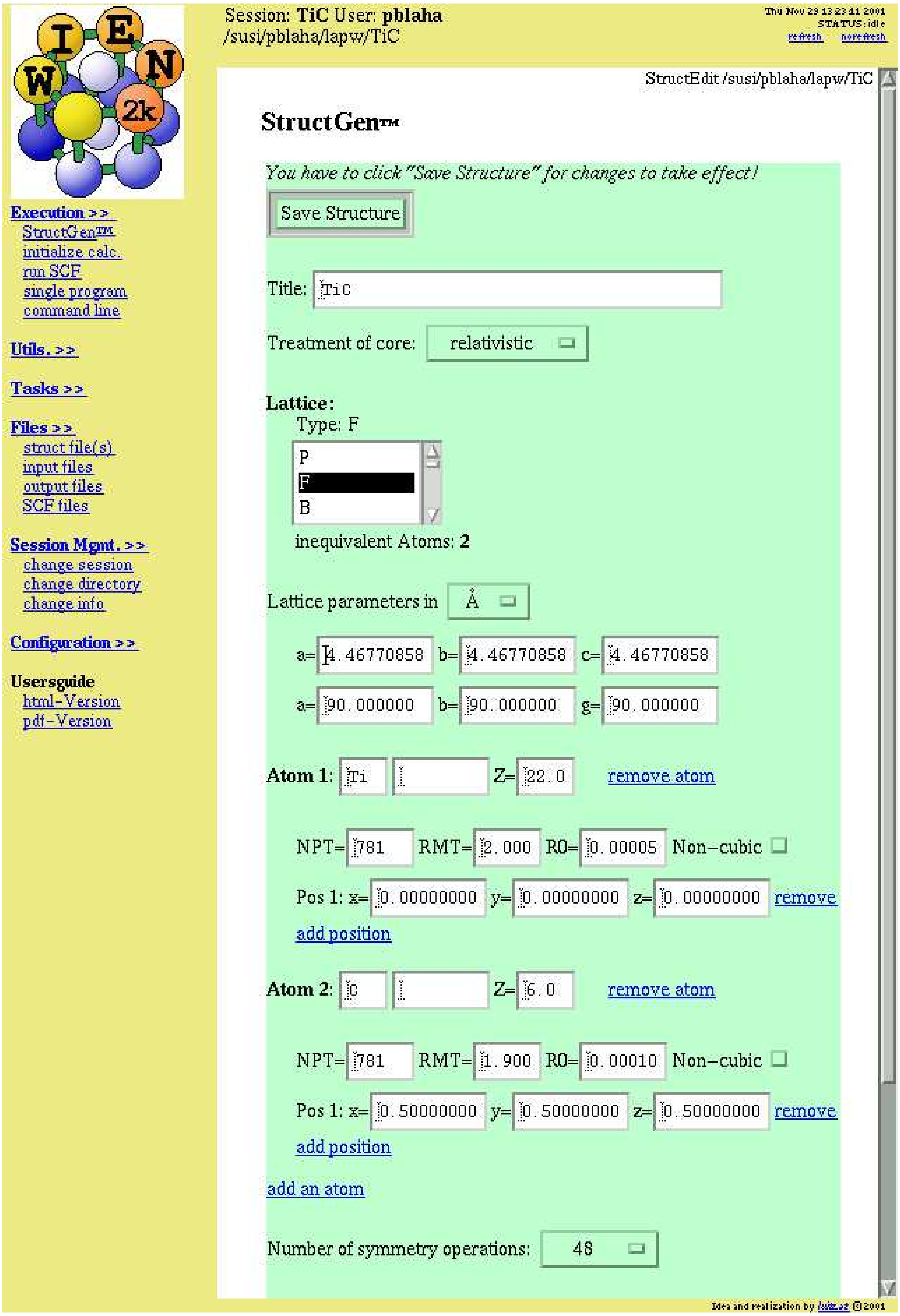

Figure 3.4: **StructGen**$^{\text{TM}}$ of **w2web**

x nn calculates the nearest neighbors up to a specified distance and thus helps to determine the atomic sphere radii (you must specify a distance factor f, e.g. 2, and all distances up to f * NN-dist. are calculated)

view TiC.outputnn : check for overlapping spheres, coordination numbers and nearest neighbor distances, (e.g. in the sodium chloride structure there must 6 nearest and 12 next nearest neighbors). Using these distances and coordinations you can check whether you put the proper positions into your struct file or if you made a mistake. **nn** also checks whether your equivalent atoms are really crystallographically equivalent and eventually writes a new struct-file which you may or may not accept. In general, this is also the time to go back to **StructGen™** and choose proper RMT values. *You can save a lot of CPU-time by changing RMT to almost touching spheres. See Sec.4.3*

x sgroup calculates the point and spacegroups for the given structure

view TiC.outputsgroup : Now you can either accept the **TiC.struct** file generated by **sgroup** (if you want to use the spacegroup information or a different cell has been found by **sgroup**) or keep your original file (default).

x symmetry generates from a raw **case.struct** file the space group symmetry operations, determines the point group of the individual atomic sites, generates the LM expansion for the lattice harmonics (in **case.in2_st**) and local rotation matrices (in **case.struct_st**).

view TiC.outputs : check the symmetry operations (they have been written to or compared with already available ones in **TiC.struct** by the program symmetry) and the point group symmetry of the atoms (You may compare them with the "International Tables for X-Ray Crystallography"). If the output does not match your expectations from the "Tables", you might have made an error in specifying the positions. The **TiC.struct** file will be updated with symmetry operations, positive or negativ atomic counter (for "cubic" point group symmetries) and the local rotation matrix.

x lstart generates atomic densities (see section 6.4) and determines how the orbitals are treated in the band structure calculations (i.e. as core or band states, with or without local orbitals, . . .). You are requested to specify the desired exchange correlation potential and an energy that separates valence from core states. For TiC select the recommended potential option "GGA of Perdew-Burke-Ernzerhof 96" and a separation energy of -6.0 Ry.

edit TiC.outputst : check the output (did you specify a proper atomic configuration, did lstart converge, are the core electrons confined to the atomic sphere?). Warnings for the radial mesh can usually be neglected since it affects only the atomic total energy. **lstart** generates **TiC.in0_st**, **in1_st**, **in2_st**, **inc_st** and **inm**. For Ti it selects automatically $1s$, $2s$, and $2p$ as core states, $3s$ and $3p$ will be treated with local orbitals together with $3d$, $4s$ and $4p$ valence states.

edit TiC.in1_st : As mentioned, the input files are generated automatically with some default values which should be a reasonable choice for most cases. Nevertheless we highly recommend that you go through these inputs and become familiar with them. The most important parameter here is RKMAX, which determines the number of basis functions (size of the matrices). Values between 5-9 (APW) and 6-10 (LAPW) are usually reasonable. You may change here the usage of APW or LAPW (set 1 or 0 after the CONT/STOP switch), since often APW is necessary only for orbitals more difficult to converge (3d, 4f). *Here we will just change EMAX of the energy window from 1.5 to 2.0 Ry in order to be able to calculate the unoccupied DOS to higher energies.*

edit TiC.in2_st : Here you may limit the LM expansion (for some speedup), change the value of GMAX (in cases with small spheres (e.g. systems with H-atoms) values of 15-24 are recommended) or specify a different BZ-integration method to determine the Fermi energy. For this example you should not change anything so that you can compare your results with the test run.

edit TiC.inm_st : For "difficult to converge systems" (several atoms with localized d- or f-electrons, magnetic systems) you should reduce the mixing factor from 0.4 to a smaller value (e.g. 0.05). (See our faq-page on www.wien2k.at what you should do when the scf cycle crashes). For TiC no changes are necessary.

Copy all generated inputs (from **`case.in*_st`** to **`case.in*`**). In cases without inversion symmetry the files **`case.in1c, in2c`** are produced.

x kgen generates a k-mesh in the Brillouin zone (BZ). You must specify the number of k-points in the whole BZ (use 1000 for comparison with the provided output, a "good" calculations needs many more). For details see section 6.5.

view TiC.klist : check the number of k-points in the irreducible wedge of the BZ (IBZ) and the energy interval specified for the first k-point. You can now either rerun **`kgen`** (and generate a different k-mesh) or continue.

x dstart generates a starting density for the SCF cycle by superposition of atomic densities generated in **`lstart`**. For details see section 6.6.

view TiC.outputd (check if gmax >gmin)

Now you are asked , whether or not you want to run a spin-polarized calculation (in such a case case **`dstart`** is re-run to generate spin-densities). For TiC say **No**.

Initialization of a calculation (running **`init_lapw`**) will create all inputs for the subsequent SCF calculation choosing some default options and values. You can find a list of input files using "*Files ⇒ input files*" (3.5).

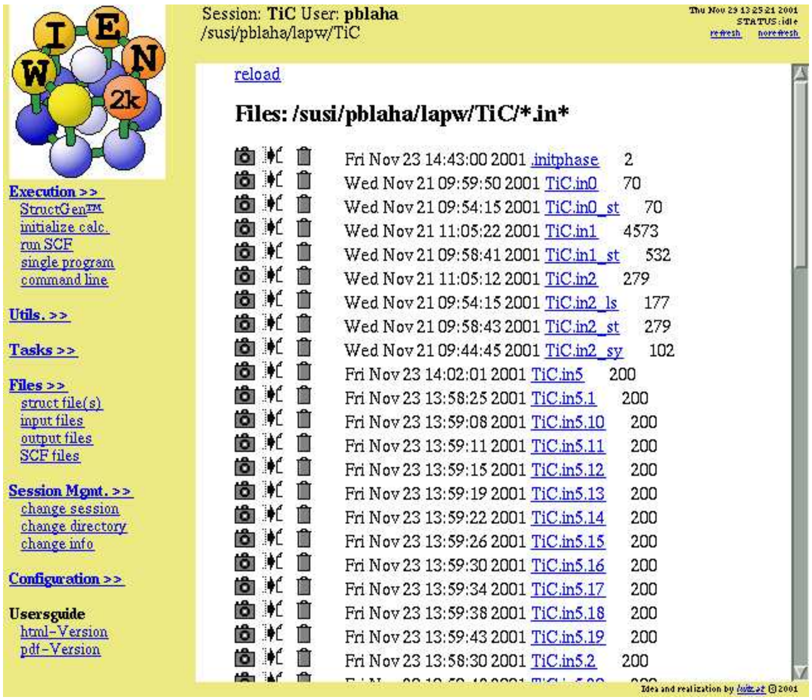

Figure 3.5: List of input files

3.8 The SCF calculation

After the case has been set up, a link to "run SCF" is added, ("*Run Programs ⇒ run SCF*" and you should invoke the self-consistency cycle (SCF). This runs the script **`run_lapw`** with the desired options.

The SCF cycle consists of the following steps:

LAPW0 (POTENTIAL) generates potential from density
LAPW1 (BANDS) calculates valence bands (eigenvalues and eigenvectors)
LAPW2 (RHO) computes valence densities from eigenvectors
LCORE computes core states and densities
MIXER mixes input and output densities

After selecting "run SCF" from the "Execution" menu, the SCF-window will open, and you can now specify additional parameters. For this example we select charge convergence to 0.0001: Specify "*charge*" to be used as convergence criterion, and select a value of 0.0001 (-cc 0.0001).

To run the SCF cycle, click on "*Run!*"

Since this might take a long time for larger systems; you can specify the "*Execution type*" to be *batch* or *submit* (if your system is configured with a queuing system and **w2web** has been properly set up, see section 11.3).

While the calculation is running (as indicated by the status frame in the top right corner of the window), you can monitor several quantities (see section 3.9).

Once the calculation is finished (11 iterations), view **case.dayfile** for timing and errors and compare your results with the files in the provided example (**TiC/case_scf**).

For magnetic systems you would run a spin-polarized calculation with the script **runsp_lapw**. The program flow of such a calculation is described in section 4.5.2 and the script itself in section 5.1.3.

3.9 The "history" file case.scf

During the SCF cycle the essential data of each iteration are appended to the file **case.scf**, in our example **TiC.scf**. For an easier retrieval of certain quantities, the essential lines carry a label of the form **:LABEL:** which can be used to monitor these quantities during a SCF run.

The information is retrieved using the UNIX grep command or using the "*Utils.* ⇓ *analyze*" menu.

While the SCF cycle of TiC is running try to monitor e.g. the total energy (label **:ENE**) or the charge distance (label **:DIS**). The calculation has converged, when the convergence criterion is met for three subsequent iterations (compare the charge distance in the example).

For a detailed description of the various labels consult section 4.4.

3.10 Saving a calculation

Before you proceed to another calculation, you should save the results of the SCF-cycle with the **save_lapw** command, which is also described in detail in section 5.2.1. This can also be done from the graphical user interface by choosing the "*Utils.* ⇓ *save_lapw*" menu.

Save the result to this example under the name "**TiC_scf**".

You can now improve your calculation and check the convergence of the most important parameters:

- increase RKMAX and GMAX in **case.in1** and **case.in2**
- increase the k-mesh with **x kgen**
- choose a different exchange-correlation potential in **case.in0**

Then just execute another **run_lapw** using "*Execution* ⇓ *run SCF*".

3.11 Calculating properties

Once the SCF cycle has converged one can calculate various properties like Density of States (DOS), band structure, Optical properties or X-ray spectra.

For the calculation of properties (which from now on will be called "*Tasks*"). We strongly encourage the user to utilize the user interface, **w2web**. This user interface automatically supplies input file templates and shows how to calculate the named properties on a step by step basis.

3.11.1 Electron density plots

Select "*El. Dens.*" from the "*Tasks*" menu and click on the buttons one by one (see figure 3.6):

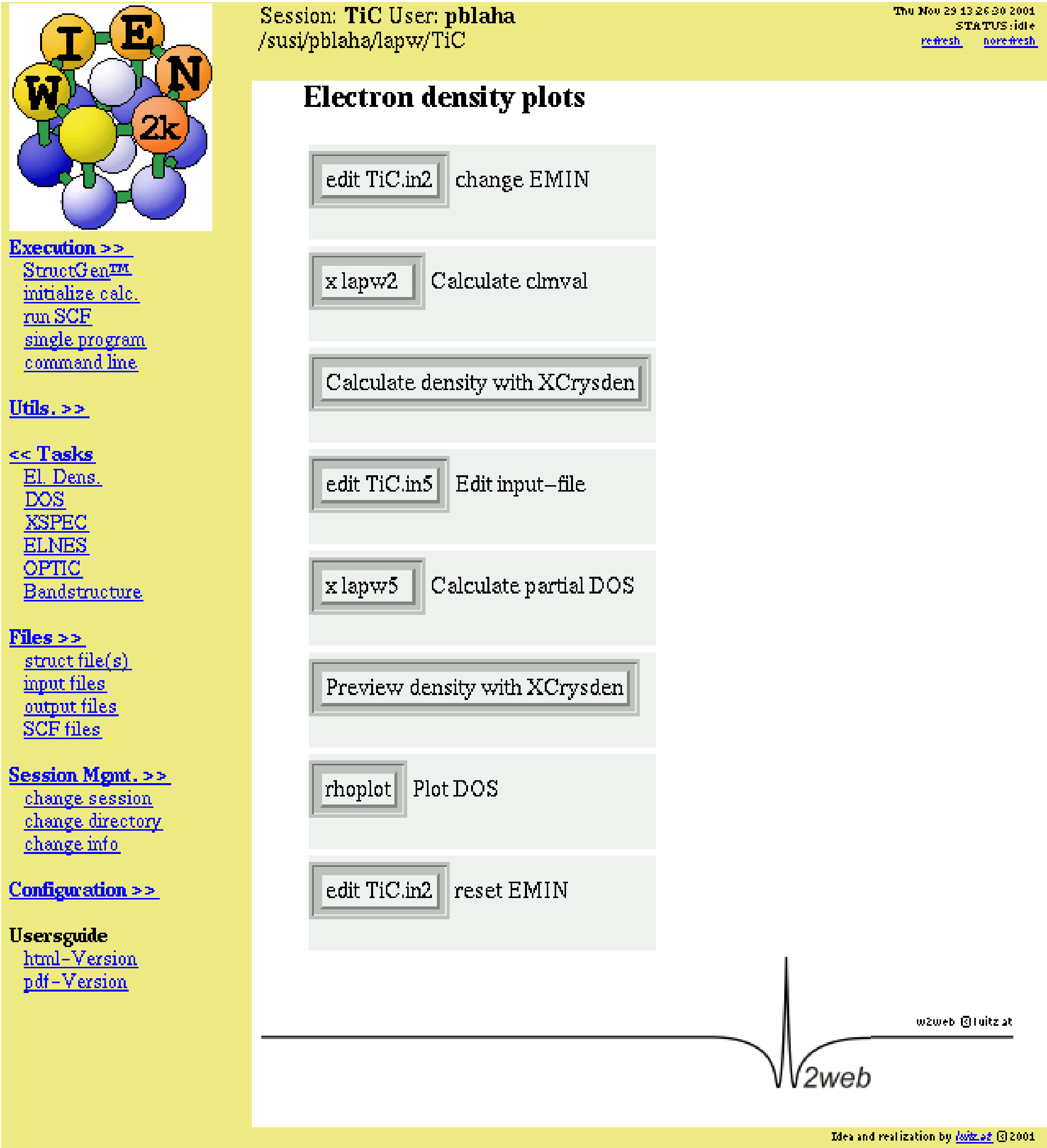

Figure 3.6: Task "Electron Density Plots"

- Edit **TiC.in2** and set EMIN to -1.0 to eliminate Ti 3s and 3p semicore states
- Recalculate the valence density without 3s and 3p (**x lapw2**). This is only possible, when you still have a valid **TiC.vector** file on a tetrahedral mesh.
- Edit **TiC.in5** choose the offered template input file. To select the (100) plane for plotting specify the following input:

```
-1 -1 0 4      # origin of plot (x,y,z,denominator)
-1  3 0 4      # x-end of plot
 3 -1 0 4      # y-end of plot
3 2 3          # x,y,z number of shells
100 100        # number of x and y points, ratio should be
               # similar to x,y length
RHO
ANG VAL NODEBUG
ORTHO
```

  For a detailed description of input options consult section 8.6.3
- Calculate electron density
- Plot output (using rhoplot), after the first preview select a range zmin=0 to zmax=2
- Reset EMIN in **TiC.in2** (don't forget this, or you will run onto troubles later on!)

Compare the result with the electron density plotted in the (100) plane (see figure 3.7). The program **gnuplot** (public domain) must be installed on your computer. For more advanced graphics use your favorite plotting package or specify other options in **gnuplot** (see **rhoplot_lapw** how gnuplot is called).

3.11.2 Density of States (DOS)

Select "*Density of States (DOS)*" from the "*Tasks*" menu and click on the buttons one by one:

- Calculate partial charges (**x lapw2 -qtl**). (This is only possible, when you still have a valid **TiC.vector** file on a tetrahedral mesh.)
- Edit **TiC.int**, choose the offered template input file and edit it to select: total DOS, Ti-d, Ti-d$_{eg}$, Ti-d$_{t2g}$, C-s and C-p-like DOS.

```
TiC
  -0.50     0.00200   1.500 0.003   EMIN, DE, EMAX, Gauss-broadening
    6                              NUMBER OF DOS-CASES
    0    1   tot                   (atom,case,description)
    1    4   Ti d
    1    5   Ti eg
    1    6   Ti t2g
    2    2   C s
    2    3   C p
```

  For a detailed description of input options consult section 8.1.3
- Calculate DOS (**x tetra**).
- Preview output using "dosplot"

If you want to use the supplied plotting interface **dosplot** to preview the results, the program **gnuplot** (public domain) must be installed on your computer.

The calculated DOS can be compared with figures 3.8 to 3.13 if you select a range of -12.5 to 3.5 eV. To calculate DOS for higher energies, you will have to increase EMAX in **case.in1** and rerun **x lapw1**.

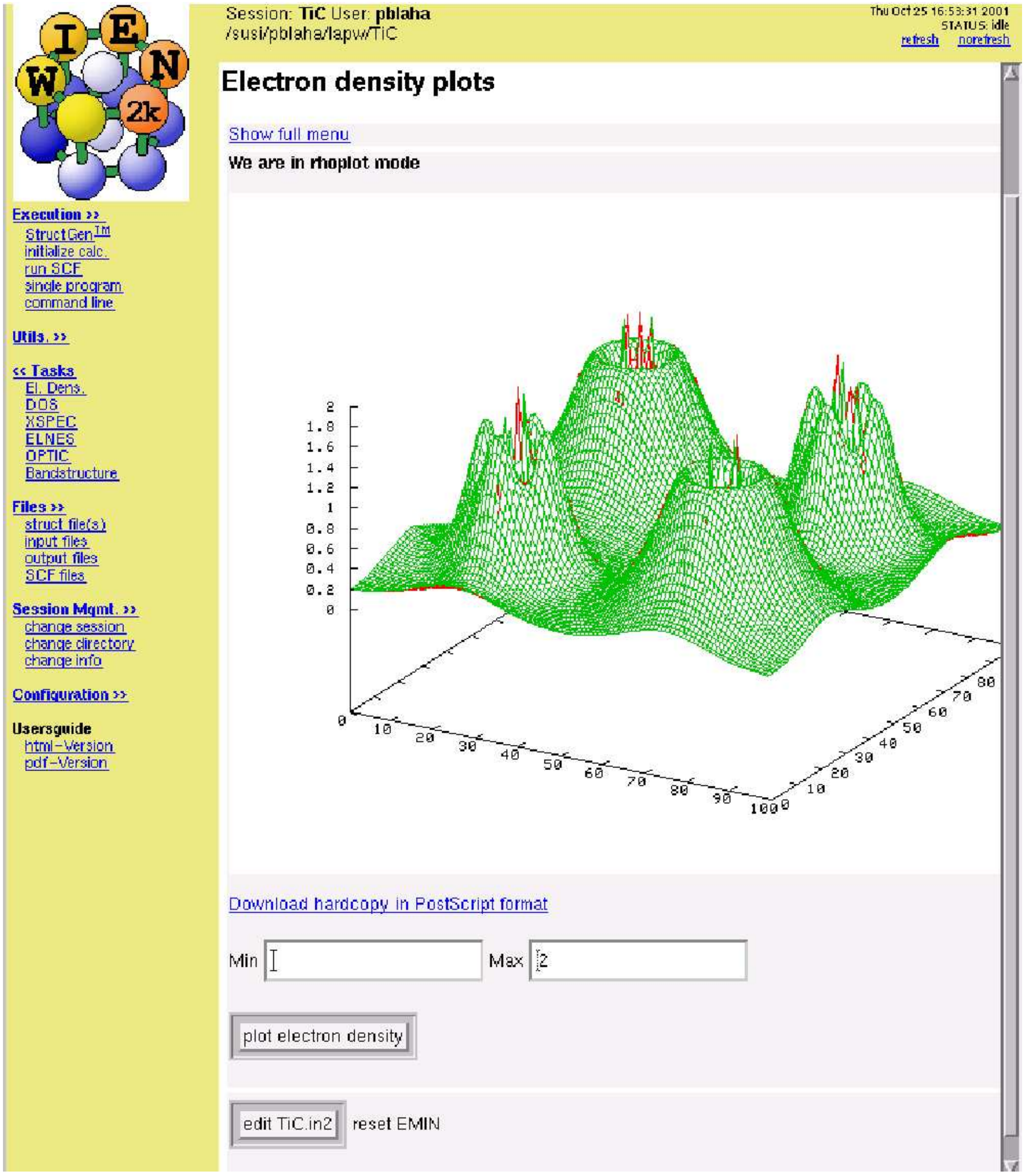

Figure 3.7: Electron density of TiC in [110] plane

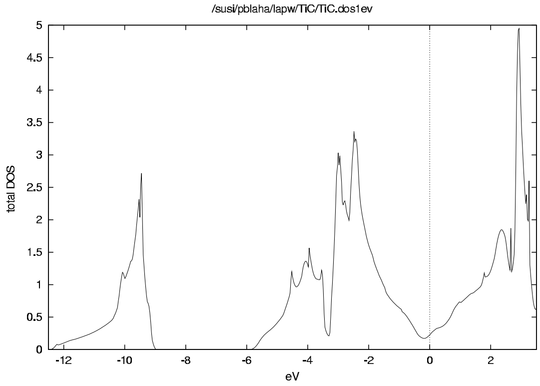

Figure 3.8: TiC: total DOS

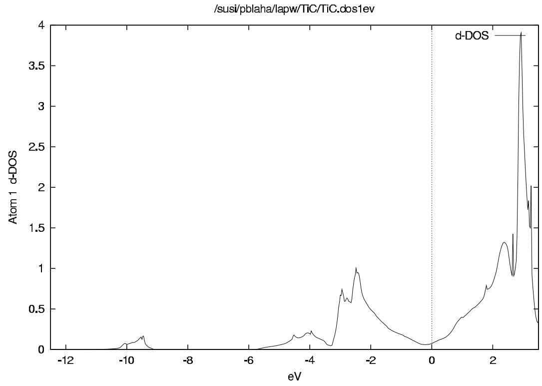

Figure 3.11: TiC: Ti partial d-DOS

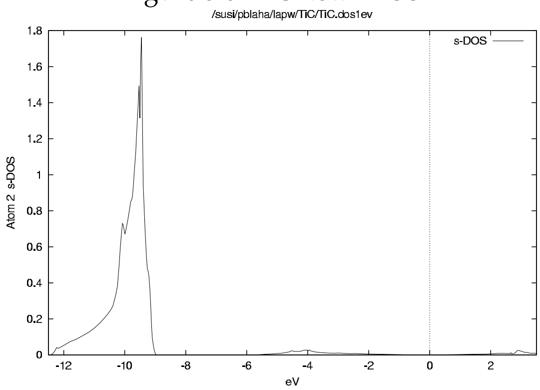

Figure 3.9: TiC: C partial s-DOS

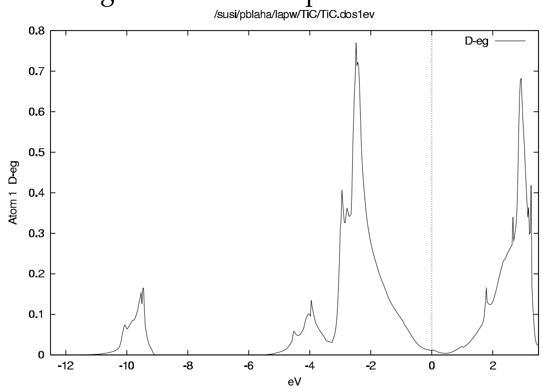

Figure 3.12: TiC: Ti partial eg-DOS

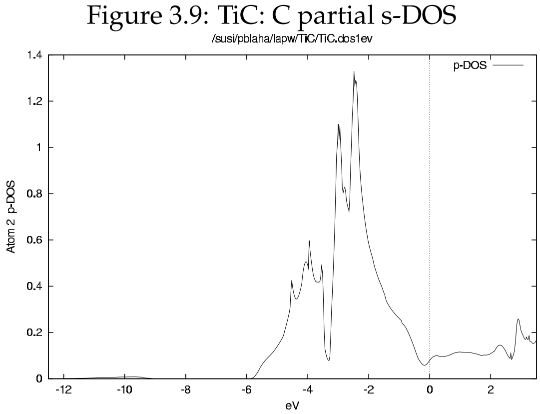

Figure 3.10: TiC: C partial p-DOS

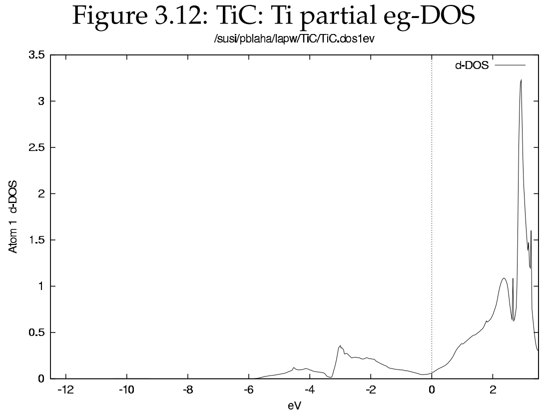

Figure 3.13: TiC: Ti partial t_{2g}-DOS

3.11.3 X-ray spectra

Select “X-Ray Spectra” from the “Tasks menu” and click on the buttons one by one:

- ▶ Calculate partial charges (**`x lapw2 -qtl`**). This is only possible, when you still have a valid **`TiC.vector`** file on a tetrahedral mesh. *To reproduce this figure you will have to increase the EMAX value in your **`TiC.in1`** to 2.5 Ry and rerun **`x lapw1`***
- ▶ Edit **`TiC.inxs`**; choose the offered template. This template will calculate the L_{III}-spectrum of the first atom (Ti in this example) in the energy range between -2 and 15 eV. For a detailed description of the contents of this input file refer to section 8.10.3.
- ▶ Calculate spectra
- ▶ Preview spectra

If you want to use the supplied plotting interface **specplot** to preview the results, the public domain program **gnuplot** must be installed on your computer. The calculated TiC Ti-L_{III}-spectrum can be compared with figure 3.14.

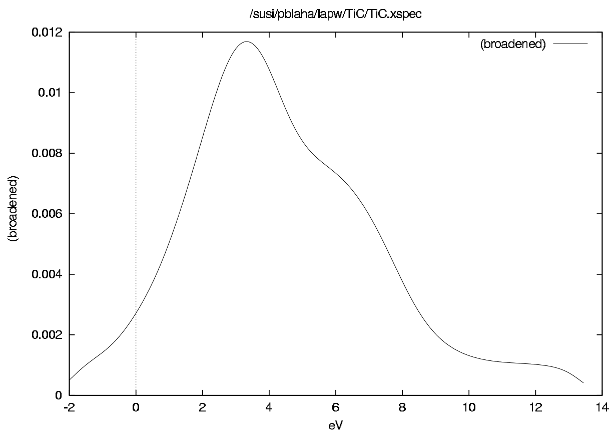

Figure 3.14: Ti L_{III} spectrum of TiC

3.11.4 Bandstructure

Select “*Bandstructure*” from the “*Tasks*” menu and click on the buttons one by one:

- ▶ Append the **`$WIENROOT/SRC_templates/fcc.klist`** file and change the entry “K-points from unit” **4** to **5** in **`TiC.in1`**. (To calculate a bandstructure a special k-mesh along high symmetry directions is necessary. For a few crystal structures template files are supplied in the **SRC**-directory, you can also use XCRYSDEN (save it as xcrasden.klist) to generate a k-mesh or type in your own mesh.
  to **`TiC.in1`** and change the entry “K-points from unit” **4** to **5**.
- ▶ Calculate Eigenvalues
  *Note: When you want to calculate DOS, charge densities or spectra after this bandstructure, you must first recalculate the **`TiC.vector`** file using the “tetrahedral” k-mesh, because the k-mesh for the band structure plots is **not** suitable for calculations of such properties.*
- ▶ Edit **`TiC.insp`**: insert the correct Fermi energy (which can be found in the saved **`scf`**-file) and specify plotting parameters. For comparison with figure 3.15 select an energy-range from -13 to 8 eV.

- Calculate Bandstructure (**`x spaghetti`**).
- Preview Bandstructure (needs **ghostscript installed**).
- Reset unit to 4 in **`TiC.in1`**, to make sure that the "tetrahedral" k-mesh is used again for subsequent calculations.

If you want to preview the bandstructure, the program **ghostview** (public domain) must be installed on your computer. You can compare your calculated bandstructure with figure 3.15.

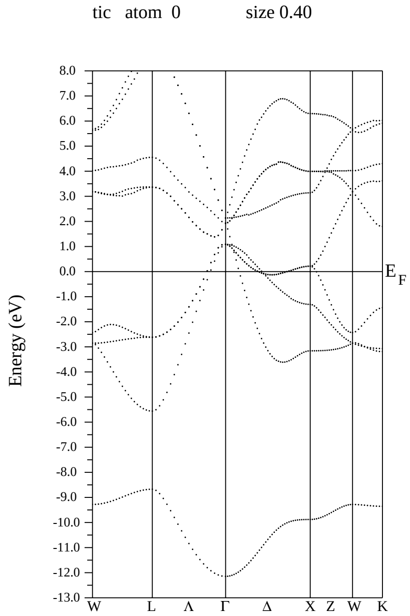

Figure 3.15: Bandstructure of TiC

3.11.5 Bandstructure with band character plotting

Select "*Bandstructure (with band character)*" from the "*Tasks*" menu and click on the buttons one by one:

- Insert k-points and change unit to 5 in **`TiC.in1`** (see previous section)
- Calculate Eigenvalues (**`x lapw1`**)
- Edit **`TiC.in2`**: Change FERMI-method (efmod) from TETRA to ROOT
- Calculate partial charges (**`x lapw2 -qtl`**)
  Note: You have to calculate the partial charges for the new special k-mesh specified above and cannot use the partial charges from the DOS calculation.
- Edit **`TiC.insp`**: insert the correct Fermi energy and specify plotting parameters. For comparison with figure 3.16 select an energy-range from -13 to 8 eV, and set jatom=1, jtype=6 and jsize=0.2 to produce a character plot of the Ti t2g-like character bands. Also check the number of bands in the **`TiC.qtl`** file to set the number of bands for character plotting accordingly.
- Calculate Bandstructure (**`x spaghetti`**)
- Preview Bandstructure
- Reset the changes made in **`TiC.in1`** and **`TiC.in2`**. (Do not forget this point, you will run into troubles later.)

You can compare your results with figure 3.16.

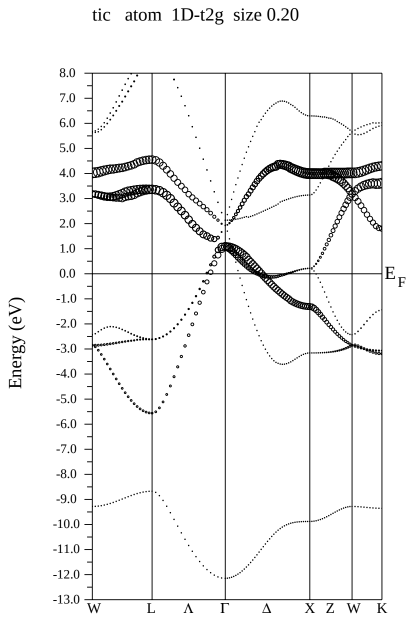

Figure 3.16: Bandstructure of TiC, showing t2g-character bands of Ti in character plotting mode

3.11.6 Volume Optimization

Select "*Optimize (V,c/a)*" from the "*Execution*" menu. Setup the shell script **`optimize.job`** script using **`x optimize`** and volume variations of -10, -5, 0, +5 and +10%. Edit this file and uncomment the **`x dstart`** line (remove the "#" character). Then run the **`optimize.job`**. When the job has finished, you should click on *Analyze results* and then preview the energy curve. Set 136.77 a.u. for the experimental V_0.

You should get an energy curve as in figure 3.17. On the screen you will find the fitting parameters for the "equation of states" (Murnaghan and the EOS2 equation, see sec. 9.6). This information is also written to **`TiC.outputeos`**.

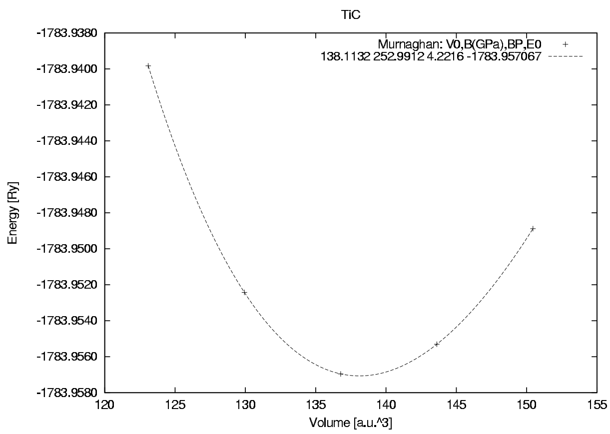

Figure 3.17: Energy vs. volume curve for TiC

3.12 Setting up a new case

In order to setup a new case you need at least the following information:

- The lattice parameters (in Bohr or Ångstroms) and angles,
- the lattice type (primitive, face-centered, hexagonal,...) or spacegroup,
- the position of all equivalent and inequivalent atoms in fractions of the unit cell.
- Alternatively with the new **StructGen**$^{\mathbf{TM}}$ you can specify the spacegroup and only the inequivalent positions. The equivalent ones will be generated automatically.

Usually this information can be collected from the "International Tables of Crystallography" once you know the space group, the Wyckoff position and the internal free coordinates.

3.12.1 Manually setting up a new case

Usually for a new "case" the input is not created from scratch, but one uses the **`struct`** and **`inst`** files from a similar case as pattern. Change into the **`lapw`** subdirectory and proceed as follows:

```
mkdir case_new
cd case_new
cp ../case_old/case_old.inst case_new.inst
cp ../case_old/case_old.struct case_new.struct
```

Now edit **`case_new.struct`** (see section 4.3) and **`case_new.inst`** (section 6.4) as necessary. Alternatively you can use **`instgen_lapw`** to generate **`case_new.inst`**.

3.12.2 Setting up a new case using w2web

Use the menu *Session Mgmt.* ⇓ *change session* of **w2web** to create a new session (enter the name of the new session and click on "*Create*"). Then you should also create a new directory and "select" it..

When you select "*Execution* ⇓ **StructGen**$^{\mathbf{TM}}$", a template file will be copied to **`case.struct`**. To create the new case using the **StructGen**$^{\mathbf{TM}}$ you simply specify cell parameters, positions of atoms, etc. When you "*save file and clean up*" the new **`case.struct`** file and the **`case.inst`** file are created automatically.

For more information on the **StructGen**$^{\mathbf{TM}}$ refer to page 136.

Part II

Detailed description of the files and programs of the WIEN2k package

4 File structure and program flow

Contents

(for naming conventions see section 3.1)

4.1 Flow of input and output files

Each program is started with (at least) one command line argument, e.g.

```
programX programX.def
```

in which the arguments specifies a filename, in which FORTRAN I/O units are connected to unix filenames. (See examples at specific programs). These "**def**"-files are generated automatically when the standard **WIEN2k** scripts **x**, **init_lapw** or **run_lapw** are used, but may be tailored by hand for special applications. Using the option

```
x program -d
```

a def-file can be created without running the program. In addition each program reads/writes the following files:

case.struct a "master" input file, which is described below (Section 4.3)
case.inX a specific input file, where X labels the program (see def-files for each program in chapter 6).
case.outputX an output file

The programs of the SCF cycle (see figure 4.1) write the following files:

case.scfX a file containing only the most significant output (see description below).
program.error error report file, should be empty after successful completion of a program (see chapter 6)

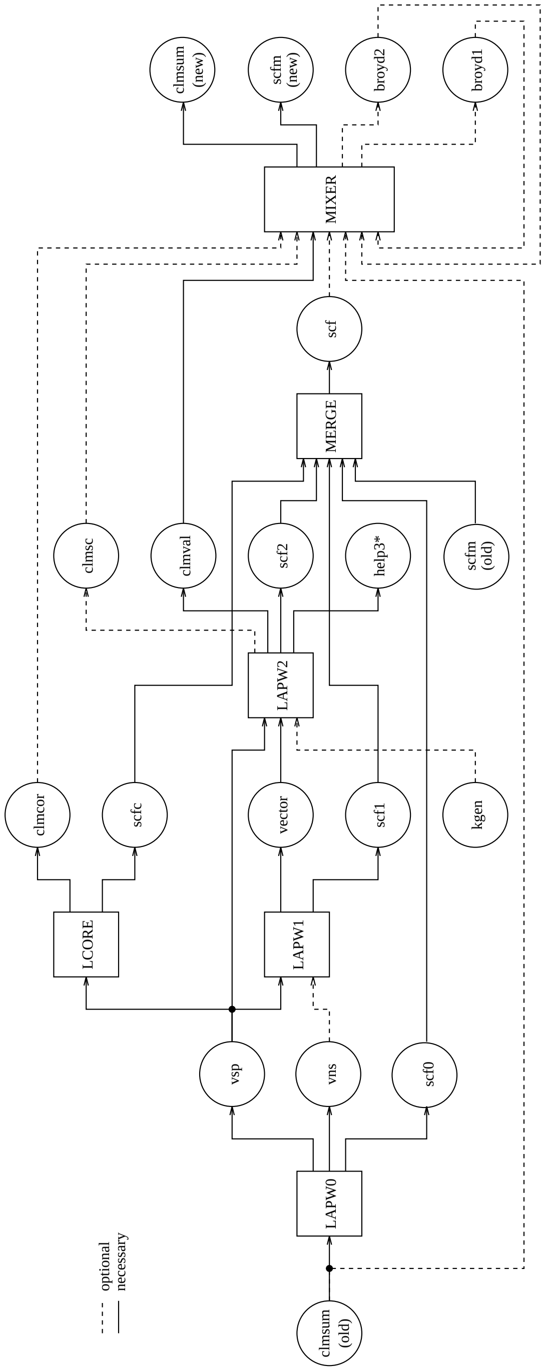

Figure 4.1: Data flow during a SCF cycle (programX.def, case.struct, case.inX, case.outputX and optional files are omitted)

The following tables describe input and output files for the initialization programs **`nn`**, **`sgroup`**, **`symmetry`**, **`lstart`**, **`kgen`**, **`dstart`** (table 4.1), the utility programs **`tetra`**, **`irrep`**, **`spaghetti`**, **`aim`**, **`lapw7`**, **`elnes`**, **`lapw3`**, **`lapw5`**, **`xspec`**, **`optic`**, **`joint`**, **`kram`**, **`optimize`** and **`mini`** (table 4.2) as well as for a SCF cycle of a non-spin-polarized case (table 4.2). Optional input and output files are used only if present in the respective case subdirectory or requested/generated by an input switch. The connection between FORTRAN units and filenames are defined in the respective **`programX.def`** files. The data flow is illustrated in Fig. 4.1.

program	needs		generates	
	necessary	optional	necessary	optional
NN	nn.def case.struct		case.outputnn	case.struct_nn
SGROUP	case.struct		case.outputsgroup	case.struct_st
SYMMETRY	symmetry.def case.struct	case.in2_st	case.outputs case.in2_st	case.struct_sgroup
LSTART	lstart.def case.struct case.inst		case.outputst case.rsp case.in0_st case.in1_st case.in2_st case.inc_st case.inm_st case.inm_restart	case.rspup case.rspdn case.vsp_st case.vspdn_st case.sigma
KGEN	kgen.def case.struct		case.outputkgen case.klist case.kgen	
DSTART	dstart.def case.struct case.rsp(up) case.in1 case.in2		case.outputd case.clmsum(up) dstart.error	

Table 4.1: Input and output files of init programs

program	needs		generates	
	necessary	optional	necessary	optional
SPAGHETTI	spaghetti.def case.insp case.struct case.output1	case.qtl	case.spaghetti_ps case.outputsp	case.spaghetti_ene
TETRA	tetra.def case.int case.qtl case.kgen		case.outputt case.dos1(2,3) case.dos1ev(1,2,3)	
LAPW3	lapw3.def case.struct case.in2 case.clmsum		case.output3 case.rho case.clmsum	
LAPW5	lapw5.def case.struct case.in5 case.clmval	case.sigma	case.output5 case.rho	case.rho.oned
XSPEC	xspec.def case.inc case.int case.vsp case.struct case.qtl		case.outputx case.dos1ev case.xspec case.txspec case.m1 case.m2	case.coredens
OPTIC	optic.def case.struct case.inop case.vsp case.vector		case.outputop case.outmat	
JOINT	joint.def case.injoint case.struct		case.outputjoint case.joint	case.sigma_intra case.intra

continued on next page

	case.kgen case.weight case.outmat			
KRAM	kram.def case.inkram case.joint		case.epsilon case.sigmak	case.eloss case.sumrules
OPTIMIZE	case.struct	case_initial.struct	optimize.job	case_vol_xxxxx.struct case_c/a_xxxxx.struct
MINI	mini.def case.inM case.finM case.scf case.struct	case.scf_mini case.tmpM case.clmsum case.clmhist	case.outputM case.tmpM1 case.scf_mini1 case.struct1	case.clmsum_inter
IRREP	case.struct case.vector		case.outputirrep case.irrep	
AIM	case.struct case.clmsum case.inaim		case.outputaim case.surf	case.crit
LAPW7	case.struct case.vector case.in7 case.vsp		case.output7 case.grid case.psink	case.abc
QTL	case.struct case.vector case.inq case.vsp		case.outputq case.qtl	

Table 4.2: Input and output files of utility programs

program	needs		generates	
	necessary	optional	necessary	optional
LAPW0	lapw0.def case.struct case.in0 case.clmsum	case.clmup/dn	case.output0 case.scf0 case.vsp(up/dn) case.vns(up/dn)	case.r2v case.vcoul
ORB	orb.def case.struct case.inorb case.dmat case.vsp	case.scf1 case.vorb_old	case.outputU case.scforb case.vorb orb.error	case.br1orb case.br2orb case.weigh
LAPW1	lapw1.def case.struct case.in1 case.vsp	case.vns case.klist	case.output1(s) case.scf1(s) case.vector(s) case.energy	case.nsh(s)
LAPWSO	lapwso.def case.struct case.inso case.vector case.vsp case.energy	 case.norm	 case.outputso case.scfso lapwso.error	 case.vectorso case.vectordum
LAPW2	lapw2.def case.struct case.in2(s) case.vector(s) case.vsp case.energy	case.kgen case.nsh(s) case.weight case.weigh	case.output2(s) case.scf2(s) case.clm[val|sc] case.help3*	case.qtl(s) case.weight case.weigh
LAPWDM	lapwdm.def case.struct case.indm case.vector case.vsp case.weigh case.energy	case.inso	case.outputdm case.scfdm case.dmat lapwdm.error	
SUMPARA	case.struct case.clmval	case.scf2p	case.outputsum case.clmval case.scf2	
LCORE	lcore.def case.struct case.inc case.vsp	case.vns	case.outputc case.scfc case.clmcor lcore.error	case.corewf
After LCORE the **`case.scfX`** files are appended to **`case.scf`** and the				
continued on next page				

case.clmsum file is renamed to **case.clmsum_old** (see **run_lapw**)				
MIXER	mixer.def case.struct case.inm case.clmval	case.clmsum_old case.clmsc case.clmcor case.scf case.broyd1 case.broyd2	case.outputm case.scfm case.clmsum mixer.error	case.broyd1 case.broyd2
After MIXER the file **case.scfm** is appended to **case.scf**, so that after an iteration is completed, the two essential files are **case.clmsum** and **case.scf**.				

Table 4.3: Input and output files of main programs in an SCF cycle

4.2 Description of general input/output files

In the following section the content of the (non-trivial) output files is described:

case.broydX Contains the charge density of previous iterations if you use Broyden's method for mixing. They are removed when using **save_lapw**. They should be removed by hand when calculational parameters (RKMAX, kmesh, ...) have been changed, or the calculation crashed due to a too large mixing and are restarted by using a new density generated by dstart.

case.clmcor Contains the core charge density (as $\sigma(r) = 4\pi r^2 \rho(r)$ and has only a spherical part). In spin-polarized calculations two files case.clmcorup and case.clmcordn are used instead.

case.clmsc Contains the semi-core charge density in a 2-window calculation, which is no longer recommended. In spin-polarized calculations two files are used instead: **case.clmscup** and **case.clmscdn**.

case.clmsum Contains the total charge density in the lattice harmonics representation and as Fourier coefficients. (The LM=0,0 term is given as $\sigma(r) = 4\pi r^2 \rho(r)$, the others as $r^2 \rho_{LM}(r)$; suitable for generating electron density plots using **lapw5** when the TOT-switch is set, (see section 8.6). In spin-polarized calculations two additional files **case.clmup** and **case.clmdn** contain the spin densities. Generated by **dstart** or **mixer**.

case.clmval Contains the valence charge density as $r^2 \rho_{LM}(r)$; suitable for generating valence electron density plots using **lapw5** when the VAL-switch is set, (see 8.6). In spin-polarized calculations two files **case.clmvalup** and **case.clmvaldn** are used instead.

case.dmatup/dn Contains the density matrix generated by **lapwdm** for LDA+U or OP calculations.

case.dosX Contains the density of states (states/Ry) and corresponding energy (in Ry at the internal energy scale) generated by **tetra**. X can be 1-3. Additional files **case.dosXev** contain the DOS in (states/eV) and the energy in eV with respect to EF.

case.help3X Contains eigenvalues and partial charges for atom number X.

case.kgen This file contains the indices of the tetrahedra in terms of the list of k-points. It is used in **lapw2** (if EFMOD switch in **case.in2** is set to TETRA, see 7.5.3) and in **tetra**.

case.klist This file contains a list of k-points in the first BZ and represents a tetrahedral (special point) mesh. It is generated in **kgen** and can either be inserted into the **case.in1** file or used directly in **kgen**.

case.qtl Contains eigenvalues and corresponding partial charges (bandwise) in a form suitable for **tetra** and band structure plots with "band character". The decomposition of these charges is controlled by ISPLIT in case.struct.

case.rho Contains the electron densities on a grid in a specified plane generated by **lapw5**. This file can be used as input for your favorite contour or 3D plotting program.

case.rsp Contains the atomic densities generated by **lstart**. They are used by **dstart** to generate a first crystalline density (**case.clmsum**).

case.r2v Contains the exchange potential (in the lattice harmonics representation as $r^2 * V_{LM}(r)$ and as Fourier coefficients) in a form suitable for plotting with **lapw5**.

case.scf_mini Contains the last scf-iteration of each individual time (geometry) step during a structural minimization using **mini**. Thus this file contains a complete history of properties (energy, forces, positions) during a structural minimization.

case.sigma Contains the atomic densities for those states with a "P" in **`case.inst`**. Generated in **`lstart`** and used for difference densities in **`lapw5`**.

case.spaghetti_ps A ps file with the energy bandstructure plot generated by **`spaghetti`**.

case.vcoul Contains the Coulomb and the total potential (in the lattice harmonics representation as $r^2 * V_{LM}(r)$ and as Fourier coefficients) in a form suitable for plotting with **`lapw5`** (split the file manually to select Coulomb or total potential).

case.vector Binary file, contains the eigenvalues and eigenvectors of all k-points calculated in **`lapw1`**. In spin-polarized calculations two files **`case.vectorup`** and **`case.vectordn`** are used instead. **`lapwso`** generates **`case.vectorso`**.

case.energy Contains the eigenvalues of all k-points calculated in **`lapw1`**. In spin-polarized calculations two files **`case.vectorup`** and **`case.vectordn`** are used instead. **`lapwso`** generates **`case.energyso`**.

case.vns Contains the non-spherical part of the total potential V. Inside the sphere the radial coefficients of the lattice harmonics representation are listed (for L greater than 0), while for the interstitial region the Fourier coefficients are given (see equ. (2.10)). In spin-polarized calculations two files **`case.vnsup`** and **`case.vnsdn`** are used instead.

case.vorbup/dn Contains the orbital dependent part of the potential in LDA+U or OP calculations. Generated in **`orb`**, used in **`lapw1`**.

case.vsp Contains the spherical part of the total potential V stored as $r * V$ (thus the first values should be close to $-2 * Z$). In spin-polarized calculations two files **`case.vspup`** and **`case.vspdn`** are used instead.

4.3 The "master input" file case.struct

The file **`case.struct`** defines the structure and is the main input file used in all programs. We provide several examples in the subdirectory

`example_struct_file`

If you are using the "*Struct Generator*" from the graphical user interface **w2web**, you don't have to bother with this file directly! However, the description of the fields of the input mask can be found here.

Note: If you are changing this file manually, please note that this is a formatted file and the proper column positions of the characters are important! Use REPLACE instead of DELETE and INSERT during edit!

We start the description of this file with an abridged example for rutile TiO_2 (adding line numbers):

```
--------------------- top of file ---------------------line #
Titaniumdioxide TiO2 (rutile):  u=0.305                      1
P   LATTICE,NONEQUIV. ATOMS: 2                               2
MODE OF CALC=RELA                                            3
 8.6817500 8.6817500 5.5916100 90.       90.       90.       4
ATOM= -1: X= 0.0000000 Y= 0.0000000 Z= 0.0000000             5
         MULT= 2          ISPLIT= 8                          6
ATOM= -1: X= 0.5000000 Y= 0.5000000 Z= 0.5000000
Titanium   NPT=  781  R0=.000022391 RMT=2.00000000   Z:22.0 7
LOCAL ROT MATRIX:    -.7071068 0.7071068 0.0000000           8
                     0.7071068 0.7071068 0.0000000           9
                     0.0000000 0.0000000 1.0000000          10
ATOM= -2: X= 0.3050000 Y= 0.3050000 Z= 0.0000000
         MULT= 4          ISPLIT= 8
ATOM= -2: X= 0.6950000 Y= 0.6950000 Z= 0.0000000
ATOM= -2: X= 0.8050000 Y= 0.1950000 Z= 0.5000000
ATOM= -2: X= 0.1950000 Y= 0.8050000 Z= 0.5000000
Oxygen     NPT=  781  R0=.000017913 RMT=1.60000000   Z: 8.0
LOCAL ROT MATRIX:    0.0000000 -.7071068 0.7071068
                     0.0000000 0.7071068 0.7071068
                     1.0000000 0.0000000 0.0000000
  16 SYMMETRY OPERATIONS:                                   11
 1 0 0  0.00                                                12
```

```
 0 1 0  0.00                                               13
 0 0 1  0.00                                               14
      1                                                    15
 1 0 0  0.00
 0 1 0  0.00
 0 0-1  0.00
      2
  ........
     15
 0 1 0  0.50
-1 0 0  0.50
 0 0 1  0.50
     16
----------------- bottom of file --------------------------
```

Interpretive comments on this file are as follows.

P	all primitive lattices except hexagonal (trigonal lattice is also supported)	[a sin(γ), a cos(γ), 0], [0, b, 0], [0, 0, c]
F	face-centered	[a/2, b/2, 0], [a/2, 0, c/2], [0, b/2, c/2]
B	body-centered	[a/2, -b/2, c/2],[a/2, b/2, -c/2], [-a/2, b/2, c/2]
CXY	c-base-centered (orthorhombic only)	[a/2, -b/2, 0], [a/2, b/2, 0], [0, 0, c]
CYZ	a-base-centered (orthorhombic only)	[a, 0, 0], [0, -b/2, c/2], [0, b/2, c/2]
CXZ	b-base-centered (orthorh. and monoclinic)	[a sin(γ)/2, a cos(γ)/2, -c/2], [0, b, 0], [a sin(γ)/2, a cos(γ)/2, c/2]
R	rhombohedral	[a/$\sqrt{3}$/2, -a/2, c/3],[a/$\sqrt{3}$/2, a/2, c/3],[-a/$\sqrt{3}$, 0, c/3]
H	hexagonal	[$\sqrt{3}$a/2, -a/2, 0],[0, a, 0],[0, 0, c]

Table 4.4: Lattice type, description and bravais matrix used in **WIEN2k**

line 1: format (A80)
title (compound)
line 2: format (A4,24X,I2)
lattice type, NAT

lattice type	as defined in table 4.4. For definitions of the triclinic lattice see **`SRC_nn/dirlat.f`**
NAT	number of inequivalent atoms in the unit cell

line 3: format (13X,A4)
mode

RELA	fully relativistic core and scalar relativistic valence
NREL	non-relativistic calculation

line 4: format (6F10.6)
a, b, c, α, β, γ

a, b, c	unit cell parameters (in a.u., 1 a.u. = 0.529177 Å). In face- or body-centered structures the non-primitive (cubic) lattice constant, for rhombohedral (R) lattices the hexagonal lattice constants must be specified. (The following may help you to convert between hexagonal and rhombohedral specifications: $a_{hex} = 2cos(\frac{\pi-\alpha_{rhomb}}{2})a_{rhomb}$ $c_{hex} = 3\sqrt{a_{rhomb}^2 - \frac{1}{3}a_{hex}^2}$ and (for fcc-like lattices) $a_{rhomb} = a_{cubic}/\sqrt{2}$
α, β, γ	angles between unit axis (if omitted, 90° is set as default). Set it only for P and CXZ lattices

line 5: format (5X,I3,4X,F10.8,3X,F10.8,3X,F10.8)
atom-index, x, y, z

atom-index	running index for inequivalent atoms positive in case of cubic symmetry negative for non-cubic symmetry this is set automatically using **symmetry**
x,y,z	position of atom in internal units, i.e. as **positive** fractions of unit cell parameters. ($0 \le x \le 1$; the positions in the unit cell are consistent with the convention used in the International Tables of Crystallography 64. In face- (body-) centered structures only one of four (two) atoms must be given, eg. in Fm3m position 8c is specified with 0.25, 0.25, 0.25 and .75, 0.75, 0.75). For R lattice use rhombohedral coordinates. (To convert from hexagonal into rhombohedral coordinates use the auxiliary program **hex2rhomb**, which can be found in "*Run Programs* ⇩ *Other Goodies*" from **w2web**):

$$\vec{X}_{ortho} = \vec{X}_{hex} \begin{pmatrix} 0 & 1 & 0 \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\vec{X}_{rhomb} = \vec{X}_{ortho} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{-2}{\sqrt{3}} \\ -1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

line 6: format (15X,I2,17X,I2)
multiplicity, isplit

multiplicity		number of equivalent atoms of this kind
isplit		this is just an output-option and is used to specify the decomposition of the lm-like charges into irreducible representations, useful for interpretation in case.qtl). This parameter is automatically set by **symmetry**:
	0	no split of l-like charge
	1	p-z, (p-x, p-y) e.g.:hcp
	2	e-g, t-2g of d-electrons e.g.:cubic
	3	d-z2, (d-xy,d-x2y2), (d-xz,dyz) e.g.:hcp
	4	combining option 1 and 3 e.g.:hcp
	5	all d symmetries separate
	6	all p symmetries separate
	8	combining option 5 and 6
	-2	d-z2, d-x2y2, d-xy, (d-xz,d-yz)
	88	split lm like charges (for **telnes**)
	99	calculate cross-terms (for **telnes**)

>>>: **line 5** must now be repeated MULT-1 times for the other positions of each equivalent atom according to the Wyckoff position in the "International Tables of Crystallography".

line 7: format (A10,5X,I5,5X,F10.8,5X,F10.5,5X,F5.2)
name of atom, NPT, R0, RMT, Z

name of atom	Use the chemical symbol. Positions 3-10 for further labeling of nonequivalent atoms (use a number in position 3)
NPT	number of radial mesh points (381 gives a good mesh for LDA calculations, but for GGA twice as many points are recommended; *always use an **odd** number of mesh points!*) the radial mesh is given on a logarithmic scale: $r(n) = R_0 * e^{[(n-1)*DX]}$
R0	first radial mesh point (typically between 0.0005 and 0.00005)

RMT	atomic sphere radius (muffin-tin radius), can easily be estimated after running NN (see 6.1). The following guidelines will be given here: Choose spheres as large as possible as this will save MUCH computer time. But: Use identical radii within a series of calculations (i.e. when you want to compare total energies) — therefore consider first how close the atoms may possibly come later on (volume or geometry optimization); do NOT make the spheres too different (even when the geometry would permit it), instead use the largest spheres for f-electron atoms, 10-20 % smaller ones for d-elements and again 10-20 % smaller for sp-elements; H is a special case, you may choose it much smaller (e.g. 0.6 and 1.2 for H and C) and systems containing H need a much smaller RKMAX value (3-5) in **`case.in1`**.
Z	atomic number

line 8-10: format (20X,3F10.7)

ROTLOC	local rotation matrix (always in an orthogonal coordinate system). Transforms the global coordinate system (of the unit cell) into the local at the given atomic site as required by point group symmetry (see in the INPUT-Section 7.5.3 of LAPW2). SYMMETRY calculates the point group symmetry and determines ROTLOC automatically. Note, that a proper ROTLOC is required, if the LM values generated by SYMMETRY are used. A more detailed description with several examples is given in the appendix A and sec. 10.3

>>>: **lines 5 thru 10** must be repeated for each inequivalent atom
line 11: format (I4)

nsym	number of symmetry operations of space group (see International Tables of Crystallography 64) If nsym is set to zero, the symmetry operations will be generated automatically by SYMMETRY.

line 12-14: format (3I2,F10.7)
matrix, tau (as listed in the International Tables of Crystallography 64)

matrix	matrix representation of (space group) symmetry operation
tau	non-primitive translation vector

line 15: format (I8)
index of symmetry operation specified above
>>>: **lines 12 thru 15** must be repeated for all other symmetry operations
(the complete list is contained in sample inputs)

4.4 The "history" file case.scf

During the self-consistent field (SCF) cycle the essential data are appended to the file **`case.scf`** in order to generate a summary of previous iterations. For an easier retrieval of certain quantities the essential lines are labeled with **:LABEL:**, which can be used to monitor these quantities during self-consistency as explained below. The most important **:LABELs** are

:ENE	total energy (Ry)
:DIS	charge distance between last 2 iterations ($\int \vert\rho_n - \rho_{n-1}\vert dr$). Good convergence criteria.
:FER	Fermi energy
:FORxx	force on atom xx in mRy/bohr (in the local (for each atom) carthesian coordinate system)
:FGLxx	force on atom xx in mRy/bohr (in the global coordinate system of the unit cell (in the same way as the atomic positions are specified))
:DTOxx	total difference charge density for atom xx between last 2 iterations

:CTOxx	total charge in sphere xx (mixed after MIXER)
:NTOxx	total charge in sphere xx (new (not mixed) from LAPW2+LCORE)
:QTLxx	partial charges in sphere xx
:EPLxx	l-like partial charges and "mean energies" in lower (semicore) energy window for atom xx. Used as energy parameters in case.in1 for next iteration
:EPHxx	l-like partial charges and "mean energies" in higher (valence) energy window for atom xx. Used as energy parameters in **case.in1** for next iteration
:EFGxx	Electric field gradient (EFG) V_{zz} for atom xx
:ETAxx	Asymmetry parameter of EFG for atom xx
:RTOxx	Density for atom xx at the nucleus (first radial mesh point)
:VZERO	Gives the total, Coulomb and xc-potential at z=0 and z=0.5 (meaningfull only for slab calculations)

To check to which type of calculation a scf file corresponds use:

:POT	Exchange-correlation potential used in this calculation
:LAT	Lattice parameters in this calculation
:VOL	Volume of the unit cell
:POSxx	Atomic positions for atom xx (as in **case.struct**)
:RKM	Actual matrix size and resulting RKmax
:NEC	normalization check of electronic charge densities. If a significant amount of electrons is missing, one might have core states, whose charge density is not completely confined within the respective atomic sphere. In such a case the corresponding states should be treated as band states (using LOs).

For spin-polarized calculations:

:MMTOT	Total spin magnetic moment/cell
:MMIxx	Spin magnetic moment of atom xx. Note, that this value depends on RMT.
:CUPxx	spin-up charge (mixed) in sphere xx
:CDNxx	spin-dn charge (mixed) in sphere xx
:NUPxx	spin-up charge (new, from lapw2+lcore) in sphere xx
:NDNxx	spin-dn charge (new, from lapw2+lcore) in sphere xx
:ORBxx	Orbital magnetic moment of atom xx (needs SO calculations and LAPWDM).
:HFFxx	Hyperfine field of atom xx (in kGauss).

One can monitor the energy eigenvalues (listed for the first k-point only), the Fermi-energy or the total energy. Often the electronic charges per atom reflect the convergence. Charge transfer between the various atomic spheres is a typical process during the SCF cycles: large oscillations should be avoided by using a smaller mixing parameter; monotonic changes in one direction suggest a larger mixing parameter.

In spin-polarized calculations the magnetic moment per atomic site is an additional crucial quantity which could be used as convergence criterion.

If a system has electric field gradients and one is interested in that quantity, one should monitor the EFGs, because these are very sensitive quantities.

It is best to monitor several quantities, because often one quantity is converged, while another still changes from iteration to iteration. The script **run_lapw** has three different convergence criteria built in, namely the total energy, the atomic forces and the charge distance (see 5.1.2, 5.1.3).

We recommend the use of UNIX commands like :

grep :ENE case.scf or use "Analysis" from **w2web**

for monitoring such quantities.

You may define an **alias** for this (see sec. 11.2), and a csh-script **`grepline_lapw`** is also available to get a quantity from several scf-files simultaneously (sec. 5.2.9 and 5.3).

4.5 Flow of programs

The **WIEN2k** package consists of several independent programs which are linked via C-SHELL SCRIPTS described below.

The flow and usage of the different programs is illustrated in the following diagram (Fig. 4.2):

The initialization consists of running a series of small auxiliary programs, which generates the inputs for the main programs. One starts in the respective **`case/`** subdirectory and defines the structure in **`case.struct`** (see 4.3). The initialization can be invoked by the script **`init_lapw`** (see sec. 3.7 and 5.1.2), and consists of running:

NN a program which lists the nearest neighbor distances up to a specified limit (defined by a distance factor f) and thus helps to determine the atomic sphere radii. In addition it is a very usefull additional check of your **`case.struct`** file (equivalency of atoms)

SGROUP determines the spacegroup of the structure defined in your **`case.struct`** file.

SYMMETRY generates from a raw case.struct file the space group symmetry operations, determines the point group of the individual atomic sites, generates the LM expansion for the lattice harmonics and determines the local rotation matrices.

LSTART generates free atomic densities and determines how the different orbitals are treated in the band structure calculations (i.e. as core or band states, with or without local orbitals,. . .).

KGEN generates a k-mesh in the irreducible part of the BZ.

DSTART generates a starting density for the scf cycle by a superposition of atomic densities generated in LSTART.

Then a self-consistency cycle is initiated and repeated until convergence criteria are met (see 3.8 and 5.1.3). This cycle can be invoked with a script **`run_lapw`**, and consists of the following steps:

LAPW0 (POTENTIAL) generates potential from density

LAPW1 (BANDS) calculates valence bands (eigenvalues and eigenvectors)

LAPW2 (RHO) computes valence densities from eigenvectors

LCORE computes core states and densities

MIXER mixes input and output densities

4.5.1 Core, semi-core and valence states

In many cases it is desirable to distinguish three types of electronic states, namely core, semi-core and valence states. For example titanium has core ($1s$, $2s$, $2p$), semi-core ($3s$, $3p$) and valence ($3d$, $4s$, $4p$) states. In our definition **core states** are only those whose charge is entirely confined inside the corresponding atomic sphere. They are deep in energy, e.g., more than 7-10 Ry below the Fermi energy. **Semi-core states** lie high enough in energy (between about 1 and 7 Ry below the Fermi energy), so that their charge is no longer completely confined inside the atomic sphere, but has a few percent outside the sphere. **Valence states** are energetically the highest (occupied) states and always have a significant amount of charge outside the spheres.

The energy cut-off specified in **`lstart`** during **`init_lapw`** (usually -6.0 Ry) defines the separation into core- and band-states (the latter contain both, semicore and valence). If a system has atoms with semi-core states, then the best way to treat them is with "local orbitals", an extension of the usual LAPW basis. An input for such a basis set will be generated automatically. (Additional LOs can also be used for valence states which have a strong variation of their radial wavefunctions with energy (e.g. d states in TM compounds) to improve the quality of the basis set, i.e. to go beyond the simple linearization).

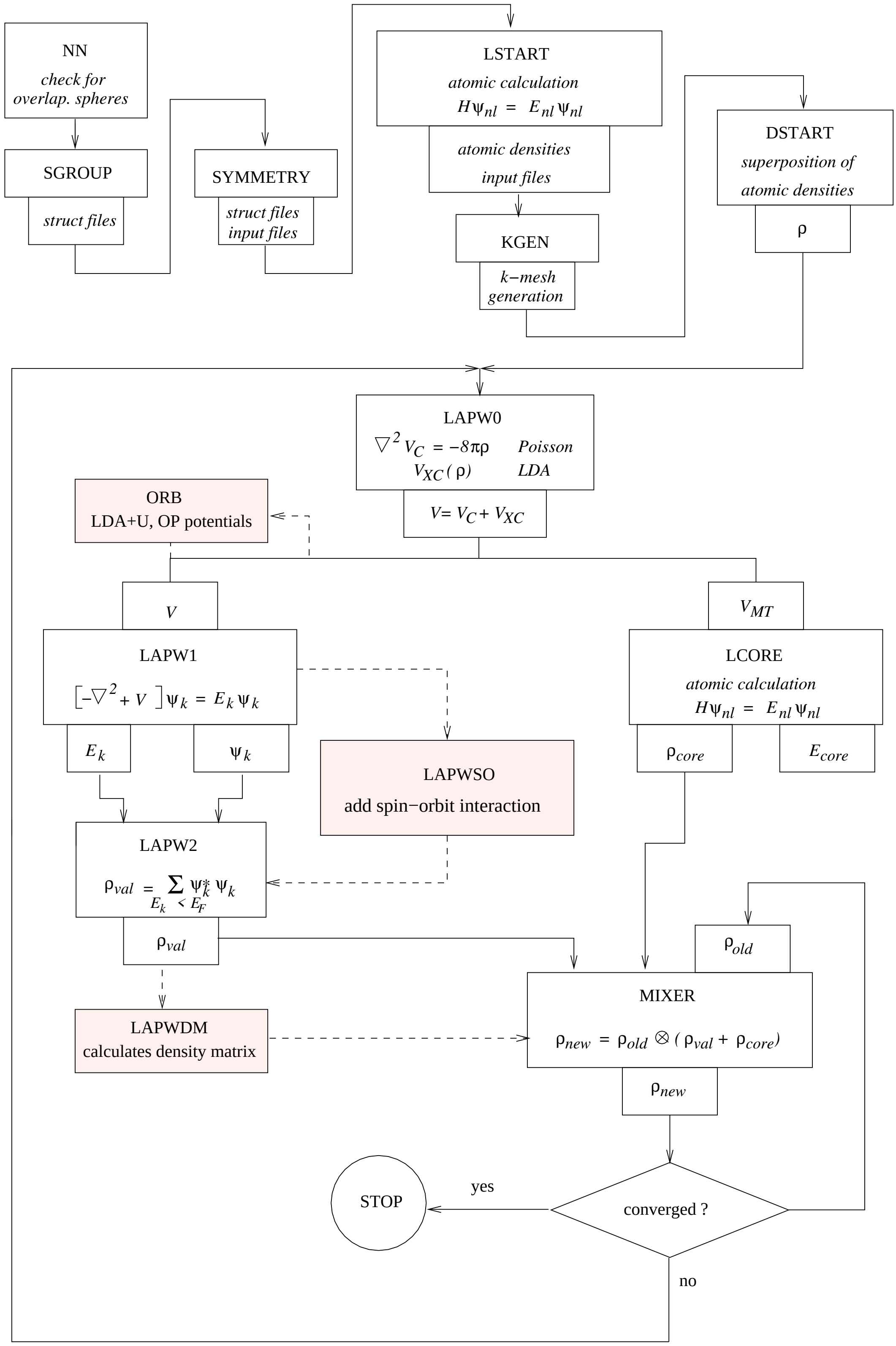

Figure 4.2: Program flow in **WIEN2k**

4.5.2 Spin-polarized calculation

For magnetic systems spin-polarized calculations can be performed. In such a case some steps are done for spin-up and spin-down electrons separately and the script **runsp_lapw** consists of the following steps:

LAPW0 (POTENTIAL) generates potential from density
LAPW1 -up (BANDS) calculates valence bands for spin-up electrons
LAPW1 -dn (BANDS) calculates valence bands for spin-down electrons
LAPW2 -up (RHO) computes valence densities for spin-up electrons
LAPW2 -dn (RHO) computes valence densities for spin-down electrons
LCORE -up computes core states and densities for spin-up electrons
LCORE -dn computes core states and densities for spin-down electrons
MIXER mixes input and output densities

The use of spin-polarized calculations is illustrated for fcc Ni (section 10.2), one of the test cases provided in the **WIEN2k** package.

4.5.3 Fixed-spin-moment (FSM) calculations

Using the script **runfsm_lapw -m XX** it is possible to constrain the total spin magnetic moment per unit cell to a fixed value XX and thus force a particular ferromagnetic solution (which may not correspond to the equillibrium). This is particularly useful for systems with several metastable (non-) magnetic solutions, where conventional spin-polarized calculation would not converge or the solution may depend on the starting density. Additional SO-interaction is not supported at the moment.

4.5.4 Antiferromagnetic (AFM) calculations

Several considerations are necessary, when you want to perform an AFM calculation.

- First you have to construct a unit cell which allows the desired AF ordering. For example for bcc Cr you must select a "P" lattice and specify both atoms, Cr1 at (0,0,0) and Cr2 at (.5,.5,.5), corresponding to a CsCl structure. Note, that it is important to label the two Cr atoms with "Cr1" and "Cr2", since only then the symmetry programs can detect that those atoms should be different (although they have the same Z).
- Edit **case.inst** and flip the spin of one of the AF atoms (i.e. invert the spin up and dn occupation numbers). In addition you must set a zero moment (identical spin up and dn occupations) for all "non-magnetic" atoms, otherwise AFMINPUT cannot determine the proper input for CLMCOPY.
- Run **init_lapw**. At the end AFMINPUT creates an input file for the program CLMCOPY. It tries to detect which spin-up density component corresponds to which spin-dn component.
- Run **runafm_lapw**. This script calls LAPW1 and LAPW2 only for spin-up but the corresponding spin-dn density is created by CLMCOPY according to the rules defined during initialization.
- Since AFMINPUT and CLMCOPY are not well tested for all possible structures or have special options, it is highly recommended that you save your work (**save_lapw**) and check the results by continuing with a regular **runsp_lapw**. If nothing changes (E-tot and other properties), then you are ok, otherwise make sure the scf calculation is well converged (-cc 0.0001 or better) and try to redefine the AFM-"rules" with another call of AFMINPUT (For numerical reasons you may have to assist the program and define two similar densities as equal or not.) or - better - by manual inspection of **case.clmup/dn**.

> *However, it is quite possible that AFMINPUT and/or CLMCOPY may not work properly for certain AFM structures and one needs to define a "special" case as implemented for AFM Rutile (MnF_2) or $FeCO_3$ structure.*

If **runafm_lapw** works, it saves you more than a factor of 2 in in computer time, since only spin-up is calculated and in addition the scf-convergence may be MUCH faster.

4.5.5 Spin-orbit interaction

You can add spin-orbit interaction in LAPWSO (called directly after LAPW1) using a second-variational method with the scalar-relativistic orbitals (from LAPW1) as basis. The number of eigenvalues will double since SO couples spin-up and dn states, so they are no longer separable. In addition, LOs with a "$p_{1/2}$" radial basis can be added. (Kunes et al. 2001)

To assist with the generation of the necessary input files and possible changes in symmetry, a script **initso_lapw** exists. For non-spinpolarized cases nothing particular must be taken into account and SO can be easily applied by running **run_lapw -so**. It will automatically use the complex version of LAPW2.

However, for spin-polarized cases, the SO interaction may change (lower) the symmetry depending on how you choose the direction of magnetization and care must be taken to get a proper setup. **initso_lapw** together with **symmetso** generates the proper symmetry.

Just a few hints what can happen:

- Suppose you have a cubic system and put the magnetization along [001]. This will create a tetragonal symmetry (and you can temporarely tell this to the initialization programs by changing the respective lattice parameter c to a tetragonal system).
- If you put the magnetization along [111], this creates most likely a rhombohedral (or hexagonal) symmetry. (Try to visualize this for a fcc lattice, XCRYSDEN is very usefull for this purpose).
- Symmetry operations can be classified into operations which invert the magnetization,others which leave it unchanged and some which do some arbitrary rotation. The program **symmetso** (part of **initso_lapw**) sorts these operations in the proper way.
- If you don't have inversion symmetry in the original structure, you must not "add inversion" in KGEN.

The recommended way to include SO in the calculations is to run a regular scf calculation first, save the results, initialize SO and run another scf cycle including SO:

- run[sp]_lapw
- save_lapw case_nrel
- initso_lapw
- run[sp]_lapw -so

4.5.6 Orbital potentials

In **WIEN2k**it is possible to go beyond standard LDA (GGA) and include orbital dependent potentials in methods like LDA+U or the "Orbital-Polarization", which are very usefull for strongly correlated systems.

To use these features you need to create input-files for LAPWDM and ORB (**case.indm, case.inorb**). You may copy a template from **SRC_templates**, but must modify it according to your needs. In particular you must select for which atoms and which orbitals (usually d-Orbitals of late transition metal atoms or f-orbitals for 4f/5f atoms) you want to add such a potential and also choose the proper U and J values for them. Once this is done, you can include this using the **-orb** switch. The density matrix (**case.dmatup/dn**) will be calculated after **lapw2** in **lapwdm**, it will be mixed in **mixer** (consistently with the "regular" charge density) and the orbital dependend potentials will be calculated on **orb** (after **lapw0**). Note, you must run spin-polarized in order to use orbital potentials.

▶ runsp_lapw -orb [-so]

Without SO, **case.vorbup/dn** will be considered in LAPW1(c). With SO, it will be applied in LAPWSO (and allows coupling of nondiagonal spin-terms).

5 Shell scripts for running programs

Contents

5.1 Job control (c-shell scripts)

In order to run **WIEN2k** several c-shell scripts are provided which link the individual programs to specific tasks.

All available (user-callable) commands have the ending **_lapw** so you can easily get a list of all commands using

ls $WIENROOT/*_lapw

in the directory of the **WIEN2k** executables. (*Note: all of the more important commands have a link to a short name omitting "_lapw".*) All these commands have at least one option, **-h**, which will print a small help indicating purpose and usage of this command.

5.1.1 Main execution script (x_lapw)

The main script, which executes a single program with automatic creation of the respective "def"-file is called **x_lapw** or **x** . You can call it with several switches to provide the proper file definitions in case of semicore, spin-polarized or complex calculations. All options are listed with the help switch

x -h or **x_lapw -h**

This script can also be run from **w2web** by using the "Single Programs" menu.

```
USAGE:  x PROGRAMNAME [flags]

PURPOSE:runs WIEN executables:                    afminput,aim,clmcopy,
        lcore,dstart,eosfit,init_xspec,hex2rhomb,irrep,joint,kgen,kram,
        lapw0,lapw1,lapw2,lapw3,lapw5,lapwdm,lapwso,lorentz,lstart,mini,
        mixer,nn,optic,optimize,orb,rhomb_in5,sgroup,spaghetti,sumpara,
```

```
        symmetry,tetra,txspec,xspec,elnes,telnes,filtvec,lapw7

FLAGS:
-f FILEHEAD ->  FILEHEAD for path of struct & input-files
-t/-T ->        suppress output of running time
-h/-H ->        help
-d    ->        create only the def-file
-up   ->        runs up-spin
-dn   ->        runs dn-spin
-sc   ->        runs semicore calculation
-c    ->        complex calculation (no inversion symmetry present)
-p    ->        run lapw1/2/so in parallel (needs .machines file)
-orb  ->        runs lapw1 with LDA+U/OP or B-ext correction
-it   ->        runs lapw1 with iterative diagonalization
-nohns->        runs lapw1 without HNS
-qtl  ->        calculates QTL in lapw2
-fermi->        calculates Fermi energy and weights in lapw2
-so   ->        runs lapw2 with def-file for spin-orbit calculation
-sel  ->        use reduced vector file in lapw7
USE: x -h PROGRAMNAME   for valid flags for a specific program
```

Note: To make use of a scratch file system, you may specify such a filesystem in the environment variable ***SCRATCH*** *(it may already have been set by your system administrator). However, you have to make sure that there is enough disk-space in the* ***SCRATCH*** *directory to hold your* ***case.vector**** *and* ***case.help**** *files.*

5.1.2 Job control for initialization (init_lapw)

In order to start a new calculation, one should make a new subdirectory and run all calculations from there. At the beginning one must provide two files (see 3), namely **case.struct** (see 4.3) and **case.inst** (see 6.4.3), then one runs a series of programs using **init_lapw**. This script is described briefly in chapter 4.5) and in detail in "Getting started" for the example TiC (see chapter 3). You can get help with switch -h. All actions of this script are logged in short in **:log** and in detail in the file **case.dayfile**, which also gives you a "restart" option when problems occurred. In order to run **init_lapw** starting from a specific point on, specify -s PROGRAM.

5.1.3 Job control for iteration (run_lapw or runsp_lapw)

In order to perform a complete SCF calculation, several types of scripts are provided with the distribution. For the specific flow of programs see chapter 4.5.

- For non-spinpolarized calculations use: **run_lapw**,
- for spin-polarized calculations use: **runsp_lapw**.
- for spin-polarized calculations but zero moment use: **runsp_c_lapw**.
- for antiferromagnetic calculations use: **runafm_lapw**
- for FSM (fixed-spin moment) calculations use: **runfsm_lapw**
- for a spin-polarized setup, where you want to constrain the moment to zero (e.g. for LDA+U calculations) use: **runsp_c_lapw**

Cases with/without inversion symmetry and with/without semicore or core states are handled automatically by these scripts. All activities of these scripts are logged in short in **:log** (appended) and in detail together with convergence information in **case.dayfile** (overwriting the old "dayfile"). You can always get help on its usage by invoking these scripts with the -h flag.

run_lapw -h

```
PROGRAM:        /zeus/lapw/WIEN2k/bin/run_lapw

PURPOSE:        running the nonmagnetic scf-cycle in WIEN
```

```
                to be called within the case-subdirectory
                has to be located in WIEN-executable directory

USAGE:          run_lapw [OPTIONS] [FLAGS]

OPTIONS:
-cc LIMIT ->    charge convercence LIMIT (0.0000)
-ec LIMIT ->    energy convercence LIMIT (0.0001 Ry)
-fc LIMIT ->    force  convercence LIMIT (0 mRy/a.u.)
-e PROGRAM ->   exit after PROGRAM ()
-i NUMBER ->    max. NUMBER (20) of iterations
-s PROGRAM ->   start with PROGRAM ()
-r NUMBER ->    restart after NUMBER (20) iterations (rm *.broyd*)
-nohns NUMBER ->do not use HNS for NUMBER iterations
-ql LIMIT ->    select LIMIT (0.05) as min.charge for E-L setting in new in1
-in1new N ->    use "new" in1 file after N iter (rewrite in1 using scf info)

FLAGS:
-h/-H ->        help
-I    ->        with initialization of in2-files to "TOT"
-p    ->        run k-points in parallel (needs .machine file [speed:name])
-so   ->        run SCF including spin-orbit coupling
-it   ->        use iterative diagonalization after first cycle
-it0  ->        use iterative diagonalization (also in first cycle)
-renorm->       start with mixer and renormalize density
-in1orig->      use case.in1_orig file (after a previous -in1new)

CONTROL FILES:
.stop           stop after SCF cycle
.fulldiag       force full diagonalization

ENVIRONMENT VARIBLES:
SCRATCH         directory  where vectors and help files should go
```

Calling **run_lapw** (after **init_lapw**) from the subdirectory **case** will perform up to 20 iterations (or what you specified with switch -i) unless convergence has been reached earlier. You can choose from three convergence criteria, -ec (the total energy convergence is the default and is set to 0.0001 Ry for at least 3 iterations), -fc (magnitude of force convergence for 3 iterations) or -cc (charge convergence, just the last iteration), but only one criterion can be specified. Be careful with these criteria, different systems will require quite different limits (e.g. fcc Li can be converged to μRy, $YBa_2Cu_3O_7$ only to 0.1 mRy). With -e PROGRAM you can run only part of one scf cycle (e.g. run lapw0, lapw1 and lapw2), with -s PROGRAM you can start at an arbitrary point in the scf cycle (e.g. after a previous cycle has crashed and you want to continue after fixing the problem) and continue to self-consistency. Before mixer is invoked, **case.clmsum** is copied to **case.clmsum_old**, and the final "important" files of the scf calculation are **case.clmsum** and **case.scf**.

Invoking

run_lapw -I -i 30 -fc 0.5

will first set in case.in2 the TOT-switch (if FOR was set) to save cpu time, then run up to 30 scf cycles till the force criterion of 0.5 mRy/a.u. is met (for 3 consecutive iterations). Then the calculation of all terms of the forces is activated (setting FOR in **case.in2**) for a final iteration.

The switch **-in1new N** preserves for N iteration the default **case.in1** file, thus using the "old" WIEN97 scheme to select the energy parameters. After the first N iterations **write_in1_lapw** is called and a new **case.in1** file is generated, where the energy parameters are set according to the :EPLxx and :EPHxx values of the last scf iteration and the **-ql** value (see sections 4.4 and 7.3). In this way you select the best possible energy-parameters and also additional LOs to improve the linearization may be generated automatically. Note, however, that this option is potentially dangerous if you have a "bad" last iteration (or large changes from one scf iteration to the next. The switch **-in1orig** can be used to switch back to the original ("old") scheme.

Parallelization is described in Sec. 5.4.

Iterative diagonalization, which can significantly save computer time in cases with "few electrons" and "large matrices (larger than 2000)", is described in Sec. 7.3. It needs the **case.vector** file from the previous scf-iteration and this file is copied to **case.vector.old** when the -it switch is set.

You can save computer time by performing the first scf-cycles without calculating the non-spherical matrix elements in lapw1. This option can be set for **N** iterations with the **-nohns N** switch.

If you have a previous scf-calculation and changed lattice parameters or positions (volume optimization or internal positions minimization), we recommend to use **-renorm** to renormalize the density prior to the first iteration.

For magnetic systems which are difficult to converge you can use the script **runfsm_lapw -m M** (see section 4.5.3) for the execution of fixed-spin moment (FSM) calculations.

5.2 Utility scripts

5.2.1 Save a calculation (save_lapw)

After self-consistency has been reached, the script

```
save_lapw head_of_save_filename
```

saves **case.clmsum**, **case.scf**, **case.dmat**, **case.vorb** and **case.struct** under the new name and removes the **case.broyd*** files. Now you are ready to modify structural parameters or input switches and rerun **run_lapw**, or calculate properties like charge densities (lapw5), total and partial DOS (tetra) or energy bandstructures (spaghetti).

For more complicated situations, where many parameters will be changed, we have extended **save_lapw** so that calculations can not only be saved under the **head_of_save_filename** but also a directory can be specified. If you use any of the possible switches (-a, -f, -d, -s) all input files will be saved as well (and can be restored using **restore_lapw**).

Options to **save_lapw** can be seen with

```
save_lapw -h
```

Currently the following options are supported

-h	help
-a	save **all** input files as well
-f	force save_lapw to overwrite previous saves
-d directory	save calculation in directory specified
-s	silent operation (no output)

5.2.2 Restoring a calculation (restore_lapw)

To restore a calculation the script **restore_lapw** can be used. This script restores the **struct**, **clmsum**, **vorb** and **dmat** files as well as all input files. **Note**: This script works only in conjunction with the new scheme of save_lapw, i.e. when you have saved a calculation in an extra directory.

Options to restore_lapw are:

-h	help
-f	force restore_lapw to overwrite previous files
-d directory	restore calculation from directory specified
-s	silent operation (no output)
-t	only test which files would be restored

5.2.3 Remove unnecessary files (clean_lapw)

Once a case has been completed you can clean up the directory with this command. Only the most important files (scf, clmsum, struct, input and some output files) are kept. It is very important to use this command when you have finished a case, since otherwise the large vector and helpXX files will quickly fill up all your disk space.

5.2.4 Generate case.inst (instgen_lapw)

This script generates **case.inst** from a **case.struct** file. It can be used instead of the "Structure-generator" of **w2web**. Note: the label "RMT" is necessary in **case.struct**.

5.2.5 scfmonitor_lapw

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

A plot of some quantities from the **case.scf** file as specified on the commandline is generated using the **analyse** program and GNUPLOT. This plot is updated in regular intervals.

For a description of how to use the script call it using

```
scfmonitor_lapw -h
```

The **scfmonitor** can be directly called from **w2web** using the default monitoring parameters (`ENE` and `DIS`)

In order to have a reasonable behavior of scfmonitor the GNUPLOT window should stay in background. This can be achieved by putting a line into your **.Xdefaults** file like:

gnuplot*raise: off

Note: It does not make sense to start MONITOR before the first cycle has finished because no ***case.scf*** *exists at this point.*

5.2.6 Check parallel execution (testpara_lapw)

testpara_lapw is a small script which helps you to determine an optimal selection for the file **.machines** for parallel calculations (see sec. 5.4).

5.2.7 Check parallel execution of lapw1 (testpara1_lapw)

testpara1_lapw is a small script which determines how far the execution of **lapw1para** has proceeded.

5.2.8 Check parallel execution of lapw2 (testpara2_lapw)

testpara2_lapw is a small script which determines how far the execution of **lapw2para** has proceeded.

5.2.9 grepline_lapw

Using

> **grepline_lapw :label 'filename*.scf' lines_for_tail** or
> **grepline :label 'filename*.scf' lines_for_tail**

you can get a list of a quantity "**:label**" (e.g. :ENE for the total energy) from several scf files at once.

5.2.10 initso_lapw

initso_lapw helps you to initialize the calculations for spin-orbit coupling. It creates all required input files (**case.inso, case.in2c**). In a spinpolarized case SO may reduce symmetry or equivalent atoms may become non-equivalent, and the script will help you to find proper symmetries and setup the respective input files. It is called using

> **initso_lapw** or
> **initso**

and you should *carefully* follow the instructions and explanations of the script.

5.2.11 oldvec2vec_lapw

oldvec2vec_lapw moves **case.vector.old** files to **case.vector**. This is useful if you used the iterative diagonalization (**run_lapw -it**) and now want to calculate qtl's,.... It also works automatically for the parallel case.

5.3 Structure optimization

5.3.1 Lattice parameters (Volume or c/a)

The auxilliary program **optimize** (**x optimize**) helps you to find the equilibrium volume or c/a ratio. It generates from an already existing **case.struct** or **case_initial.struct** a series of struct files with various volumes (c/a ratios) (depending on your input) and a shell-script **optimize.job** which looks similar to:

```
#!/bin/csh -f
 foreach i ( \
        tic_vol_-10.0  \
        tic_vol__-5.0  \
        tic_vol___0.0  \
        tic_vol___5.0  \
        tic_vol__10.0  \
 )
     cp  $i.struct tic.struct
 #    cp  $i.clmsum tic.clmsum
```

```
#    x dstart
#    run_lapw -ec 0.0001 -in1new 3 -in1orig -renorm
    run_lapw -ec 0.0001
    set stat = $status
    if ($stat) then
       echo "ERROR status in" $i
       exit 1
    endif
    save_lapw  $i
#    save_lapw  -f -d XXX $i
end
```

You may modify this script according to your needs (use runsp_lapw or even min_lapw, specify different convergence parameters, save into a directory to separate e.g. "gga" and "lda" results, activate the line "**x dstart**" or " **cp $i.clmsum case.clmsum**" to use a previously saved clmsum file, e.g. from a calculation with smaller RKmax, ...)

*Note: You must have a **case.clmsum** file (either from **init_lapw** or from a previous scf calculation) in order to run **optimize.job**.*

Using the script **grepline** (or the "*Analysis* ⇓ *Analyze multiple SCF-files*" menu of **w2web**) you get a summary of the total energy vs. volume (c/a). The file **case.analysis** can be used in **eplot_lapw** to find the minimum total energy and the equilibrium volume (c/a).

grepline :ENE '*.scf' 1 > case.analysis

Using such strategies also higher-dimensional optimizations (e.g. c/a ratio and volume) are possible in combination with the -d option of **save_lapw**.

For the determination of elastic constants see the description of ELAST in sec 8.13.

5.3.2 Minimization of internal parameters (min_lapw)

Most of the more complicated structures have free internal structural parameters, which can either be taken from experiment or optimized using the calculated **forces on the nuclei**. The shell script **min_lapw** is provided which, together with the program **mini**, automatically determines the equilibrium position of all individual atoms (obeying the symmetry constraints of a certain space group). Note, that **mini** requires an input file **case.inM** (see Sec. 8.14). When you detect large oszillations or too small changes of the forces during geometry optimization, you will have to decrease/increase the DELTAs in this file and restart using the -I switch (or rm case.tmpM). The last iteration of each geometry step is appended to **case.scf_mini**, so that this file contains the complete history of the minimization.

You can get help on its usage with:

min -h or **min_lapw -h**

```
PROGRAM:        min

USAGE:          min [OPTIONS]

OPTIONS:
-j JOB ->       job-file JOB (run_lapw -I -fc 1. -renorm )
-m ->           extract force-input and execute mini (without JOB) and exit
-mo ->          like -m but without copying of case.tmpM1 to case.tmpM
-h/-H ->        help
-NI/-I ->       without/with initialization of input-files
-i NUMBER ->    max. NUMBER (50) of structure changes
-s NUMBER ->    save_lapw after NUMBER of structure changes

CONTROL FILES:
.minstop        stop after next structure change
```

For instance for a spin-polarized case, which converges more difficultly, you would use:

min -j ''runsp_lapw -I -fc 1.0 -i 40''

5.4 Running programs in parallel mode

This section describes two methods for running **WIEN2k** on parallel computers. One method, parallelizing k-points over processors, utilizes c-shell scripts. This method works with all standard flavors of Unix without any special requirements. This parallelization was already available in **WIEN97** and is very efficient even on heterogeneous computing environments, e. g. on heterogeneous clusters of workstations, but also on dedicated parallel computers.

The other parallelization method, which comes new with **WIEN2k**, is based on fine grained methods. It is especially useful for large systems, if the required memory size is no longer available on a single computer or in situations where more processors than k-points are available.

The k-point parallelization uses a dynamic load balancing scheme and is therefore often preferred on heterogeneous compute environments and on networks of workstations or PCs, if interactive users contribute to the processors' work load. The fine grained parallelization method relies on static load balancing, therefore, in a heterogeneous environment, the slowest processor sets the pace. In many cases, a combination of both parallelization methods is favorable (always use k-point parallelism if you have more than 1 k-point).

5.4.1 k-Point Parallelization

Parts of the code are executed in parallel, namely **LAPW1, LAPWSO, LAPW2, LAPWDM,** and **OPTIC**. These are the numerically intensive parts of most calculations.

Parallelization is achieved on the k-point level by distributing subsets of the k-mesh to different processors and subsequent summation of the results. The implemented strategy can be used both on a multiprocessor architecture and on a heterogeneous (even multiplatform) network.

To make use of the k-point parallelization, make sure that your system meets the following requirements:

NFS: All files for the calculation must be accessible under the same name and path. Therefore you should set up your NFS mounts in such a way, that on all machines the path names are the same.

Remote login: rlogin or **ssh** to all machines to be used must be possible **without** specifying a password. Therefore you must either edit your **.rhosts** file to include all machines you intend to use (not necessary for a shared memory machine), or correctly set up the directories **.ssh** or **.ssh2**.
Unfortunately the command for launching a remote shell is platform dependent, and can be '**rsh**' or '**remsh**'. On some systems 'rsh' refers to the restricted shell. Please check these commands on your system and change the line

set remote = rsh or **remsh** or **ssh**

in the scripts **lapw1para_lapw**, **lapwsopara_lapw**, **lapw2para_lapw**, **lapwdmpara_lapw** and **opticpara_lapw** accordingly (In the following we use the shortcut without _lapw). This modification is done automatically by **siteconfig_lapw** during installation (see chapter 11).

5.4.2 Fine grained parallelization

Fine grained parallel versions are available for the programs **lapw0, lapw1,** and **lapw2**. This parallelization method is based on parallelization libraries, including MPI, ScaLapack, and PBlas. The required libraries are not included with **WIEN2k**. On parallel computers, however, they are usually installed. Otherwise, free versions of these libraries are available[1].

[1] http://www-unix.mcs.anl.gov/mpi/mpich,http://www.netlib.org/scalapack

The parallelization affects the naming scheme of the executable programs: the fine grained parallel versions of **lapw0/1/2** are called **lapw0_mpi**, **lapw1[c]_mpi**, and **lapw2[c]_mpi**. These programs are executed by calls to the local execution environments, as in the sequential case, by the scripts **x, lapw0para, lapw1para,** and **lapw2para**. On most computers this is done by calling **mpirun**.

5.4.3 How to use WIEN2k as a parallel program

To start the calculation in parallel, a switch must be set and an input file has to be prepared by the user.

- ▶ The switch **-p** switches on the parallelization in the scripts **x**, **run_lapw**, and **runsp_lapw**.
- ▶ In addition to this switch the file **.machines** has to be present in the current work directory. In this file the machine names on which the parallel processes should be launched, and their respective relative speeds must be specified.

If the **.machines** file does not exist, or if the **-p** switch is omitted, the serial versions of the programs are executed.

Generation of all necessary files, starting of the processes and summation of the results is done by the appropriate scripts **lapw1para**, **lapwsopara**,**lapwdmpara** and **lapw2para** (when using **-p**), and parallel programs **lapw0_mpi**, **lapw1_mpi**, and **lapw2_mpi** (when using fine grained parallelization has been selected in the **.machines** file).

5.4.4 The .machines file

The following **.machines** file describes a simple example. We assume to have 5 computers, (alpha, ... epsilon), where epsilon has 4, and delta and gamma 2 cpus. In addition, gamma, delta and epsilon are 3 times faster than alpha and beta.:

```
# This is a valid .machines file
#
granularity:1
1:alpha
1:beta
3:gamma:2 delta
3:delta:1 epsilon:4
residue:delta:2
lapw0:gamma:2 delta:2 epsilon:4
```

To each set of processors, defined by a single line in this file, a certain number of k-points is assigned, which are computed in parallel. In each line the weight (relative speed) and computers are specified in the following form:

```
weight:machine_name1:number1 machine_name2:number2 ...
```

where **weight** is an integer (e.g. a three times more powerful machine should have a three times higher weight). The name of the computer is **machine_name[1/2/...]**, and the number of processors to be used on these computers are **number[1/2/...]**. If there is only one processor on a given computer, the **:1** may be omitted. Empty lines are skipped, comment lines start with #.

Assuming there are 8 k-points to be distributed in the above example, they are distributed as follows. The computers **alpha** and **beta** get 1 each. Two processors of computer **gamma** and one processor of computer **delta** cooperate in a fine grained parallelization on the solution of 3 k-points, and one processor of computer **delta** plus four processors of computer **epsilon** cooperate on the solution of 3 k-points. If there were additional k-points, they would be calculated by the first processor (or set of processors) becoming available. With higher numbers of k-points, this method ensures dynamic load balancing. If a processor is busy doing other (e. g., interactive) work, the overall calculation will not stall, but most of its work will be done by other processors (or sets of processors using MPI). This is, however, not an implementation for fail safety: if a process does not terminate (e. g., due to shutdown of a computer) the calculation will never terminate. It is up to the user to handle with such hardware failures by modifying the **.machines** file and restarting the calculation at the appropriate point.

During the run of **lapw1para** the file **.processes** is generated. This file is used by **lapw2para** to determine which **case.vector*** to read.

By default **lapw1para** will generate approximately 3 vector-files per processor, if enough k-points are available for distribution. The factor 3 is called "granularity" and should allow some load balancing in heterogeneous environments. If during **siteconfig_lapw** a shared memory system was selected, "granularity" will be set by default to 1.

For performance reasons a different "granularity" can be specified, by adding the line

```
granularity:new_granularity
```

to the **.machines** file. In particular on shared memory machines it is advisable to add a "residue machine" to calculate the surplus (residual) k-points (given by the expression MOD($klist, \sum_j newweight_j$) and rely on the operating system's load balancing scheme. Such a "residue machine" is specified as

```
residue:machine_name:number
```

in the **.machines** file.

Alternatively, it is also possible to distribute the remaining k-points one-by-one (and not in one junk) over all processors. The option

```
extrafine:1
```

can be set in the **.machines** file. Note, each (set of) process(es) in the k-point parallelization gets their own input files and creates a set of output files. To keep the number of files small, the number for **extrafine** can be increased and the number for **granularity** can be decreased. The line

```
lapw0:gamma:2 delta:2 epsilon:4
```

defines the computers used for running **lapw0_mpi**. In this example the 6 processors of the computers **gamma**, **delta**, and **epsilon** run **lapw0_mpi** in parallel.

If fine grained parallelization is used, each set of processors defined in the **.machines** file is converted to a single file **.machine[1/2/...]**, which is used in a call to **mpirun** (or another parallel execution environment).

5.4.5 How the list of k-points is split

In the setup of the k-point parallel version of LAPW1 the list of k-points in **case.klist** (*Note, that the k-list from* ***case.in1*** *cannot be used for parallel calculations*) is split into subsets according to the weights specified in the **.machines** file:

$$newweight_i = \left\lfloor \frac{weight_i * klist}{granularity * \sum_j weight_j} \right\rfloor$$

where $newweight_i$ is the number of k-points to be calculated on processor i. $newweight_i$ is always set to a value greater equal one.

A loop over all i processors is repeated until all k-points have been processed.

Speedup in a parallel program is intrinsically dependent on the serial or parallel parts of the code according to Amdahl's law:

$$speedup = \frac{1}{(1-P) + \frac{P}{N}}$$

whereas N is the number of processors and P the percentage of code executed in parallel.

In **WIEN2k** usually only a small part of time is spent in the programs **`lapw0, lcore`** and **`mixer`** which is very small (negligible) in comparison to the times spent in **`lapw1`** and **`lapw2`**. The time for waiting until all parallel **`lapw1`** and **`lapw2`** processes have finished is important too. For a good performance it is therefore necessary to have a good load balancing by estimating properly the speed and *availability* of the machines used. We encourage the use of **`testpara_lapw`** or *"Utils. ⇓ testpara"* from **w2web** to check the k-point distribution over the machines *before* actually running the programs in parallel.

While running **`lapw1`** and **`lapw2`** in parallel mode, the scripts **`testpara1_lapw`** (see 5.2.7) and **`testpara2_lapw`** (see 5.2.8) can be used to monitor the succession of parallel execution.

5.4.6 Flow chart of the parallel scripts

To see how files are handled by the scripts **`lapw1para`** and **`lapw2para`** refer to figures 5.1 and 5.2. After the **`lapw2`** calculations are completed the densities and the informations from the **`case.scf2_x`** files are summarized by **`sumpara`**.

*Note: parallel **`lapw2`** and **`sumpara`** take two command line arguments, namely the **`case.def`** file but also a **`number_of_processor`** indicator.*

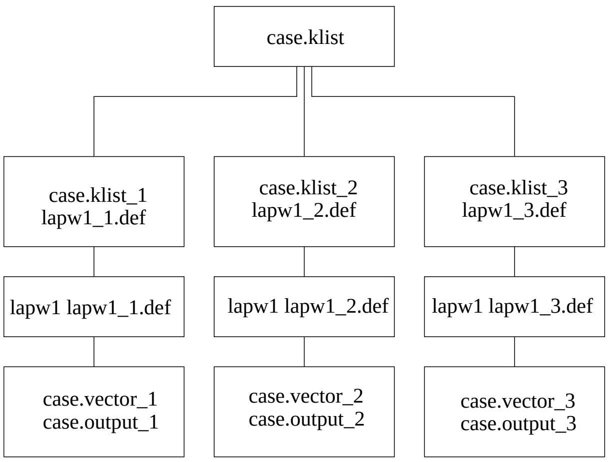

Figure 5.1: Flow chart of **`lapw1para`**

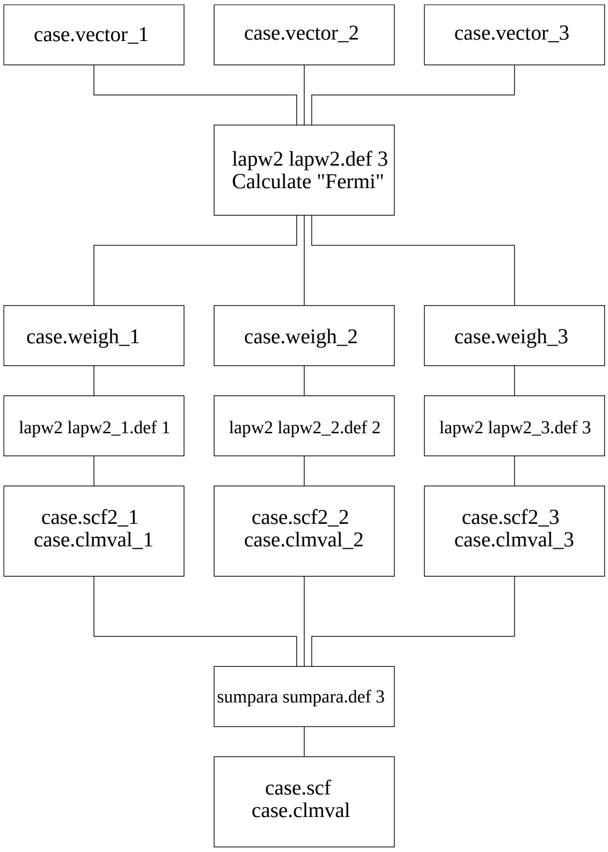

Figure 5.2: Flow chart of **lapw2para**

5.4.7 On the fine grained parallelization

The following parallel programs use different parallelization strategies:

lapw0_mpi is parallelized over the number of atoms. This method leads to good scalability as long as there are more atoms than processors. For very many processors, however, the speedup is limited, which is not at all critical, since the overall computing time of **`lapw0_mpi`** will be nearly negligible.

lapw1_mpi uses a two-dimensional processor setup to distribute the Hamilton and overlap matrices. For higher numbers of processors two-dimensional communication patterns are clearly preferable to one-dimensional communication patterns.
Let us assume, for example, 64 processors. In a given processing step, one of these processors has to communicate with the other 63 processors if a one-dimensional setup was chosen. In the case of a two-dimensional processor setup it is usually sufficient to communicate with the processors of the same processor row (7) or the same processor column (7), i. e. with 14 processors.
In some cases a price has to be paid for these preferable communication patterns: Assume that 17 processors are available to calculate one k-point. In this case **`lapw1_mpi`** will choose a 4×4 processor setup, which leaves one processor to contribute only to the calculation of some intermediate results.
In general the processor array $P \times Q$ is chosen as follows: $P = \lfloor\sqrt{\text{number of processors}}\rfloor$, $Q = \left\lfloor\frac{\text{number of processors}}{P}\right\rfloor$.

lapw2_mpi is parallelized in two main parts: (i) each eigenvector is distributed evenly to all the processors, and (ii) the fast Fourier transforms are done in parallel.

If more than one k-point is distributed at once to **`lapw1_mpi`** or **`lapw2_mpi`**, these will be treated consecutively.

Depending on the parallel computer system and the problem size, speedups will vary in a wide range. Running the fine grained parallelization over a 10 Mbit/s Ethernet network is not recommended, even for large problem sizes.

5.5 Getting on-line help

- As mentioned before, all **WIEN2k** csh-shell scripts have a **"help"-switch -h**, which gives a brief summary of all options for the respective script.
- To obtain online help on input-parameters, program description, . . . use

  `help_lapw`

  which opens the pdf-version of the users guide (using **`acroread`** or what is defined in $PDF-READER). You can search for a specific keyword using "^f keyword". This procedure substitutes an "Index" and should make it possible to find a specific information without reading through the complete users guide.
- In addition there is a html-version of the UG and its starting page is: **`$WIENROOT/SRC_usersguide_html/usersguide.html`**
- When using the user interface **w2web**, you have access to the html and pdf-version (the latter requires an X-windows environment) of the usersguide.
- At our webserver *http://www.wien2k.at/reg_user* we put informations for the registered user:
  - A "FAQ" page with answers to some common problems.
  - Update information: When you think the program has an error, please check wether newer versions are available, which might have fixed the problem you encounter.

– A mailing list:

Please check the "digest"! In many cases your questions may have been answered before.

Locate your problem: If a calculation crashes, please locate the problem. Check the content of files like **`case.dayfile, *.error, case.scf, case.scfX, case.outputX`** where X specifies the program which crashed.

Posting questions: Please provide enough information so that somebody can help you. A question like: "My calculation crashed. Please help me!" will most likely not be answered.

5.6 Interface scripts

We have included a few "interface scripts" into the current **WIEN2k** distribution, to simplify the previewing of results. In order to use these scripts the public domain program "**gnuplot**" has to be installed on your system.

5.6.1 eplot_lapw

The script **`eplot_lapw`** plots total energy vs. volume or total energy vs. c/a-ratio using the file **`case.analysis`**. The latter should have been created with **`grepline`** or the "*Analysis ⇓ Analyze multiple SCF-files*" menu of **w2web** and the file names must be generated (or compatible) with "optimize.job".

For a description of how to use the script for batch like execution call the script using

```
eplot_lapw -h
```

5.6.2 dosplot_lapw

The script **`dosplot_lapw`** plots total or partial Density of States depending on the input used by **`case.int`** and the interactive input.

For a description of how to use the script for batch like execution call the script using

```
dosplot_lapw -h
```

5.6.3 specplot_lapw

`specplot_lapw` provides an interface for plotting X-ray spectra from the output of the **`xspec`** or **`txspec`** program.

For a description of how to use the script for batch like execution call the script using

```
specplot_lapw -h
```

5.6.4 rhoplot_lapw

The script **`rhoplot_lapw`** produces a surface plot of the electron density from the file **`case.rho`** created by lapw5.

*Note: To use this script you must have installed the C-program **`reformat`** supplied in **`SRC_reformat`**.*

5.6.5 opticplot_lapw

The script **opticplot_lapw** produces XY plots from the output files of the optics package using the **case.joint**, **case.epsilon**, **case.eloss**, **case.sumrules** or **case.sigmak**. For a description of how to use the script for batch like execution call the script using

```
opticplot_lapw -h
```

6 Programs for the initialization

Contents

In sections (6.1-6.6) we describe the initial utility programs. These programs are used to set up a calculation.

6.1 NN (nearest neighbor distances)

This program uses the **`case.struct`** file (see 4.3) in which the atomic positions in the unit cell are specified, calculates the nearest neighbor distances of all atoms, and checks that the corresponding atomic spheres (radii) are not overlapping. If an overlap occurs, an error message is shown on the screen. In addition, the next nearest-neighbor distances up to f times the nearest-neighbor distance (f is provided interactively) are written to an output file named **`case.outputnn`**. It is highly recommended in many cases that you change your sphere sizes and NOT use the default of 2.0. An increase from 2.0 to 2.1 may already result in drastically reduced computing time. More recommendations are given in chapter 4.3.

`nn` also checks if equivalent atoms are specified correctly in **`case.struct`**. At the bottom of **`case.outputnn`** the coordination shell-structure is listed and from that a comparison with the input is made verifying that equivalent atoms really have equivalent environments. If this is not the case, an ERROR will be printed and a new structure file **`case.struct_nn`** is generated. You have to recheck your input and then decide whether you want to accept the new structure file, or reject it (because the equivalency may just be an artefact due to a special choice of lattice parameters). It also may be that you have made a simple input error. If you want to force two atoms of the same kind (e.g. 2 Fe atoms) to be nonequivalent (e.g. because you want to do an antiferromagnetic calculation), label the atoms as “Fe1” and “Fe2” in **`case.struct`**.

Thus this program helps to generate proper **`struct`**-files especially in the case of artificial unit cells, e.g. a supercell simulating an impurity or a surface.

6.1.1 Execution

The program **`nn`** is executed by invoking the command:

`nn nn.def` or **`x nn`**

6.2 SGROUP

This program was contributed by:

Bogdan Yanchitsky and Andrei Timoshevskii
Institute of Magnetism, Kiev, Ukraine
email: yan@imag.kiev.ua and tim@ukron.kiev.ua
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

It was published in Yanchitsky and Timoshevskii 2001, and is written in C.

This program uses information from **case.struct** (lattice type, lattice constants, atomic positions) and determines the spacegroup as well as all pointgroups of non-equivalent sites. It uses the nuclear charges Z or the "label" in the 3rd place of the atomic name (Si1, Si2) to distinguish different atoms uniquely. It is able to find possible smaller unit cells, shift the origin of the cell and can even produce a new struct file **case.struct_sgroup** based on your input **case.struct** with proper lattice types and equivalency. It is thus most usefull in particular for "handmade" structures.

For more information see also the README in SRC_sgroup.

6.2.1 Execution

The program sgroup is executed by invoking the command:

sgroup -wi case.struct [-wo case.struct_sgroup] case.outputsgen
or **x sgroup**

6.3 SYMMETRY

This program uses information from **case.struct** (lattice type, atomic positions). If NSYM was set to zero it generates the space group symmetry operations and writes them to **case.struct_st** to complete this file. Otherwise (NSYM > 0) it compares the generated symmetry operations with the already present ones. If they disagree a warning is given in the output. In addition the point group of each atomic site is determined and the respective symmetry operations and LM values of the lattice harmonics representation are printed. The latter information is written into **case.in2_sy**, while the local rotation matrix, the positive or negative IATNR values and the proper ISPLIT parameter are written to **case.struct_st**. (See appendix A and Sec. 4.3).

6.3.1 Execution

The program symmetry is executed by invoking the command:

symmetry symmetry.def or **x symmetry**

6.4 LSTART (atomic LSDA program)

lstart is a relativistic atomic LSDA code originally written by Desclaux (69, 75) and modified for the present purpose. Internally it uses Hartree atomic units, but all output has been converted to Rydberg units. **lstart** generates atomic densities which are used by **dstart** to generate a starting density for a scf calculation and all the input files for the scf run: **in0**, **in1**, **in2**, **inc** and **inm** (according to the atomic eigenvalues). In addition it creates atomic potentials (which are truncated at their corresponding atomic radii and could be used to run **lapw1**) and optional atomic valence densities, which can be used in **lapw5** for a difference density plot. The atomic total energies are also printed, but it can only be used for cohesive energy calculations of light elements. Already for second-row elements the different treatment of relativistic effects in **lstart** and **lapwso** yields inconsistent data and you must calculate the atomic total energy consistently by a supercell approach via a "bandstructure calculation (Put a single atom in a sufficiently large fcc-type unit cell).

If the program stops with some lines:

```
NSTOP= .....
```

in **case.outputst**, this means, that a proper solution for at least one orbital could not be obtained. In such a case the input must be changed and one should provide different occupation numbers for these states (e.g. Cu can not be started with $3d^{10}4s^1$, but it works with $3d^94s^2$).

Warnings about the radial mesh can usually be ignored. They can be avoided by larger dimension parameters NPT and NPT00, so that the radial mesh will reach up to RMAX0.

6.4.1 Execution

The program **lstart** is executed by invoking the command:

lstart lstart.def or **x lstart**

The files **case.rsp(up|dn)** are generated and contain the atomic (spin) densities, which will be used by DSTART later on.

6.4.2 Dimensioning parameters

The following parameters are defined in file **param.inc** (static and not allocatable arrays):

NPT	total number of radial mesh points, must be gt.(NRAD+NPT00), where NRAD is the number of mesh-points up to RMT specfied in case.struct.
NPT00	max. number of radial mesh points beyond RMT
RMAX0	max. distance of radial mesh

6.4.3 Input

When running **lstart** you will first be asked interactively to specify an XC-potential switch. Currently 5 (LSDA, Perdew and Wang 92) as well as 13 and 14 (two GGAs, Perdew et al. 96 and Perdew et al. 92, respectively) are officially supported, but 13 is recommended.

In addition the program asks for an energy cut-off, separating core from valence states. Usually -6.0 Ry is a good choice, but you should check for each atom how much core charge leaks out of the sphere (bottom of **case.outputs**). If this is the case one should lower this energy cut-off and thus include these low lying states into the valence region.

The rest of the input is described in the sample input below.

Note: Only the data at the beginning of the line are read whereas the comment describes the respective orbitals. This file can be generated automatically in **w2web** using "*RunPrograms* ⇒ *Struct Generator*" or with the script **instgen_lapw**. To edit this file by hand choose "*View/Edit* ⇒ *Input Files*" and choose **case.inst**.

```
------------------ top of file: case.inst -------------------
 ZINC
Ne 6         (inert gas, # OF VALENCE ORBITALS not counting spin)
3,-1,1.0  N        ( N,KAPPA,OCCUP; = 3S UP, 1 ELECTRON)
3,-1,1.0  N                          3S DN
3,-2,2.0  N                          3P UP
3,-2,2.0  N                          3P DN
3, 1,1.0  N                          3P*UP
3, 1,1.0  N                          3P*DN
3,-3,3.0  P                          3D UP
3,-3,3.0  P                          3D DN
3, 2,2.0  P                          3D*UP
3, 2,2.0  P                          3D*DN
4,-1,1.0  P                          4S UP
4,-1,1.0  P                          4S DN
****               END OF Input
****               END OF Input
------------------- bottom of file --------------------------
```

Interpretive comments follow:

line 1: format(a20) title
line 2: free format
config

config	specifies the core state configuration by an inert gas (He, Ne, Ar, Kr, Xe, Rn) and the number of (valence) orbitals (without spin). (In the example given above one could also use **Ar 3** and omit the $3s$ and $3p$ states.) The atomic configurations are listed in the appendix and can also be found online using **periodic_table**, a shell script which displays **SRC/periodic.ps** with ghostview)

line 3: format(i1,1x,i2,1x,f5.3,a1)
n, kappa, occup, plot

n	the principle quantum number
kappa	the relativistic quantum number (see below)
occup	occupation number (per spin)
plot	**P** specifies that the density of the respective orbital is written to the file **case.sigma**, which can be used for difference density plots in **lapw5**. **N** or an empty field will exempt density of the respective orbital from being printed to file.

>>>:**line 3** is repeated for the other spin and for all orbitals specified above by config.
>>>**: the last two lines** must be
****
****

The quantum numbers are defined as follows (see e.g. Liberman et al 65):

Spin quantum number: $s = +1$ or $s = -1$

Orbital quantum number $j = l + s/2$

Relativistic quantum number $\kappa = -s(j + 1/2)$

		$j = l + s/2$		κ		max. occupation	
	l	$s = -1$	$s = +1$	$s = -1$	$s = +1$	$s = -1$	$s = +1$
s	0		1/2		-1		2
p	1	1/2	3/2	1	-2	2	4
d	2	3/2	5/2	2	-3	4	6
f	3	5/2	7/2	3	-4	6	8

Table 6.4: Relativistic quantum numbers

6.5 KGEN (generates k mesh)

This program generates the k-mesh in the irreducible wedge of the Brillouin zone (IBZ) on a special point grid, which can be used in a modified tetrahedron integration scheme (Blöchl et al 1994).

kgen needs as interactive input the total number of k-points in the BZ and, if inversion symmetry is not present, asks whether or not it should include this symmetry when generating the k-mesh. One should usually add inversion here except for certain magnetic cases including SO interaction. If symmetry permits, it further asks whether or not the k-mesh should be shifted away from high symmetry directions. The file **case.klist** is used in **lapw1** and **case.kgen** is used in **tetra** and **lapw2**, if the EF switch is set to TETRA, i.e. the tetrahedron method for the k-space integration is used. For the format of the **case.klist** see page 82.

6.5.1 Execution

The program kgen is executed by invoking the command:

kgen kgen.def or **x kgen [-so]**

With the switch **-so** it uses a file **case.ksym** (usually generated by **symmetso** instead of **case.struct**.

6.5.2 Dimensioning parameters

The following parameters are used in **main.f, ord1.f** (static arrays):

IDKP	number of inequivalent k-points (like NKPT in other programs)
NWX	internal parameter, must be increased for very large k-meshes
INDEXM	internal parameter, must be increased for very large k-meshes

6.6 DSTART (superposition of atomic densities)

This program generates an initial crystalline charge density **case.clmsum** by a superposition of atomic densities (**case.rsp**) generated with **lstart**. Information about LM values of the lattice harmonics representation and number of Fourier coefficients of the interstitial charge density are taken from **case.in1** and **case.in2**. In the case of a spin-polarized calculation it must also be run for the spin-up charge density **case.clmup** and spin-down charge density **case.clmdn**.

6.6.1 Execution

The program **`dstart`** is executed by invoking the command:

`dstart dstart.def` or **`x dstart [-up|dn -c]`**

6.6.2 Dimensioning parameters

The following parameters are collected in file **`param.inc`**, but usually need not to be changed:

IPINST	number of r-mesh points beyond Rmt (should be NPT00 as in LSTART)
NCOM	number of LM terms in density
NRAD	number of radial mesh points
NSYM	order of point group

7 Programs for running an SCF cycle

Contents

In sections 7.1-7.9 we describe the main programs to run an SCF cycle as illustrated in figure 4.1.

7.1 LAPW0 (generates potential)

lapw0 computes the total potential V_{tot} as the sum of the Coulomb V_c and the exchange-correlation potential V_{xc} using the total electron (spin) density as input. It generates the spherical part (l=0) as **case.vsp** and the non-spherical part as **case.vns**. For spin-polarized systems, the spin-densities **case.clmup** and **case.clmdn** lead to two pairs of potential files. These files are called: **case.vspup**, **case.vnsup** and **case.vspdn**, **case.vnsdn**.

The Coulomb potential is calculated by the multipolar Fourier expansion introduced by Weinert (81). Utilizing the spatial partitioning of the unit cell and the dual representation of the charge density [equ. 2.10], firstly the multipole moments inside the spheres are calculated (Q-sp). The Fourier series of the charge density in the interstitial also represent SOME density inside the spheres, but certainly NOT the correct density there. Nevertheless, the multipole moments of this artificial plane-wave density inside each sphere are also calculated (Q-pw). By subtracting Q-pw from Q-sp one obtains pseudo-multipole moments Q. Next a new plane-wave series is generated which has two properties, namely zero density in the interstitial region and a charge distribution inside the spheres that reproduces the pseudo-multipole moments Q. This series is added to the original interstitial Fourier series for the density to form a new series which has two desirable properties: it simultaneously represents the interstitial charge density AND it has the same multipole moments inside the spheres as the actual density. Using this Fourier series the interstitial Coulomb potential follows immediately by dividing the Fourier coefficients by K^2 (up to a constant).

Inside the spheres the Coulomb potential is obtained by a straightforward classical Green's function method for the solution of the boundary value problem.

The exchange-correlation potential is computed numerically on a grid. Inside the atomic spheres a least squares procedure is used to reproduce the potential using a lattice harmonics representation (the linear equations are solved with modified LINPACK routines). In the interstitial region a 3-dimensional fast Fourier transformation (FFT) is used.

The total potential V is obtained by summation of the Coulomb V_C and exchange-correlation potentials V_{xc}.

In order to find the contribution from the plane wave representation to the Hamilton matrix elements we reanalyze the Fourier series in such a way that the new series represents a potential which is zero inside the spheres but keeps the original value in the interstitial region.

The contribution to the total energy which involves integrals of the form $\rho * V$ is calculated according to the formalism of Weinert et al (82).

The Hellmann-Feynman force contribution to the total force is also calculated (Yu et al 91).

Finally, the electric field gradient (EFG) is calculated in case you have an L=2 term in the density expansion. The EFG tensor is given in both, the "local-rotation-matrix" coordinate system, and then diagonalized. The resulting eigenvectors of this rotation are given by columns.

For surface calculations the total and electrostatic potential at z=0 and z=0.5 is calculated and can be used as energy-zero for the determination of the workfunction. (It is assumed that the middle of your vacuum region is either at z=0 or z=0.5).

7.1.1 Execution

The program **lapw0** is executed by invoking the command:

lapw0 lapw0.def or **x lapw0**

7.1.2 Dimensioning parameters

The following parameters are used (they are collected in file **param.inc**, but usually need not to be changed:

NCOM	number of lm components in charge density and potential representation; it must satisfy the following condition: NCOM+3 .gt. $\{$[number of l, m with $m = 0$] + [2 * number of l, m with $m > 0$]$\}$
NRAD	number of radial mesh points
NSTD	defines the angular grid points used in fitting the xc-potential inside spheres
LMAX1D	defines the angular grid points used in fitting the xc-potential inside spheres
LMAX2	highest L in the LM expansion of charge and potential
NSYM	order of point group

7.1.3 Input

The input is very simple. It is generated automatically by **init_lapw**, and needs to be changed only if a different exchange-correlation potential should be used:

```
------------------ top of file: case.in0 --------------------
TOT   13             MULT/COUL/EXCH/POT /TOT ;  VXC-SWITCH
NR2V    (R2V / NR2V)
0 0.0     (#of FK in E-field expansion, EFELD (Ry)
0         (list of K-vectors)

------------------- bottom of file --------------------------
```

Interpretive comments follow:

line 1: format(A4,I4)
switch, indxc

switch		
	TOT	total energy contributions and total potential calculated
	POT	total potential is calculated, but not the total energy
	MULT	multipole moments calculated only
	COUL	Coulomb potential calculated only
	EXCH	exchange correlation potential calculated only NOTE: MULT, COUL, and EXCH are for testing only, whereas POT, saves some CPU time if total energy is not needed
indxc		index to specify type of exchange and correlation potential. Supported options include:
	1	Moruzzi, Janak, Williams(78)
	5	Perdew and Wang 92, reparameterization of Ceperly-Alder data, the recommended LDA option
	13	Generalized Gradient approximation (Perdew-Bourke-Ernzerhof 96)
	14	Generalized Gradient approximation (Perdew-Wang 91)
	12	Meta GGA (Perdew et al. 2000). You must have a **`case.inm_vresp`** file (**`cp case.inm case.inm_vresp`** and set **`NORM = NO`**) to generate the required input files for this option. In addition you must use a very large GMAX (24.9), but even so it might be numerically unstable.

line 2: format(A4)
option

NR2V	no additional output
R2V	Exchange-correlation (**`case.r2v`**), Coulomb and total potentials (**`case.vcoul`**) are written as (r^2V) to a file for plotting with **`lapw5`**

The following 2 lines are optional and can be omitted. They are used to introduce an electric field via a zig-zag potential (see J.Stahn et al. 2000):

line 3: free format
IEFIELD, EFIELD

IEFIELD	number of Fourier coefficients to model the zig-zag potential
EFIELD	value of the electric field (mRy) Please note: The zig-zag potential is only implemented for the LDA functionals.

line 4: free format

KFIELD	Indices of K-vectors to be used in the zig-zag E-field description. I.e.: 2,3,4 means that you model this field by using the 2-4 th K-vector in **`case.clmsum`**, which are usually vectors like (0,0,1), (0,0,2),...)

7.2 ORB (Calculate orbital dependent potentials)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

orb calculates the orbital dependent potentials, i.e. potentials which are nonzero in the atomic spheres only and depend on the orbital state numbers l, m. In the present version the potential is assumed to be independent of the radius vector und needs the density matrix calculated in **lapwdm**. Three different potentials are implemented in this package:

- LDA+U. There are three variants of this method, two of them are discussed in Novák et al. 2001
  1. LDA+U(SIC) - introduced by Anisimov et al. 1993, with an approximate correction for the self-interaction correction.
  2. LDA+U(AMF) - introduced by Czyzyk and Sawatzky 1994 as 'Around the Mean Field' method. (In Novák et al. 2001 it is denoted as LDA+U(DFT)). This version is (probably) more suitable for full potential methods.
  3. LDA+U(HMF) - in addition the Hubbard model in the mean field approximation, as introduced by Anisimov et al. 1991 is also implemented. Note, however, that it is to be used with the LDA (not LSDA) exchange-correlation potential in spin polarized calculations!

  All variants are implemented in the rotationally invariant way (Liechtenstein et al. 1995). If LDA+U is used in an unrestricted, general way, it introduces an orbital field in the calculation (in analogy to the exchange field in spin-polarized calculations, but it interacts with the orbital, instead of spin momentum). The presence of such an orbital field may lower the symmetry. In particular the complex version of LAPW1 must be used. Care is needed when dealing with the LDA+U orbital field. It may be quite large, and without specifying its direction it may fluctuate, leading to oscilations of scf procedure or/and to false solutions. It is therefore necessary to use it in combination with the spin-orbit coupling, preferably running first LSDA+(s-o) and then slowly switching on the LDA+U orbital field. If the LDA+U orbital polarization is not needed, it is sufficient to run real version of LAPW1, which then automatically puts the orbital field equal to zero. For systems without the centre of inversion, when LAPW1 must be complex, an extra averaging of the LDA+U potential is necessary.
- Orbital polarization. The additional potential has the form (Brooks 1985, Eriksson et al. 1989):
  $$V_{OP} = c_{OP} < L_z > l_z \tag{7.1}$$
  where c_{OP} is the orbital polarization parameter, $< L_z >$ is projection of the orbital momentum on the magnetization direction and l_z is single electron orbital momentum component z parallel to $\vec{M}$.
- Interaction with the external magnetic field. In this case the additional potential has a simple form:
  $$V_{Bext} = \mu_B \vec{B}_{ext}(\vec{l} + 2\vec{s}). \tag{7.2}$$
  The interaction with the electronic spin is taken into account by shifting the spin up and spin down exchange correlation potentials in LAPW0 by the energy $+\mu_B B_{ext} - \mu_B B_{ext}$, respectively. The interaction of B_{ext} with spin could be as well calculated using the 'Fixed spin moment' method. For an interaction with the orbital momentum it is necessary to specify the atoms and angular momentum numbers for which this interaction will be considered. Caution is needed when considering interaction of the orbital momentum with B_{ext} in metallic or metallic-like systems. For the analysis see the paper by Hirst 1997

In all cases the resulting potential for a given atom and orbital number l is a Hermitean, $(2l+1)$x$(2l+1)$ matrix. In general this matrix is complex, but in special cases it may be real.

7.2.1 Execution

The program **orb** is executed by invoking the command:

x orb [-up/-dn/-du] or **orb up/dnorb.def**

7.2.2 Dimensioning parameters

The following parameters are used (collected in file **param.inc**):

LABC	highest l+1 value of orbital dependent potentials
NRAD	number of radial mesh points

7.2.3 Input

Since this program can handle three different cases, examples and descriptions for all cases are given below:

Input for all potentials

line 1: free format
nmod,natorb,ipr

nmod	defines the type of potential 1...LDA+U, 2...OP, 3...B_{ext}
natorb	number of atoms for which orbital potential V_{orb} is calculated
ipr	printing option, the larger ipr, the longer the output

line 2: (A5,f8.2)
mixmod,amix

mixmod	BROYD or PRATT (see MIXER for more information)
amix	coefficient for the Pratt mixing (and first BROYD iteration) of V_{orb} This option is now only used for testing. The mixing should be set to PRATT, 1.0

line 3: free format
iatom(i),nlorb(i),(lorb(li,i),li=1,nlorb(i))

iatom	index of atom in struct file
nlorb	number of orbital moments for which Vorb shall be applied
lorb	orbital numbers (repeated nlorb-times)

3rd line repeated natorb-times

Input for LDA+U (nmod=1)

line 4: free format

nsic		defines 'double counting correction'
	nsic=0	'AMF method' (Czyzyk et al. 1994)
	nsic=1	'SIC method' (Anisimov et al. 1993, Liechtenstein et al. 1995)
	nsic=2	'HMF method' (Anisimov et al. 1991)

line 5: free format

U(li,i), J(li,i)	Coulomb and exchange parameters, U and J, for LDA+U in Ry for atom type i and orbital number li

5th line repeated natorb-times, for each natorb repeated nlorb-times

Example of the input file for NiO (LDA+U included for two inequivalent Ni atoms that have indexes 1 and 2 in the structure file):

```
1  2  0                         nmod, natorb, ipr
PRATT,1.0                       mixmod, amix
1 1 2                           iatom nlorb, lorb
2 1 2                           iatom nlorb, lorb
1                               nsic (LDA+U(SIC) used)
0.59 0.07                       U J
0.59 0.07                       U J
```

Input for Orbital Polarization (nmod=2)

line 4: (free format)

nmodop		defines mode of 'OP'
	1	average L_z taken separatelly for spin up, spin down
	0	average L_z is the sum for spin up and spin down

line 5: (free format)

Ncalc(i)		
	1	Orb.pol. parameters are calculated ab-initio
	0	Orb.pol. parameters are read from input

this line is repeated natorb-times
line 6: (free format) (only if Ncalc=0, then repeated nlorb-times)

pop(li,i)	OP parameter in Ry

line 7: (free format)
xms(1), xms(2), xms(3)

direction of magnetization expressed in terms of lattice vectors

Example of the input file for NiO (total $< L_z >$ used in (1), OP parameters calculated ab-initio, $\vec{M}$ along [001]):

```
2  2  0                         nmod, natorb, ipr
PRATT, 1.0                      mixmod, amix
1 1 2                           iatom nlorb, lorb
```

```
2 1 2                          iatom nlorb, lorb
0                              nmodop
1                              Ncalc
1                              Ncalc
0. 0. 1.                       direction of M in terms of lattice vectors
```

Input for interaction with B_{ext} (nmod=3)

line 4: (free format)

B_{ext}	external field in Tesla

line 5: (free format)
xms(1), xms(2), xms(3)

direction of magnetization expressed in terms of lattice vectors

Example of the input file for NiO, (B_{ext}= 4 T, along [001]):

```
3  2  0                        nmod, natorb, ipr
PRATT, 1.0                     mixmod, amix
1 1 2                          iatom nlorb, lorb
2 1 2                          iatom nlorb, lorb
4.                             Bext in T
0. 0. 1.                       direction of Bext in terms of lattice vectors
```

7.3 LAPW1 (generates eigenvalues and eigenvectors)

lapw1 sets up the Hamiltonian and the overlap matrix (Koelling and Arbman 75) and finds by diagonalization eigenvalues and eigenvectors which are written to **case.vector**. Besides the standard LAPW basis set, also the APW+lo method (see Sjöstedt et al 2000, Madsen et al. 2001) is supported and the basis sets can be mixed for maximal efficiency. If the file **case.vns** exists (i.e. non-spherical terms in the potential), a full-potential calculation is performed.

For structures without inversion symmetry, where the hamilton and overlap matrix elements are complex numbers, the corresponding program version **lapw1c** must be used in connection with **lapw2c**.

Since usually the diagonalization is the most time consuming part of the calculations, several options exist here. In **WIEN2k** we include highly optimized modifications of LAPACK routines. We call all these routines “full diagonalization”, but we also provide an option to do an “iterative diagonalization” using a block-Davidson method (see Singh 89). This scheme starts from an old eigenvector (previous scf-iteration), needs additional memory and produces only approximate eigenvalues/vectors, but can be significantly faster than LAPACK, in particular if the ratio of matrix size to number of relevant (e.g. occupied) eigenvalues is large. In any case, it is recommended that convergence is checked by another scf-iteration with “full diagonalization”. Often the best performance can be obtained by first running to a crude convergence, next doing a “full diagonalization” and finally continuing iteratively to self consistency. (e. g. use first: **run_lapw -it -fc 10** and then **run_lapw -it -fc 1**)

Parallel execution (fine grain and on the k-point level) is also possible and is described in detail in Sec. 5.4.

7.3.1 Execution

The program **lapw1** is executed by invoking the command:

> **x lapw1 [-c -up|dn -it -p -nohns -orb]** or
> **lapw1 lapw1.def** or **lapw1c lapw1.def**

In cases without inversion symmetry, the default input filename is **case.in1c**. For semi-core calculations the **lapw1s.def** file uses a **case.in1s** file and creates the files **case.output1s** and **case.vectors**. For the spin-polarized case lapw1 is called twice with **uplapw1.def** and **dnlapw1.def**. To all relevant files the keywords "**up**" or "**dn**" are appended (see the fcc Ni test case in the **WIEN2k** package). The switch **-nohns** skips the calculation of the nonspherical matrix elements inside the sphere. This may be used to save computer time during the first scf cycles.

7.3.2 Dimensioning parameters

The following parameters (collected in file **param.inc_r** or **param.inc_c**) are used:

KMAX1START	a first guess for the largest h,k,l Fourier components of the potential
KMAX2START	
KMAX3START	
LMAX	highest l+1 in basis function inside sphere (consistent with input in case.in1)
LMMX	number of LM terms in potential (should be at least NCOM-1)
LOMAX	highest l for local orbital basis (consistent with input in case.in1)
NGAU	number of Gaunt coefficients for the non-spherical contributions to the matrix elements
NKPTSTART	a starting guess for the total number of k-points in irreducible wedge of Brillouin zone
NMATMAX	maximum size of H,S-matrix (defines size of program, should be chosen according to the memory of your hardware!)
NRAD	number of radial mesh points
NSLMAX	highest l+1 in basis functions for non-muffin-tin matrix elements (consistent with input in case.in1)
NSYM	order of point group
NUME	maximum number of energy eigenvalues per k-point
NVEC1	defines the largest triple of integers which define reciprocal
NVEC2	K-vectors when multiplied with the reciprocal Bravais matrix
NVEC3	
NLOAT	max number of LOs for one l-quantum number

7.3.3 Input

Below a sample input is shown for TiO_2 (rutile), one of the test cases provided in the **WIEN2k** package. The input file is written automatically by LSTART, but was modified to set APW only for Ti-3d and O-2p orbitals. In addition UNIT was changed to 5 and k-points where inserted by hand for bandstructure plotting.

```
------------------ top of file: case.in1 --------------------
WFFIL       (WFPRI,WFFIL,SUPWF ; wave fct. print,file,suppress
  7.500   10    4  (R-mt*K-max; MAX l, max l for hns )
  0.30    5 0 (global energy parameter E(l), with 5 other choices,   LAPW)
 0   -3.00      0.020 CONT 0   ENERGY PARAMETER for s,               LAPW
 0    0.30      0.000 CONT 0   ENERGY PARAMETER for s-local orbital, LAPW-LO
 1   -1.90      0.020 CONT 0   ENERGY PARAMETER for p                LAPW
```

```
 1    0.30      0.000 CONT 0   ENERGY PARAMETER for p-local orbitals LAPW-LO
 2    0.20      0.020 CONT 1                                         APW
  0.20    3 0 (global energy parameter E(1), with 1 other choice,    LAPW)
 0   -0.90      0.020 STOP 0                                         LAPW
 0    0.30      0.000 CONT 0                                         LAPW-LO
 1    0.30      0.000 CONT 1                                         APW
K-VECTORS FROM UNIT:5   -9.0      1.5         IUNIT, Emin, Emax
GAMMA         0    0    0    2 1.00
              0    0    1   10 2.00
              0    0    2   10 2.00
              0    0    3   10 2.00
              0    0    4   10 2.00
Z             0    0    5   10 1.00
END
------------------- bottom of file -----------------------
```

Interpretive comments follow:

line 1: format(A5)
switch

WFFIL	standard option, writes wave functions to file **`case.vector`** (needed in **`lapw2`**)
SUPWF	suppresses wave function calculation (faster for testing eigenvalues only)
WFPRI	prints eigenvectors to **`case.output1`** and writes **`case.vector`** (produces long outputs!)

line 2: free format
rkmax, lmax, lnsmax

rkmax	$R_{mt} * K_{max}$ determines matrix size (convergence), where Kmax is the plane wave cut-off, Rmt is the smallest of all atomic sphere radii. Usually this value should be between 5 and 9 (APW+lo) or 6 - 10. (LAPW-basis) (K_{max}^2 would be the plane wave cut-off parameter in Ry used in pseudopotential calculations.) Note that d (f) wavefunctions converge slower than s and p. For systems including hydrogen with short bondlength and thus a very small R_{mt} (e.g. 0.7 a.u.), RKmax = 3 might already be reasonable, but convergence must be checked for a new type of system. Note, that the actual matrix size is written on case.scf1. It is determined by whatever is smaller, the plane wave cut-off (specified with RKmax) or the maximum matrix dimension NMATMAX, (see previous section).
lmax	maximum l value for partial waves used inside atomic spheres (should be between 8 and 12)
lnsmax	maximum l value for partial waves used in the computation of non-muffin-tin matrix elements (lnsmax=4 is quite good)

line 3: free format
Etrial, ndiff, Napw

Etrial	default energy used for all E_l to obtain $u_l(r, E_l)$ as regular solution of the radial Schrödinger equation [used in equ.2.4,2.7] (see figure 7.1).
ndiff	number of exceptions (specified in the next ndiff lines)
Napw	0 ... use LAPW basis, 1 ... use APW-basis for all "global" l values of this atom. We recommend to use LAPW here.

line 4: format(I2,2F10.5,A4)

l, El, de, switch, NAPWL

l		l of partial wave
El		E_l for L=l
de		energy increment de=0: this E(l) overwrites the default energy (from line 3) de≠ 0: a search for a resonance energy using this increment is done. The radial function $u_l(r, E)$ up to the muffin-tin radius RMT varies with the energy. A typical case is schematically shown in Fig. 7.1. At the bottom of the energy bands u has a zero slope (bonding state), but it has a zero value (antibonding state) at the top of the bands. One can search up and down in energy starting with E_l using the increment de to find where $u_l(R_{MT}, E)$ changes sign in value to determine E_{top} and in slope to specify E_{bottom}. If both are found E_l is taken as the arithmetic mean and replaces the trial energy. Otherwise E_l keeps the specified value. For E_{top} and E_{bottom} bounds of +1 and -10 Ry are defined respectively, and if they are not found, they remain at the initial value set to -200.
switch		used only if de.ne.0
	CONT	calculation continues, even if either E_{top} or E_{bottom} are not found
	STOP	calculation stops if not both E_{top} and E_{bottom} are found (especially useful for semi-core states)
NAPWL		0 ... use LAPW basis, 1 ... use APW-basis for this *l* value of this atom. We recommend to use APW+lo when the corresponding wavefunction is "localized" and thus difficult to converge with standard LAPW (like 3d functions) and/or when the respective atomic sphere is small compared to the other spheres in the unit cell.

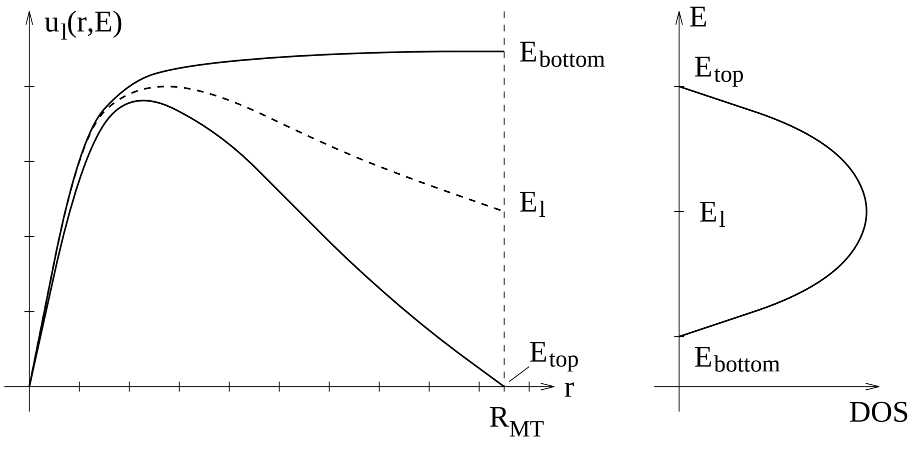

Figure 7.1: Schematic dependence of DOS and $u_l(r, E_l)$ on the energy

>>>:**line 4** is repeated ndiff times (see line 3) for each exception. If the same l value is specified twice, local orbitals are added to the (L)APW basis. The first energy (E_1) is used for the usual LAPW's and the second energy (E_2) for the LOs, which are formed according to (see equ. 2.7): $u_{E_1} + \dot{u}_{E_1} + u_{E_2}$.
Note: You may change the automatically created input and add d- or f-local orbitals to reduce the linearization error (e.g. in late transition metals you could put E_{3d} at 0.0 and 1.0 Ry) or s, p, d, and/or f-LOs at very high energy (e.g. 2.0 - 3.0 Ry) to better describe unoccupied states. This input is also adapted during scf when -in1new is specified, while the original in1 file is saved in **`case.in1_orig`**.

>>>**:lines 3 and 4** are repeated for each non equivalent atom

line 5: format (20x,i1,2f10.1)
unit-number, Emin, Emax

unit-number	file number from which the k-vectors in the irreducible wedge of the Brillouin zone are read. 5 specifies the input file itself (as shown in the example), default is 4, for which the corresponding information is contained in **`case.klist`** (generated by KGEN).
EMIN, EMAX	energy window in which eigenvalues shall be searched (overrides setting in **`case.klist`**. A small window saves computer time, but it also limits the energy range for the DOS calculation of unoccupied states.

line 6: format (A10,4I5,3F5.2)
name, ix,iy,iz, idv, weight

name	name of k-vector (optional) >>>: the last line must be END !!
ix,iy,iz, idv	defines the k-vector, where x= ix/idv etc. We use carthesian coordinates in units of $2\pi/a$, $2\pi/b$, $2\pi/c$ for P,C,F and B cubic, tetragonal and orthorhombic lattices, but internal coordinates for H and monoclinic/triclinic lattices
weight	of k-vector (order of group of k)

>>>: **line 6** is repeated for each k-vector in the IBZ, but Emin and Emax may be omitted after the first k point. The utility program **`kgen`** (see section 6.5) provides a list of such vectors (on a tetrahedral mesh) in **`case.klist`**.
>>>: **the last line** must be END

7.4 LAPWSO (adds spin orbit coupling)

`lapwso` includes spin-orbit (SO) coupling in a second-variational procedure and computes eigenvalues and eigenvectors (stored in **`case.vectorso`**) using the scalar-relativistic wavefunctions from **`lapw1`**. For reference see Singh 94 and Novák 97. The SO coupling must be small, as it is diagonalized in the space of the scalar relativistic eigenstates. For large spin orbit effects it might be necessary to include many more eigenstates from **`lapw1`** by increasing EMAX in **`case.in1`** (up to 10 Ry!). We also provide an additional basisfunction, namely an LO with a $p_{1/2}$ radial wavefunction, which improves the basis and removes to a large degree the dependency of the results on EMAX and RMT (see Kuneš et al. 2001). SO is considered only within the atomic spheres and thus the results may depend to some extent on the choice of atomic spheres radii. The nonspherical potential is neglected when calculating $\frac{dV}{dr}$. Orbital dependend potentials (LDA+U or OP) can be added to the hamiltonian in a cheap and siomple way.

In spin-polarized calculations the presence of spin-orbit coupling may reduce symmetry and even split equivalent atoms into non-equivalent ones. It is then necessary to consider a larger part of the Brillouin zone and the input for **lapw2** should also be modified since the potential has lower symmetry than in the non-relativistic case. The following inputs may change:

- ▶ **case.struct**
- ▶ **case.klist**
- ▶ **case.kgen**
- ▶ **case.in2c**
- ▶ **case.in1**

We recommend to use **initso** (see Sec.5.2.10) which helps you together with **symmetso** (see Sec.9.1) to setup spinorbit calculations.

Note: SO eigenvectors are complex and thus ***lapw2c*** *must be used in a selfconsistent calculation.*

7.4.1 Execution

The program **lapwso** is executed by invoking the command:

> **x lapwso [-up -p -c -orb]** or
> **lapwso lapwso.def**

where here -up indicates a spin-polarized calculation (no "-dn" is needed, since spin-orbit will mix spin-up and dn states in one calculation).

7.4.2 Dimensioning parameters

The following parameters are used (collected in file **param.inc**):

FLMAX	constant = 3
LMAX	highest l of wave function inside sphere (consistent with **lapw1**)
LABC	highest l of wave function inside sphere where SO is considered
LOMAX	max l for local orbital basis
NRAD	number of radial mesh points
NLOAT	number of local orbitals

7.4.3 Input

A sample input for lapwso is given below. It will be generated automatically by **initso**

```
------------------ top of file: case.inso --------------------
WFFIL
 4  0  0                      llmax,ipr,kpot
 -10.0000   1.5000           Emin, Emax
     0 0 1                       h,k,l (direction of magnetization)
   2                             number of atoms with RLO
 1    -3.5      0.005 STOP       atom-number, E-param for RLO
 3    -4.5      0.005 STOP       atom-number, E-param for RLO
 1   2                           number of atoms without SO, atomnumbers
-------------------- bottom of file -----------------------
```

Interpretive comments on this file are as follows:

line 1: format(A5)
switch

WFFIL		wavefunctions will also be calculated for scf-calculation. Otherwise only eigenvalues are calculated.

line 2: free format
LLMAX, IPR, KPOT

LLMAX		maximum l for wavefunctions
IPR		print switch, larger numbers give additional output.
KPOT	0	V(dn) potential is used for $< dn\|V\|dn >$ elements, V(up) for $< up\|V\|up >$ and [V(dn)+V(up)]/2 for $< up\|V\|dn >$.
	1	averaged potential used for all matrix elements.

line 3: free format
Emin, Emax

Emin		minimum energy for which the output eigenvectors and eigenenergies will be printed (Ry)
Emax		maximum energy

line 4: free format

h,k,l		vector describing the direction of magnetization. For R lattice use h,k,l in rhombohedral coordinates (not in hexagonal)

line 5: free format

nlr		number of atoms for which a $p_{1/2}$ LO should be added

line 6: free format
nlri, El, de, switch

nlri		atom-number for which RLO should be added
El		E_l for L=l
de		energy increment (see **`lapw1`**)
switch		used only if de.ne.0
	CONT	calculation continues, even if either E_{top} or E_{bottom} are not found
	STOP	calculation stops if not both E_{top} and E_{bottom} are found (especially useful for semi-core states)

$>>>$**: line 6** is repeated "nlr" times.

line 7: free format
noff, (iatoff(i),i=1,noff)

noff		number of atoms for which SO is switched off (for "light" elements, saves time)
iatoff		atom-numbers

7.5 LAPW2 (generates valence charge density expansions)

lapw2 uses the file **case.vector** and computes the Fermi-energy and the expansions of the electronic charge densities in a representation according to eqn. 2.10 for each occupied state and each k-vector; then the corresponding (partial) charges inside the atomic spheres are obtained by integration. The partial charges for each state (energy eigenvalue) and each k-vector are written to files **case.help31**, **case.help32** etc., where the last digit gives the atomic index of inequivalent atoms. In addition "Pulay-corrections" to the forces at the nuclei are calculated here. For systems without inversion symmetry you have to use the program **lapw2c** (in connection with **lapw1c**).

7.5.1 Execution

The program **lapw2** is executed by invoking the command:

> **x lapw2 [-c -up|dn -p -so -qtl -fermi]** or
> **lapw2 lapw2.def [proc#]** or **lapw2c lapw2.def [proc#]**

where proc# is the i-th processor number in case of parallel execution (see Fig. 5.2). The **-so** switch sets **-c** automatically.

For each inequivalent atom a file **case.helpXX** is defined, starting with XX=31. For complex calculations `case.in2c` is used, for semi-core calculations `lapw2s.def` differs from the regular file **lapw2.def** only in few points, namely **case.in2** must be replaced by `case.in2s` and **case.clmval** by `case.clmsc`. For a spin-polarized case see the fcc Ni test case in the **WIEN2k** package.

7.5.2 Dimensioning parameters

The following parameters are used (collected in file param.inc):

IBLCK	Blocking parameter (32-255) in **fourier.frc**, optimize for best performance
IBLOCK	Blocking parameter (32-255) in **l2main.frc**, optimize for best performance
LMAX2	highest l in wave function inside sphere (smaller than in **lapw1**, at present must be .le. 6)
LOMAX	max l for local orbital basis
NCOM	number of LM terms in density
NGAU	max. number of Gaunt numbers
NRAD	number of radial mesh points

7.5.3 Input

A sample input for **lapw2** is listed below, it is generated automatically by the programs **lstart** and **symmetry**.

```
------------------ top of file: case.in2 --------------------
TOT                          (TOT,FOR,QTL,EFG)
-1.2       32.000   0.5  0.05  (EMIN, # of electrons,ESEPERMIN, ESEPER0 )
TETRA       0.0      (EF-method (ROOT,TEMP,GAUSS,TETRA,ALL),value)
 0 0 2 0 2 2 4 0 4 2 4 4
 0 0 1 0 2 0 2 2 3 0 3 2 4 0 4 2 4 4
14.0      (GMAX)
FILE      (NOFILE, optional)
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: format(A5)
switch

TOT	total valence charge density expansion inside and outside spheres
FOR	same as TOT, but in addition a "Pulay" force contribution is calculated (this option costs extra computing time and thus should be performed only at the final scf cycles, see **run_lapw** script in sec. 5.1.3)
QTL	partial charges only (generates file **case.qtl** for DOS calculations)
EFG	computes decomposition of electric field gradient (EFG), contributions from inside spheres (the total EFG is computed in **lapw0**).
CLM	CLM coefficients only
FERMI	Fermi energy only, this produces weight files for parallel execution and for the **optics** package.
>>>:	TOT and FOR are the standard options, QTL is used for density of states (or energy bandstructure) calculations, EFG for analysis, while FOURI, CLM are for testing only.

line 2: free format
emin, ne, esepermin, eseper0

emin	lower energy cut-off for defining the range of occupied states
ne	number of electrons (per unit cell) in that energy range
esepermin	LAPW2 tries to find the "mean" energies for each l channel, for both the valence and the semicore states. To define "valence" and "semicore" it starts at (EF - "esepermin") and searches for a "gap" with a width of at least "eseper0" and defines this as seperation energy of valence and semicore
eseper0	minimum gap width (see above). The values esepermin and eseper0 will only influence results if the option -in1new is used

line 3: format(a5,f10.5)
efmod, eval

efmod		determines how E_F is determined
	ROOT	E_F is calculated and k space integration is done by root sampling (this can be used for insulators, but for metals poor convergence is found)
	TEMP	E_F is calculated where each eigenvalue is temperature broadened using a Fermi function with a broadening parameter of eval Ry. (e.g. eval=0.002 gives good total energy convergence, but has no "physical" justification).
	GAUSS	E_F is calculated as above but a Gaussian smearing method is used with a width of eval Ry. (e.g. eval=0.002 gives good total energy convergence, but has no "physical" justification).
	TETRA	E_F is calculated and k space integration is done by the modified (if eval is .lt. 100) or standard (eval .gt. 100) tetrahedron-method (Blöchl 94). This "standard" scheme is recommended for **optic**. In this case the file **case.kgen**, consistent with the k-mesh used in **lapw1**, must be provided (see Sec. 7.3). This is the recommended option although convergence may be slower than with Gauss- or temperature-smearing.
	ALL	All states up to eval are used. This can be used to generate charge densities in a specified energy interval.

eval — when efmod is set to TEMP or GAUSS, eval specifies the width of the broadening (in Ry), if efmod is set to ALL, eval specifies the upper limit of the energy window, if efmod is set to TETRA, eval .gt. 100 specifies the use of the standard tetrahedron method instead of the modified one (see above).

line 4: format (20I2)

L,M — LM values of lattice harmonics expansion (equ. 2.10), defined according to the point symmetry of the corresponding atom; generated in SYMMETRY, MUST be consistent with the local rotation matrix defined in **`case.struct`** (details can be found in Kara and Kurki-Suonio 81). CAUTION: additional LM terms which do not belong to the lattice harmonics will in general not vanish and thus such terms must be omitted. Automatic termination of the lm series occurs when a second 0,0 pair appears within the list. When you change the l, m list during an SCF calculation the Broyden-Mixing is restarted in MIXER.

>>>**line 4:** must be repeated for each inequivalent atom

Symmetry	LM combinations
23	0 0, 4 0, 4 4, 6 0, 6 4,-3 2, 6 2, 6 6,-7 2,-7 6, 8 0, 8 4, 8 8,-9 2,-9 6,-9 4,-9 8,10 0, 10 4,10 8, 10 2, 10 6, 10 10
M3	0 0, 4 0, 4 4, 6 0, 6 4, 6 2, 6 6, 8 0, 8 4, 8 8,10 0, 10 4,10 8, 10 2, 10 6, 10 10
432	0 0, 4 0, 4 4, 6 0, 6 4, 8 0, 8 4, 8 8,-9 4,-9 8,10 0, 10 4,10 8
-43M	0 0, 4 0, 4 4, 6 0, 6 4,-3 2,-7 2,-7 6, 8 0, 8 4, 8 8,-9 2,-9 6,10 0, 10 4,10 8
M3M	0 0, 4 0, 4 4, 6 0, 6 4, 8 0, 8 4, 8 8,10 0, 10 4,10 8

Table 7.39: LM combinations of "Cubic groups" (3∥(111)) direction, requires "positive atomic index" in case.struct. Terms that should be combined (Kara and Kurki-Suonio 81) must follow one another.

Symmetry	Coordinate axes	Indices of $Y_{\pm LM}$	crystal system
1	any	ALL (±l,m)	triclinic
-1	any	(±2l,m)	
2	2∥ z	(±l,2m)	monoclinic
M	m⊥z	(±l,l-2m)	
2/M	2∥z, m⊥z	(±2l,2m)	
222	2∥z, 2∥y, (2∥x)	(+2l,2m), (-2l+1,2m)	orthorhombic
MM2	2∥z, m⊥y, (2⊥x)	(+l,2m)	
MMM	2⊥z, m⊥y, 2⊥x	(+2l,2m)	
4	4∥z	(±l,4m)	tetragonal
-4	-4∥z	(±2l,4m), (±2l+1,4m+2)	
4/M	4∥z, m⊥z	(±2l,4m)	
422	4∥z, 2∥y, (2∥x)	(+2l,4m), (-2l+1,4m)	
4MM	4∥z, m⊥y, (2⊥x)	(+l,4m)	
-42M	-4∥z, 2∥x (m=xy→yx)	(+2l,4m), (-2l+1,4m+2)	
4MMM	4∥z, m⊥z, m⊥x	(+2l,4m)	
3	3∥z	(±l,3m)	rhombohedral
-3	-3∥z	(±2l,3m)	
32	3∥z, 2∥y	(+2l,3m), (-2l+1,3m)	
3M	3∥z, m⊥y	(+l,3m)	
-3M	-3∥z, m⊥y	(+2l,3m)	
6	6∥z	(±l,6m)	hexagonal
-6	-6∥z	(+2l,6m), (±2l+1,6m+3)	
6/M	6∥z, m⊥z	(±2l,6m)	
622	6∥zm, 2∥y, (2∥x)	(+2l,6m), (-2l+1,6m)	
6MM	6∥z, m∥y, (m⊥x)	(+l,6m)	
-62M	-6∥z, m⊥y, (2∥x)	(+2l,6m), (+2l+1,6m+3)	
6MMM	6∥z, m⊥z, m⊥y, (m⊥x)	(+2l,6m)	

Table 7.40: LM combination and local coordinate system of "non-cubic groups" (requires "negative atomic index" in case.struct)

line 5: free format

GMAX		max. G (magnitude of largest vector) in charge density Fourier expansion. For systems with short H bonds larger values (e.g. GMAX up to 25) could be necessary. Calculations using GGA (potential option 13 or 14 in case.in0) should also employ a larger GMAX value (e.g. 14), since the gradients are calculated numerically on a mesh determined by GMAX. When you change GMAX during an scf calculation the Broyden-Mixing is restarted in **mixer**.

line 6: A4

reclist	FILE	writes list of K-vectors into file `case.recprlist` or reuses this list if the file exists. The saved list will be recalculated whenever GMAX, or a lattice parameter has been changed.
	NOFILE	always calculate new list of K-vectors

7.6 SUMPARA (summation of files from parallel execution)

sumpara is a small program which (in parallel execution of **WIEN2k**) sums up the densities (**case.clmval_***) and quantities from the **case.scf2_*** files of the different parallel runs.

7.6.1 Execution

The program **sumpara** is executed by invoking the 2 commands as follows:

x sumpara -d [-up/-dn/-du] and then
sumpara sumpara.def #_of_proc

where **#_of_proc** is the numbers of parallel processors used. It is usually called automatically from **lapw2para** or **x lapw2 -p**.

7.6.2 Dimensioning parameters

The following parameters are listend in file **param.inc**, but usually they need not to be modified:

NCOM	number of LM terms in density
NRAD	number of radial mesh points
NSYM	order of point group

7.7 LAPWDM (calculate density matrix)

This program was contributed by:

J.Kuneš and P.Novák
Inst. of Physics, Acad.Science, Prague, Czeck Republic
email: novakp@fzu.cz

Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

lapwdm calculates the density matrix needed for the orbital dependent potentials generated in **orb**. Optionally it also provides orbital moments, orbital and dipolar contributions to the hyperfine field (only for the specified atoms AND orbitals). It calculates the average value of the operator X which behaves in the same way as the spin-orbit coupling operator: it must be nonzero only within the atomic spheres and can be written as a product of two operators - radial and angular:

$X = X_r(r) * X_{ls}(\vec{l}, \vec{s})$

$X_r(r)$ and $X_{ls}(\vec{l}, \vec{s})$ are determined by RINDEX and LSINDEX in the input as described below:

- RINDEX=0 LSINDEX=0: only the density matrix is calculated
- RINDEX=1 LSINDEX=1: <X> is number of electrons inside the atomic sphere (for test)
- RINDEX=2 LSINDEX=1: <X> is the $< 1/r^3 >$ expectation value inside the atomic sphere
- RINDEX=1 LSINDEX=2: <X> is the projection of the spin moment inside the atomic sphere
- RINDEX=1 LSINDEX=3: <X> is the projection of the orbital moment inside the atomic sphere
- RINDEX=3 LSINDEX=3: <X> is the orbital part of the hyperfine field at the nucleus
- RINDEX=3 LSINDEX=5: <X> is the spin dipolar part of the hyperfine field at the nucleus

To use the different operators, set the appropriate input. More information and extentions to operators of similar behavior may be obtained directly from P. Novák (97)

7.7.1 Execution

The program **lapwdm** is executed by invoking the command:

> **x lapwdm [-up/dn -p -c -so]** or
> **lapwdm lapwdm.def**

7.7.2 Dimensioning parameters

The following parameters are used (collected in file **param.inc**):

FLMAX	constant = 3
LMAX	highest l of wave function inside sphere (consistent with **lapw1**)
LABC	highest l of wave function inside sphere where SO is considered
LOMAX	max l for local orbital basis
NRAD	number of radial mesh points

7.7.3 Input

A sample input for **lapwdm** is given below.

```
------------------ top of file: case.indm --------------------
-9.                     Emin cutoff energy
 1                      number of atoms for which density matrix is calculated
 1  1  2      index of 1st atom, number of L's, L1
 0 0          r-index, (l,s)-index
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: free format

emin	lower energy cutoff (usually set to very low number).

line 2: free format

natom	number of atoms for which the density matrix is calculated

line 3: free format
iatom, nl, l

iatom	index of atom for which the density matrix should be calculated
nl	number of l-values for which the density matrix should be calculated
l	l-values for which the density matrix should be calculated

line 3 is repeated natom times t
line 4: free format, optional
RINDEX, LSINDEX

RINDEX	0-3, as described in the introduction to **lapwdm**
LSINDEX	0-5, as described in the introduction to **lapwdm**

7.8 LCORE (generates core states)

lcore is a modified version of the Desclaux (69, 75) relativistic LSDA atomic code. It computes the core states (relativistically including SO, or non-relativistically if "NREL" is set in **case.struct**) for the current spherical part of the potential (**case.vsp**). It yields core eigenvalues, the file **case.clmcor** with the corresponding core densities, and the core contribution to the atomic forces.

7.8.1 Execution

The program **lcore** is executed by invoking the command:

lcore lcore.def or **x lcore [-up|-dn]**

For the spin-polarized case see fcc Ni on the distribution tape.

7.8.2 Dimensioning parameters

The following parameter is listend in file **param.inc**:

NRAD	number of radial mesh points

7.8.3 Input

Below is a sample input (written automatically by **lstart**)
for TiO_2 (rutile), one of the test cases provided with the **WIEN2k**
package.

```
------------------ top of file: case.inc --------------------
 4 0.0       # of orbitals,  shift of potential
 1,-1,2      n (principal quantum number), kappa, occup. number
 2,-1,2      2s
 2,-2,4      2p
 2, 1,2      2p*
 1   0.0         # of orbital of second atom
 1,-1,2      1s
 0           end switch
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: free format
nrorb, shift

nrorb	number of core orbitals
shift	shift of potential for "positive" eigenvalues (e.g. for 4f states as core states in lanthanides)

line 2: free format
n, kappa, occup

n	principle quantum number
kappa	relativistic quantum number (see Table 6.4)
occup	occupation number (including spin), fractial occupations supported

>>>: **line 2** is repeated for each orbital (nrorb times; see line 1)
>>>: **line 1 and 2** are repeated for each inequivalent atom. Atoms without core states (e.g. H or Li) must still include a 1s orbital, but with occupation zero.
line 3: free format

0	zero indicating end of job

7.9 MIXER (adding and mixing of charge densities)

In **mixer** the electron densities of core, semi-core, and valence states are added to yield the total new (output) density (in some calculations only one or two types will exist). Proper normalization of the densities is checked and enforced (by adding a constant charge density in the interstitial). As it is well known, simply taking the new densities leads to instabilities in the iterative SCF process. Therefore it is necessary to stabilize the SCF cycle. In **WIEN2k** this is done by mixing the output density with the (old) input density to obtain the new density to be used in the next iteration. Two mixing schemes are implemented:

1. straight mixing as originally proposed by Pratt (52) with a mixing factor Q

$$\rho_{new}(r) = (1-Q)\rho_{old}(r) + Q\rho_{output}(r)$$

2. the Broyden-II mixing scheme (Singh et al., 86), in which all the expansion coefficients of the density from several preceding iterations are utilized to calculate an optimal mixing fraction for each coefficient in each iteration.

At the outset of a new calculation (for any changed computational parameter such as k-mesh, matrix size, lattice constant etc.), any existing **case.broydX** files must be deleted (since the iterative history which they contain refers to a "different" incompatible calculation). In addition, in some cases better convergence can be achieved, if these files are removed every 15-20 iterations. Usually the Broyden scheme is much better than Pratt's scheme and thus is recommended.

After modifications to the **case.struct** file (lattice parameters, atomic positions) a run with mixing factor 0.0 can be used to renormalize the **case.clmsum_old** file from the previous case. If the file **case.clmsum_old** can not be found by **mixer**, a "PRATT-mixing" with mixing factor 1.0 is done.

*Note: a **case.clmval** file must always be present, since the LM values and the K-vectors are read from this file.*

The total energy and the atomic forces are computed in mixer by reading the **case.scf** file and adding the various contributions computed in preceding steps of the last iteration. Therefore **case.scf** must not contain a certain "iteration-number" more than once and the number of iterations in the scf file must not be greater than 99.

7.9.1 Execution

The program **mixer** is executed by invoking the command:

mixer mixer.def or **x mixer**

A spin-polarized case will be detected automatically by **x** due to the presence of a case.clmvalup file. For an example see fccNi (sec. 10.2) in the **WIEN2k** package.

7.9.2 Dimensioning parameters

The following parameters are collected in file **param.inc**, :

NCOM	number of LM terms in density
NRAD	number of radial mesh points
NSYM	order of point group

7.9.3 Input

Below a sample input (written automatically by **lstart**) is provided for TiO_2 (rutile), one of the test cases provided with the **WIEN2k** package.

```
------------------ top of file: case.inm --------------------
BROYD 0.d0  YES  (PRATT/BROYD, background charge (+1 for additional e), NORM
  0.4            MIXING FACTOR
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: (A5,f8.2,A5)
switch, bgch, norm

switch	BROYD	Broyden's scheme
	PRATT	Pratt's scheme
bgch		Background charge for charged cells (+1 for additional electron, -1 for core hole, if not neutralized by additional valence electron)
norm	YES	Charge densities are normalized to sum of Z
	NO	Charge densities are not normalized

line 2: free format

factor		mixing parameter Q (for Pratt and in the first iteration of Broyden). In the first iteration using Broyden's scheme: Q is automatically reduced by the program depending on the average charge distance :DIS and the number of non-equivalent TM (f)-elements. In case that the scf cycle fails due to large charge fluctuations, this factor must be further reduced (sometimes by an order of magnitude) before the calculations can be restarted (see sect.12

8 Programs for analysis, calculation of properties, and geometry optimization

Contents

8.1 TETRA (density of states)

This program calculates total and partial density of states (DOS) by means of the modified tetrahedron method (Blöchl et al 1994). It uses the partial charges in **`case.qtl`** generated by **`lapw2`** (switch QTL) and generates the DOS in states/Ry (files **`case.dos1/2/3`**) and in states/eV (with respect to the Fermi energy; files **`case.dos1/2/3ev`**). In spin-polarized calculations the DOS is given in states/Ry/spin (or states/eV/spin).

It is strongly recommended that you use "*Run Programs* ⇓ *Tasks* ⇓ *Density of States*" from **w2web**.

8.1.1 Execution

The program **tetra** is executed by invoking the command:

tetra tetra.def or **x tetra [-up|dn]**

8.1.2 Dimensioning parameters

The following parameters are listed in file **param.inc**:

MG	max. number of DOS cases (usually 21)
LXDOS	usually 1, except for "cross-DOS" (TELNES program) = 3

8.1.3 Input

An example is given below:

```
------------------ top of file: case.int ------------------
TiO2                          # Title
 -1.000     0.00250   1.200 0.003  # EMIN, DE, EMAX for DOS, GAUSS-Broad
    7                         # NUMBER OF DOS-CASES
    0    1   tot              # jatom, doscase, description
    1    2   Ti-s
    1    3   Ti-p
    1    4   Ti-px
    1    5   Ti-py
    1    6   Ti-pz
    2    1   O-tot
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: free format
title
line 2: free format
emin, delta, emax, broad

emin, delta, emax	specifies the energy mesh (in Ry) where the DOS is calculated. (emin should be set slightly below the lowest valence band; emax will be checked against the lowest energy of the highest band in **case.qtl**, and set to the minimum of these two values; delta is the energy increment.
broad	Gauss-broadening factor. Must be greater than delta to have any effect.

line 3: free format
ndos

ndos	specifies the number of DOS cases to be calculated. It should be at least 1 and can get up to 21. The corresponding output is written in groups of 7 to respective **case.dosX** files

line 4: (2i5,3x,a6)
jatom, jcol, description

jatom	specifies for which atom the DOS is calculated. 0 means total DOS, $jatom = nat + 1$ means DOS in the interstitial, where nat is the number of inequivalent atoms.
jcol	specifies the column to be used in the respective QTL-file. 1 means total, 2 . . . s, 3 . . . p, . . . The further assignment depends on the value of ISPLIT set in **case.struct** (see sec. 4.3); the respective description can be found in the header of **case.qtl**.
description	text used for further identification.

>>>**:line 4** is repeated "ndos" times

8.2 QTL (calculates special partial charges)

This program was contributed by:

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Inst. of Physics, Acad.Science, Prague, Czeck Republic
email: kunes@fzu.cz

Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

qtl creates the input for calculating total density of states, spin projected densities of states and densities of states projected on an arbitrary basis of a given l-subshell of any atom (including the relativistic jj_z basis) using **tetra**. For example it supports calculations of "$p_{1/2}$" or "$p_{3/2}$" DOS or an "approximate e_g/t_{2g}" splitting in a distrorted structure. The calculation is based on the spectral decomposition of a density matrix on a given atomic site and its transformation to the required basis. There are three types of input, which determine the results of the program:

a) the ordinary input file described below,

b) the unitary transformation matrix from the standard $_{lms}$-basis to the required one. For the most common bases (e.g. $_{jj_z}$, $_{lms}$, or $e_g - t_{2g}$) these matrices are supplied with the code in **$WIENROOT/SRC_templates/case.cf_*** and must be copied to **case.cf$iatom** . For less common cases these must be generated by hand.

c) the proper setting of the local rotation matrix in the **case.struct** file, which may be different from the setting for the scf calculation. In the special case of jj_z projected densities of states the local z-axis must coincide with the magnetization direction defined in **case.inso**. This is not done automaticaly but a message is written in the output together with the spin coordinate matrix.

qtl can use "parallel" vector-files and the output is written to **case.qtl$iatom**, which is used as an input for **tetra**.

8.2.1 Execution

The program **qtl** is executed by invoking the command:

x qtl [-up/dn -so -p] or
qtl qtl.def

8.2.2 Dimensioning parameters

LMAX	highest l of wave function inside sphere (consistent with **lapw1**)
LABC	highest l of wave function inside sphere where SO is considered
LOMAX	max l for local orbital basis
NRAD	number of radial mesh points

8.2.3 Input

A sample input for **case.inq** is given below.

```
------------------ top of file: case.inq --------------------
FULL                (SUMA,SPIN,TOTA)
DOSYM               (NOSYM)
0.0 1.2             Emin, Emax
0.768               Fermi energy
 2                  number of atoms for which density matrix is calculated
 1  2               index of 1st atom, L
 4  3
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: formatA4

FULL	all $2(2l+1)$ components of l-subshell are calculated
SUMA	only sums defined by stars in the **case.cf$n** file calculated
SPIN	projections of total DOS on up/dn subspaces for the case of a calculation with SOC
TOTA	shortcut for calculating total DOS only.

line 2: formatA5

DOSYM	standard option
NOSYM	symmetrization schwiched off. Allowed only in special cases.

line 3: free format

emin,emax	energy window

line 4: free format

ef	Fermi energy

line 5: free format

natom	number of atom for which projected DOS is calculated

line 6: free format
iatom, l

iatom	index of atom for which projected DOS should be calculated
l	l-value for which projected DOS should be calculated

line 6: is repeated natom times

8.3 SPAGHETTI (energy bandstructure plots)

This program generates an energy bandstructure plot (postscript file) using the eigenvalues printed in **case.output1** or **case.outputso**. Using the SCF potentials one runs **lapw1** with a special k-mesh along some high-symmetry lines (some sample inputs can be found in **SRC_templates/*.klist**). As an option, one can emphasize the character of the bands by additionally supplying corresponding partial charges (file **case.qtl** which can be obtained using **lapw2** with the QTL option and efmod set to ALL, see 7.5). This will be called "band-character plotting" below, in which each energy is drawn by a circle whose radius is proportional to the specified character of that state. It allows to analyze the character of bands (see also figures 3.15 and 3.16).

C.Persson has modifified this program and it allows now also to draw connected lines. For this purpose it uses the irreduzible representations (from file **case.irrep** produced by program **irrep** together with a table of "compatibility relations" to decide which points should be connected (non-crossing rule !). *(Note: The latter may not be complete leading to incorrect connections between high symmetry points and neighboring points in the BZ. Please inform us of such cases)*

It is strongly recommended that you use "*Run Programs ⇓ Tasks ⇓ Bandstructure*" from **w2web**.

8.3.1 Execution

The program **spaghetti** is executed by invoking the command:

spaghetti spaghetti.def or **x spaghetti [-up|dn] [-so]**

8.3.2 Input

An example is given below:

```
----------------- top of file: case.insp -------------------
### Figure configuration
 5.0   3.0                      # paper offset of plot
10.0  15.0                      # xsize,ysize [cm]
 1.0   4                        # major ticks, minor ticks
 1.0   1                        # character height, font switch
 1.1   2    4                   # line width, line switch, color switch
### Data configuration
-25.0 15.0  2                   # energy range, energy switch (1:Ry, 2:eV)
1      0.74250                  # Fermi switch,  Fermi-level (in Ry units)
1   999                         # number of bands for heavier plotting   1,1
0      1    0.02                # jatom, jtype, size  of heavier plotting
------------------- bottom of file ------------------------
```

for "character plotting"

Interpretive comments on this file are as follows:

line 1: free format
test

test	line must start with '###'. Begin of figure description. This tests also if you use the new input (different from WIEN97 or early WIEN2k versions)

line 2: free format
xoffset, yoffset

xoffset		x offset (in cm) of origin of plot
yoffset		y offset (in cm) of origin of plot

line 3: free format
xsize,ysize

xsize		plotsize in x direction (cm)
ysize		plotsize in y direction (cm)

line 4: free format
eincr, mtick

eincr		energy increment where y-axis labels are printed (major ticks)
mtick		number of minor ticks of y-axis

line 5: free format
charh, font

charh		scaling factor for size of labels
font	0	no text
	1	Times and Symbol
	2	Times,Times-Italic and Symbol
	3	Helvetica, Symbol, and Helvetica-Italic
	4	include your own fonts in defins.f

line 6: free format
linew, ilin, icol

linew		line width
ilin	0	dots or open circles (WIEN97 style)
	1	lines
	2	lines and open circles
	3	lines and filled circles
icol	0	black
	1	one-color plot
	2	three-color plot
	3	multi-color plot
	4	multi-color plot,one color for each irred. representation

line 7: free format
test

test		line must start with '###'. Begin of data description.

line 8: free format
emin, emax, iunits

emin		energy minimum of plot
emax		energy maximum of plot
iunits		
	1	energies in Ry (internal scale)
	2	energies in eV with respect to E_f

line 9: free format

iferm, efermi

iferm	0	no line at EF
	1	solid line at EF
	2	dashed line at EF
	3	dotted line at EF
efermi		Fermi energy (Ry); can be found in the respective **case.scf** file. If set to 999., E_f is not plotted (and iunits=2 cannot be used)

line 10: free format

nband1, nband2	lower and upper band index for bands which should show "band-character plotting" (if **case.qtl** is present and the proper switch is set, see below). In addition the corresponding x and y coordinates are written to file **case.spaghetti_ene** (which can be used for plotting with an external xy-plotting program).

line 11: free format
jatom, jcol, jsize

jatom	If a **case.qtl** file is present, jatom indicates the atom whose character (selected by jcol) is used for "band-character plotting" (dots are replaced by circles with radii proportional to the corresponding weight). If set to zero or if **case.qtl** is not present, "band-character plotting" does not occur.
jcol	specifies the column to be used in the respective QTL-file. 1 means total, 2 . . . s, 3 . . . p, . . . The further assignment depends on the value of ISPLIT set in **case.struct**. (ignored for jatom=0). The description can be found in the header of **case.qtl**.
jsize	size factor for radii of circles used in "band-character plotting"

if line 11 is repeated, averaging of QTLs for degenerate states is performed (useful in SO-calculations).

8.4 IRREP (Determine irreducible representations)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

This program determines the irreducible representation for each eigenvalue and all your k-points. It is in particular usefull to analyse energy bands and their connectivity.

You need a valid vector file, but no other input is required. The output can be found in **case.outputir** and **case.irrep**. For nonmagnetic SO calculations you must set IPR=1 in **case.inso**.

The output of this program is needed when you want to draw bandstructures with connected lines (instead of "dots").

It will not work in cases of non-symmorphic spacegroups AND k-points at the surface of the BZ. See also **$WIENROOT/SRC_irrep/README**.

8.4.1 Execution

The program **irrep** is executed by invoking the command:

irrep [up/dn]irrep.def or **x irrep [-so -up/dn]**

8.4.2 Dimensioning parameters

The following parameters are listend in file **param.inc**:

LOMAX	max. no. of local orbital. should be consistent with lapw1 and lapwso
NLOAT	number of different types of LOs
MSTP	max. step to describe k as a fraction
MAXDG	max. no. of degenerate eigenfunctions
MAXIRDG	max. no. of degenerate irr. representations
FLMAX	size of flag (FL) array (should be 4)
MAXIR	max. no. of irreducible representations
NSYM	max. no. of symmetry operations
TOLDG	min. energy deviation of degenerate states, in units of Rydberg

8.5 LAPW3 (X-ray structure factors)

This program calculates X-ray structure factors from the charge density by Fourier transformation.

You have to specify interactively valence or total charge density (because of the different normalization of **case.clmsum** and **case.clmval**) and a maximum $sin\theta/\lambda$ value.

8.5.1 Execution

The program **lapw3** is executed by invoking the command:

lapw3 lapw3.def or **lapw3c lapw3.def** or **x lapw3 [-c]**

8.5.2 Dimensioning parameters

The following parameters are listend in file **param.inc_r** or **param.inc_c** :

LMAX2	highest L in in LM expansion of charge and potential
NCOM	number of LM terms in density
NRAD	number of radial mesh points

8.6 LAPW5 (electron density plots)

This program generates the charge density (or the potential) in a specified plane of the crystal on a two dimensional grid which can be used for plotting with an external contour line program of your choice. Depending on the input files one can generate valence (**case.clmval**) or difference densities (i.e. crystalline minus superposed atomic densities) using the additional file (**case.sigma**). It is also possible to plot total densities (**case.clmsum**), Coulomb (**case.vcoul**), exchange-correlation or total (**case.r2v**) potentials, but in those cases the file **lapw5.def** has to be edited and you must replace **case.clmval** by the respective filename. The file **case.rho** contains in the first line

npx, npy, xlength, ylength;

and then the density (potential) written with:

```
      write(21,11) ((charge(i,j),j=1,npy),i=1,npx)
 11   format(5e16.8)
```

It is strongly recommended that you use *"Run Programs ⇓ Tasks ⇓ Electron density plots"* from **w2web**, see the TiC example inFig.3.6 .

8.6.1 Execution

The program **lapw5** is executed by invoking the command:

lapw5 lapw5.def or **lapw5c lapw5.def** or **x lapw5 [-c -up|dn]**

8.6.2 Dimensioning parameters

The following parameters are listend in file **param.inc**:

LMAX2	highest L in in LM expansion of charge and potential
NCOM	number of LM terms in density
NRAD	number of radial mesh points
NPT00	number of radial mesh points beyond RMT
NSYM	order of point group

8.6.3 Input

An example is given below. You may want to use XCRYSDEN by T.Kokalj to generate this file (see sect. 9.11.2).

```
---------------- top of file: case.inc --------------------
0 0 0 1           # origin of plot: x,y,z,denominator
1 1 0 1           # x-end of plot
0 0 1 2           # y-end of plot
3 3 3             # x,y,z nshells (of unit cells)
100 100           # nx,ny
RHO               # RHO/DIFF/OVER; ADD/SUB or blank
ANG VAL NODEBUG   # ANG/ATU, VAL/TOT, DEBUG/NODEBUG
NONORTHO          # optional line: ORTHO|NONORTHO
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: free format

ix,iy,iz,idv	The plane and section of the plot is specified by three points in the unit cell, an origin of the plot, an x-end and an y-end. The first line specifies the coordinates of the origin, where x=ix/idv, . . . in units of the lattice vectors (except fc, bc and c lattices, where the lattice vectors of the conventional cell are used)

line 2: free format

ix,iy,iz,idv	coordinates of x-end

line 3: free format

ix,iy,iz,idv	coordinates of y-end (The two directions x and y must be orthogonal to each other unless NONORTHO is selected). Since it is quite difficult to specify those 3 points for a rhombohedral lattice, an auxiliary program **`rhomb_in5`** is provided, which creates those points when you specify 3 atomic positions which will define your plane. You can find this program using "*Run Programs ⇓ Other Goodies*" from **w2web**.

line 4: free format

nxsh, nysh, nzsh	specifies the number of nearest neighbor cells (in x,y,z direction) where atomic positions are generated (needs to be increased for very large plot sections, otherwise some "atoms" are not found in the plot)

line 5: free format

npx, npy	specifies number of grid points in plot. npy=1 produces a file **`case.rho_onedim`** containing the distance r (from the origin) and the respective density, which can be used in a standard x-y plotting program.

line 6: format (2a4)
switch, addsub

switch	RHO	charge (or potential) plots, no atomic density is used (regular case)
	DIFF	difference density plot (crystalline - superposed atomic densities), needs file **`case.sigma`** (which is generated with LSTART, see section 6.4)
	OVER	superposition of atomic densities, needs file **`case.sigma`**
addsub	ADD	adds densities from units 9 and 11 (if present), e.g. to add spin-up and down densities.
	SUB	subtracts density of unit 11 (if present) from that of unit 9 (e.g. for the spin-density, which is the difference between spin-up and down densities). This is the default if this field is blank.

line 7: format (3a4)
iunits, cnorm, debug

iunits	ATU	density (potential) in atomic units e/a.u.^{3} (or Ry)

	ANG	density in e/Å^3 (do not use this option for potentials)
cnorm		determines normalization factor
	VAL	used for files **case.clmval**, **r2v**, **vcoul**
	TOT	used for files **case.clmsum**
debug	DEBU	debugging information is printed (large output)

line 8: free format

noorth1	ORTHO	(default) enforces directions to be orthogonal
	NONORTH	directions can be arbitrary; use this option only if your plotting program supports non orthogonal plots (e.g. for XCYSDENS).

In order to plot total densities or potentials (see cnorm as above) you have to create **lapw5.def** using **x lapw5 -d**, then edit **lapw5.def** and insert proper filenames (**case.clmval**, **case.r2v**, **case.vcoul**) for units 9 and 11, and finally run **lapw5 lapw5.def**.

8.7 AIM (atoms in molecules)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

This program analyses the topology of the electron density according to Bader's "Atoms in molecules" theory. For more information see Bader 2001 and Sofo and Fuhr 2001.

Basically it performs two different tasks, namely searching for "critical points" (CP) and/or determination of the atomic basins with an integration of the respective charge density.

It is important that you provide a "good" charge density, i.e. one which is well converged with respect to LMMAX in the CLM-expansion (you may have to increase the default LM-list to LM=8 or 10) and with as little "core-leakage" as possible (see **lstart**, sect. 6.4), otherwise discontinuities appear at the sphere boundary.

8.7.1 Execution

The program **aim** is executed by invoking the command:

aim aim.def or **aimc aim.def** or **x aim [-c]**

8.7.2 Dimensioning parameters

The following parameters are listend in file **param.inc**:

LMAX2	highest L in in LM expansion of charge and potential
NRAD	number of radial mesh points
NPT00	number of radial mesh points beyond RMT
NSYM	order of point group

8.7.3 Input

The input file contains “SWITCHES”, followed by the necessary parameters until an END-switch has been reached.

Examples for “critical-point” searches and “charge-integration” are given below:

```
---------------- top of file: case.inaim --------------------
CRIT
1                 # index of the atom (counting multiplicity)
ALL               # TWO/THRE/ALL /FOUR
3 3 3             # x,y,z nshells (of unit cells)
END
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: A4

CRIT — Keyword to calculate critical points

line 2: free format

iatom — index of the atom from where the search should be started. This count includes the multiplicity, i.e. if the first atom has MULT=2, the “second atom” has iatom=3 (Do not use simply the atom-numbers from **`case.struct`**)

line 3: A4

KEY — TWO, THRE, ALL, or FOUR
defines the starting point for the CP search to be in the middle of 2, 3 or 4 atoms. ALL combines option TWO and THRE together.

line 4: free format
nxsh, nysh, nzsh

specifies the number of nearest neighbor cells (in x,y,z direction) where atomic positions are generated.

lines 1-4 can be repeated with different atoms or KEYs
line 5: A4

END — specifies end of job.

In **`case.outputaim`** the critical points are marked with a label **`:PC`**

```
:PC a1 a2 a3 l1 l2 l3 c lap rho
```

where a1,a2,a3 are the coordinates of the CP in lattice vectors; l1 l2 l3 are the eigenvalues of the Hessian at the CP; c is the character of the CP (-3, -1, 1 or 3); lap is the Laplacian of the density at the CP (lap=l1+l2+l3) and rho is the density at the CP (all in atomic units).

```
---------------- top of file: case.inaim --------------------
SURF
3                                 atom in center of surface (including MULT)
40 0.0 3.1415926536               theta, 40 points, from zero to pi
40 -0.7853981634 2.3561944902     phi
0.07 1.0 4                        step along gradient line, rmin, check
1.65 0.1                          initial R for search, step (a.u)
3 3 3                             nshell
IRHO                              "INTEGRATE" rho
WEIT                              WEIT (surface weights from case.surf), NOWEIT
30                                30 radial points outside min(RMIN,RMT)
END
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: A4

SURF — Keyword to calculate the Bader surface.

line 2: free format

iatom — index of the atom from where the search should be started. This count includes the multiplicity, i.e. if the first atom has MULT=2, the “second atom” has iatom=3 (Do not use simply the atom-numbers from **case.struct**)

line 3: free format
ntheta, thmin, thmax

ntheta	number of theta directions for the surface determination
thmin	starting angle for theta
thmax	ending angle for theta. If you have higher symmetry, you can change thmin/max and use only the “irreducible” part, i.e. when you have a mirror plane normal to z, restrict thmax to $\pi/2$.

line 4: free format
nphi, phimin, phimax

nphi	number of phi directions for the surface determination
phimin	starting angle
phimax	ending angle. (see comments for theta to reduce phi from the full $0-2\pi$ integration).

line 5: free format
h0, frmin, nstep

h0	step in real space to follow the gradient (˜ 0.1)
frmin	defines the radius, for which the routine assumes that the search path has entered an atom, given as “rmin = frmin * rmt” (0.8-1.0)
nstep	number of steps between testing the position being inside or outside of the surface (4-8).

line 6: free format
r0, dr0

r0	initial radius for the search of the surface radius (1.5)
dr0	step for the search of the surface radius(0.1)

line 7: free format
nxsh, nysh, nzsh

specifies the number of nearest neighbor cells (in x,y,z direction) where atomic positions are generated.

line 8: A4

IRHO	integrate function on "unit 9" (usually **`case.clmsum`**) inside previously defined surface (stored in **`case.surf`**).

line 9: A4

WEIT	specifies the use of weights in **`case.surf`**.

line 9: free format

npt	specifies number of points for radial integration outside the MT (30)

line 8: A4

END	specifies end of job.

8.8 LAPW7 (wave functions on grids / plotting)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

The program **`lapw7`** generates wave function data on spatial grids for a given set of k-points and electronic bands. **`lapw7`** uses the wave function information stored in **`case.vector`** (or in reduced (filtered) form in **`case.vectorf`** which can be obtained from **`case.vector`** by running the program **`filtvec`**). Depending on the options set in the input file **`case.in7(c)`** one can generate the real or imaginary part of the wave functions, it's modulus (absolute value) or argument, or the complex wave function itself. For scalar-relativistic calculations both the large and the small component of the wave functions can be generated (only one at a time). The wave functions are generated on a grid which is to be specified in the input file(s). The grid can either be any arbitrary list of points (to be specified free-formatted in a separate file **case.grid**) or any n-dimensional grid ($n = 0...3$). The operating mode and grid parameters are specified in the input file **case.in7(c)**. As output **lapw7** writes the specified wave function data for further processing – e.g. for plotting the wave functions with some graphical tools such as gnuplot – in raw format to **case.psink**. For quick inspection, a subset of this data is echoed to the standard output file **case.outputf** (the amount of data can be controlled in the input). In case, **lapw7** is called many times for one and the same wave function, program overhead can be reduced, by first storing the atomic augmentation coefficients A_{lm}, B_{lm} (and C_{lm}) to a binary file **case.abc**. For the spin-polarized case two different calculations have to be performed using either the spin-up or the spin-down wave function data as input.

It should be easy to run **lapw7** in parallel mode, and/or to apply it to wave function data obtained by a spin-orbit interaction calculation. None of these options have been implemented so far. Also, **lapw7** has not yet been adapted for **w2web**.

Please note: **lapw7** requires an LAPW basis set and does not work with APW+lo yet.

8.8.1 Execution

The program **lapw7** is executed by invoking the command:

lapw7 lapw7.def or **lapw7c lapw7.def** or **x lapw7 [-c] [-up|dn] [-sel]**

With the **-sel** option **lapw7** expects data from the reduced (filtered) wave function file **case.vectorf**, otherwise the standard wave function file **case.vector** is used. The reduced vector file **case.vectorf** is assumed to resist in the current working directory, while the standard vector file **case.vector** (which may become quite large) is looked for in the `WIEN` scratch directory. For details see **lapw7.def**.

8.8.2 Dimensioning parameters

The following parameters are listed in file **param.inc_(r/c)**:

NRAD	number of radial mesh points
NSYM	order of point group
LMAX7	maximum L value used for plane wave augmentation
LOMAX	maximum L value used for local orbitals

The meaning of `LMAX7` is the same as that of `LMAX2` in **lapw2** and that of `LMAX-1` in `lapw1`. Rather than being an upper bound it directly defines the number of augmentation functions to be used. It may be set different to `LMAX2` in **lapw2** or `LMAX-1` in **lapw1**, but it must not exceed the latter one. Note that, the degree of continuity of the wave functions across the boundary of the muffin tin sphere is quite sensitive to the choice of the parameter `LMAX7`. A value of 8 for `LMAX7` turned out to be a good compromise.

8.8.3 Input

A sample input is given below. It shows how to plot a set of wave functions on a 2-dim. grid.

```
- - - - - - - - - - - - - - - - - - top of file - - - - - - - - - - - - - - - - - -
2D ORTHO                # mode  O(RTHOGONAL)|N(ON-ORTHOGONAL)
0 0 0 2                 # x, y, z, divisor of origin
3 3 0 2                 # x, y, z, divisor of x-end
0 0 3 2                 # x, y, z, divisor of y-end
141 101 35 25           # grid points and echo increments
NO                      # DEP(HASING)|NO (POST-PROCESSING)
RE  ANG LARGE           # switch  ANG|ATU|AU  LARGE|SMALL
1 0                     # k-point, band index
- - - - - - - - - - - - - - - - - - end of file - - - - - - - - - - - - - - - - - -
```

Interpretive comments on this file are as follows.

line 1:	format(A3,A1)		
	mode flag		
	mode		the type of grid to be used
		ANY	An arbitrary list of grid points is used.
		0D, 1D, 2D, or 3D	An n-dim. grid of points is used. $n = 0, 1, 2,$ or 3.
	flag		orthogonality checking flag (for n-dim. grids only)
		N	The axes of the n-dim. grid are allowed to be non-orthogonal.
		O or ⟨blank⟩	The axes of the n-dim. grid have to be mutual orthogonal.
line 2:	free format — (for n-dim. grids only)		
	ix iy iz idiv		Coordinates of origin of the grid, where x=ix/idv etc. in units of the *conventional* lattice vectors.
line 3:	free format — (for n-dim. grids with $n > 0$ only)		
	ix iy iz idiv		Coordinates of the end points of each grid axis. This input line has to be repeated n-times.
line 4:	free format — (not for 0-dim. grids)		
	np ... npo ...		In case of an n-dim. grid, first the number of grid points along each axis, and then the increments for the output echo for each axis. Zero increments means that only the first and last point on each axis are taken. In case of an arbitrary list of grid points, the total number of grid points and the increment for the output echo. Again a zero increments means that only the first and last grid point are taken. Hence, for n-dim. grids, altogether, $2*n$ integers must be provided; for arbitrary lists of grid points two intergers are expected.

line 5: format(A3)

tool		post-processing of the wave functions
	DEP	Each wave function is multiplied by a complex phase factor to align it (as most as possible) along the real axis (the so-called DEP(hasing) option).
	NO	No post-processing is applied to the wave functions.

line 6: format(A3,1X,A3,1X,A5)
switch iunit whpsi

switch		the type of wave function data to generate
	RE	The real part of the wave functions is evaluated.
	IM	The imaginary part of the wave functions is evaluated.
	ABS	The absolute value of the wave functions is evaluated.
	ARG	The argument the wave functions in the complex plane is evaluated.
	PSI	The complex wave functions are evaluated.
iunit		the physical units for wave function output
	ANG	Å units are used for the wave functions.
	AU or ATU	Atomic units are used for the wave functions.
whpsi		the relativistic component to be evaluated
	LARGE	The large relativistic component of wave function is evaluated.
	SMALL	The small relativistic component of wave function is evaluated.

line 7: free format
iskpt iseig

iskpt	The k-points for which wave functions are to be evaluated. Even if the wave function information is read from **`case.vectorf`**, iskpt refers to the index of the k-point in the original **`case.vector`** file! If iskpt is set to zero, all k-points in **`case.vector(f)`** are considered.
iseig	The band index for which wave functions are to be evaluated. Even if the wave function information is read from **`case.vectorf`**, iseig refers to the band index in the original **`case.vector`** file! If iseig is set to zero, all bands (for the selected k-point(s)) which can found in **`case.vector(f)`** are considered.

line 8: format(A4) — this line is optional

handle	augmentation coefficient control flag
SAVE or STOR(E)	Augmentation coefficients are stored in **case.abc**). No wave function data is generated in this case. This option is only allowed if a *single* wave function is selected in the previous input line.
READ or REPL(OT)	Previously stored augmentation coefficients are read in (from **case.abc**). This option is only allowed if the *same* single wave function as the one who's augmentation coefficients are stored in **case.abc** is selected in the previous input line.
anything else	Augmentation coefficients are generated from the wave function information in **case.vector(f)**.

8.9 FILTVEC (wave function filter / reduction of case.vector)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

The program **filtvec** reduces the information stored in **case.vector** files by filtering out a user-specified selection of wave functions. Either a fixed set of band indices can be selected which is used for all selected k-points (global selection mode), or the band indices can be selected individually for each selected k-point (individual selection mode). The complete wave function and band structure information for the selected k-points and bands is transferred to **case.vectorf**. The information on all other wave functions in the original file is discarded. The structure of the generated **case.vectorf** file is identical to that of the original **case.vector** file. Hence, it should be possible to use **case.vectorf** as substitutes for **case.vector** anywhere in the **WIEN** program package. (This has only been tested for **lapw7**.and **filtvec**.) To filter vector files from spin-polarized calculations, **filtvec** has to be run separately for both the spin-up and the spin-down files.

filtvec has not yet been adapted for **w2web**.

8.9.1 Execution

The program **filtvec** is executed by invoking the command:

filtvec filtvec.def or **filtvecc filtvec.def** or **x filtvec [-c] [-up|dn]**

In accordance with the file handling for **lapw1** and **lapw7** the input vector file **case.vector** is assumed to be located in the WIEN scratch directory, while the reduced output vector file **case.vectorf** is written to the current working directory. See **filtvec.def** for details.

8.9.2 Dimensioning parameters

The following parameters are listed in file **param.inc_(r/c)**:

NKPT	number of k-points
LMAX	maximum number of L values used (as in **lapw1**)
LOMAX	maximum L value used for local orbitals (as in **lapw1**)

The parameter LMAX and LOMAX must be set precisely as in **lapw1**; all other parameters must not be chosen smaller than the corresponding parameters in **lapw1**.

8.9.3 Input

Two examples are given below. The first uses global selection mode; the second individual selection mode.

I. Global Selection Mode

```
------------------- top of file -------------------
3  1 17 33    # number of k-points, k-points
2  11 -18     # number of bands, band indices
------------------- end of file -------------------
```

Interpretive comments on this file are as follows.

line 1:	free format	
	kmax ik(1) ... ik(kmax)	Number of k-point list items, followed by the list items themselves. Positive list items mean selection of the k-point with the specified index; negative list items mean selection of a range of k-points with indices running from the previous list item to the absolute value of the current one. E.g. the sequence 2 -5 stands for 2, 3, 4, and 5.
line 2:	free format	
	nmax ie(1) ... ie(nmax)	Number of band index items, followed by the list items themselves. Again, positive list items mean selection of a single band index; negative list items mean selection of a range of band indices.

II. Individual Selection Mode

```
------------------- top of file -------------------
2 :                     # number of k-points
17    4  11 13 15 17    # k-point, number of bands, band indices
33    3  11 -14 18      # k-point, number of bands, band indices
------------------- end of file -------------------
```

Interpretive comments on this file are as follows.

line 1:	free format	
	kmax	the number of individual k-points to be selected. This number must be followed by any text, e.g. 'SELECTIONS' or simply ':', to indicate individual selection mode.
line 2:	free format	
	ik nmax ie(1) ... ie(nmax)	First the index of the selected k-point, then the number of band index items, followed by the list items for the current k-point themselves. Positive list items mean selection of the band with the specified index; negative list items mean selection of a range of band indices running from the previous list item to the absolute value of the current one. E.g. the sequence 3 -7 stands for 3, 4, 5, and 7. This input line has to be repeated *kmax*-times.

8.10 XSPEC (calculation of X-ray Spectra)

This program calculates near edge structure of x-ray absorption or emission spectra according to the formalism described by Neckel et al.75, Schwarz et al. 79 and 80. For a brief introduction see below. It uses the partial charges in **case.qtl**. This file must be generated separately using **lapw2**. Partial densities of states in **case.dos1ev** are generated using the **tetra** program. Spectra are calculated for the dipole allowed transitions, generating matrix elements, which are multiplied with a radial transition probability and the partial densities of states. Unbroadened spectra are found in the file **case.txspec**, broadened spectra in the file **case.xspec**. Other generated files are: **case.m1** (matrix element for the selection rule L+1) and **case.m2** (matrix element for the selection rule L-1) and **case.corewfx** (radial function of the core state). The calculation is done with several individual programs (**initxspec**, **tetra**, **txspec**, and **lorentz**). which are linked together with the c-shell script **xspec**.

It is strongly recommended that you use "*Run Programs □ Tasks □ X-ray spectra*" from **w2web**.

8.10.1 Execution

Execution of the shell script xspec

The program **xspec** is executed by invoking the command:

xspec xspec.def or **x xspec [-up|-dn]**

Sequential execution of the programs

Besides calculating the X-ray spectra in one run using the **xspec** script, calculations can be done "by hand", i.e. step by step, for the sake of flexibility.

initxspec This program generates the appropriate input file **case.int**, according to the dipole selection rule, for the subsequent execution of the tetra program.
The program **initxspec** is executed by invoking the command:

initxspec xspec.def or **x initxspec [-up|-dn]**

tetra The appropriate densities of states for (L+1) and (L-1) states respectively are generated by execution of the **tetra** program.
The program **tetra** is executed by invoking the command:

tetra tetra.def or **x tetra [-up|-dn]**

txspec This program calculates energy dependent dipole matrix elements. Theoretical X-ray spectra are generated using the partial densities of states (in the **case.dos1ev** file) and multiplying them with the corresponding dipole matrix elements.
The program **txspec** is executed by invoking the command:

txspec xspec.def or **x txspec [-up|-dn]**

lorentz The calculated spectra must be convoluted to account for lifetime broadening and for a finite resolution of the spectrometer before they can be compared with experimental spectra. In the **lorentz** program a Lorentzian is used to achieve this broadening.
The program **lorentz** is executed by invoking the command:

lorentz xspec.def or **x lorentz [-up|-dn]**

8.10.2 Dimensioning parameters

The following dimensioning parameters are collected in the files **param.inc** of **SRC_txspec** and **SRC_lorentz**:

IEMAX0	maximum number of energy steps in the spectrum (SRC_lorentz)
NRAD	number of radial mesh points
LMAX	highest l+1 in basis function inside sphere (consistent with input in case.in1)

8.10.3 Input

Two examples are given below; one for emission spectra and one for absorption spectra:

Input for Emission Spectra:

```
---------------- top of file: nbc.inxs --------------------
NbC: C K                   (Title)
2                (number of inequivalent atom)
1                (n core)
0                (l core)
0,0.5,0.5        (split, int1, int2)
-20,0.1,3        (EMIN,DE,EMAX   in eV)
EMIS             (type of spectrum, EMIS or ABS)
0.35             (S)
0.25             (gamma0)
0.3              (W)
AUTO             (generate band ranges AUTOmatically or MANually
-7.21            (E0 in eV)
-10.04           (E1 in eV)
-13.37           (E2 in eV)
------------------- bottom of file ------------------------
```

Input for Absorption Spectra:

```
---------------- top of file: nbc.inxs --------------------
NbC: C K         (Title)
```

```
2               (number of inequivalent atom)
1               (n core)
0               (l core)
0,0.5,0.5       (split, int1, int2)
-2,0.1,30       (EMIN,DE,EMAX   in eV)
ABS             (type of spectrum)
1.0             (S)
------------------- bottom of file ------------------------
```

Interpretive comments on these files are as follows.

line 1: free format

TITLE	Title

line 2: free format

NATO	Number of the selected atom (in case.struct file)

line 3: free format

NC	principle quantum number of the core state

line 4: free format

LC	azimuthal quantum number of the core state

The table below lists the most commonly used spectra:

Spectrum	n	l
K	1	0
$L_{II,III}$	2	1
M_V	3	2

Table 8.56: Quantum numbers of the core state involved in the x-ray spectra

line 5 free format

SPLIT, INT1, INT2	split in eV between e.g. L_{II} and L_{III} spectrum (compare with the respective core eigenvalues), INT1 and INT2 specifies the relative intensity between these spectra. Values of 0, 0.5, 0.5 give unshifted spectra.

line 6: free format

EMIN, DE, EMAX	minimum energy, energy increment for spectrum, maximum energy; all energies are in eV and with respect to the Fermi level EMIN and EMAX are only used as limits if the energy range created by the **lapw2** calculation (using the QTL switch) is greater than the selected range.

line 7: Format A4

TYPE	EMIS	X-ray emission spectrum
	ABS	X-ray absorption spectrum (default)

line 8: free format

S	broadening parameter for the spectrometer broadening. For absorption spectra S includes both experimental and core broadening. Set S to zero for no broadening.

line 9: free format

GAMMA0	broadening parameter for the life-time broadening of the core states. Set GAMMA0 to zero to avoid lifetime broadening of the core states.

line 10: free format

W	broadening parameter for the life-time broadening of valence states. Set W to zero to avoid lifetime broadening of the valence states.

line 11: format A4

BANDRA		
	AUTO	band ranges are determined AUTOmatically (default)
	MAN	band ranges have to be entered MANually

line 12: free format

E0	Emission spectra: onset energy for broadening, E0, generated automatically if AUTO was set in line 10 Absorption spectra: not used

line 13: free format

E1	Emission spectra: onset energy for broadening, E1, generated automatically if AUTO was set in line 10 Absorption spectra: not used

line 14: free format

E2	Emission spectra: onset energy for broadening, E2, generated automatically if AUTO was set in line 10 Absorption spectra: not used

8.11 ELNES (calculation of energy loss near edge structure)

This program was contributed by:

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schatt@atp6000.tuwien.ac.at
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

This program calculates energy loss near edge structures (ELNES) according to the formalism described by Nelhiebel M. et al. 1999.

To calculate orientation dependent spectra the option formula must be set to "F" or "H" in the input. For systems with lower symmetry than orthorombic, "H" has to be selected and the following steps must be performed: generate a "full-k mesh" (make all positions inequivalent, set symmetry operations only to the identity), run **`x kgen`**, edit **`case.struct`** and set ISPLIT=99, rerun **`x lapw1`** and **`x lapw2 -qtl`**. For Formula "F" ISPLIT=88 is required.

8.11.1 Execution

Execution of the shell script elnes

The program **`elnes`** is executed by invoking the command:

`elnes elnes.def` or **`x elnes [-up|-dn]`**

Sequential execution of the programs

Besides calculating the ELNES in one run using the **`elnes`** script, calculations can be done "by hand", i.e. step by step, for the sake of flexibility.

initelnes This program generates the appropriate input file **`case.int`**, according to the dipole selection rule, for the subsequent execution of the tetra program. The program **`initelnes`** is executed by invoking the command:

`initelnes elnes.def` or **`x initelnes [-up|-dn]`**

tetra The appropriate densities of states for (L+1) and (L-1) states respectively are generated by execution of the **`tetra`** program. The program **`tetra`** is executed by invoking the command:

`tetra tetra.def` or **`x tetra [-up|-dn]`**

telnes This program calculates the electron energy loss spectrum. The program **`telnes`** is executed by invoking the command:

`telnes elnes.def` or **`x telnes [-up|-dn]`**

8.11.2 Dimensioning parameters

The following dimensioning parameters are collected in the file **`param.inc`** of **`SRC_telnes`**:

IEMAX0	maximum number of energy steps in the spectrum
NRAD	number of radial mesh points
LMAX	highest l+1 in basis function inside sphere (consistent with input in case.in1)
LMMX	number of LM terms in potential (should be at least NCOM-1)
NATO	number of inequivalent atoms
NDIF	total number of atoms per unit cell
NGAU	number of Gaunt coefficients for the non-spherical contributions to the matrix elements
NSLMAX	highest l+1 in basis functions for non-muffin-tin matrix elements (consistent with input in case.in1)
NPOSMAX	max. number of postions for simulation of a series of spectra
LAMBMAX	max. dimension of λ in the $3j$ Symbol

8.11.3 Input

An example input for the B-K edge of BN is given below:

```
---------------- top of file: bn.innes --------------------
Title: Atom 1 K Peak
1, 1            (atom)
1               (n core)
0               (l core)
0,0.05,30       (EMIN,DE,EMAX)
190, 0, .8      (E-Loss, Split between edges, precision; all in [eV])
200             (energy of the incident electrons (keV))
0, 0            (ThetaX, ThetaY in mrad)
0               (double of Bragg angle in mrad)
0, 0, 0         (DeltaX, DeltaY, Number of cases - 1: (0=1 case))
4               (LambdaMax)
L               (L for Line and P for Plane)
N               (N: Normal; F: Fine; H: HyperFine)
00.D0, 00.D0, 00.D0     (Euler angles)
0               (Spectrometer aperture in mrad)
0               (collection angle in mrad)
1, 1            (NR, NT)
------------------- bottom of file ------------------------
```

Interpretive comments on these files are as follows.

line 1: free format

TITLE	Title

line 2: free format

NATO, NEQ	Number of the selected atom (in case.struct file), number of the equivalent position (set to 0 to sum over all equivalent positions)

line 3: free format

NC	principle quantum number of the core state

line 4: free format

LC	azimuthal quantum number of the core state

line 5 free format

EMIN,DE,EMAX	Simulation of the edge will be performed from EMIN to EMAX with a step size of DE (in eV with respect to E_F)

line 6 free format

DeltaE, SPLIT, PreV	DeltaE is the energy loss of the first edge. SPLIT is the energy difference between the 2 edges of the same l′ with 2 possible j, first edge: $j = l' + 1/2$, second $j = l' - 1/2$. Their occupancy is $\frac{2j+1}{2(2l'+1)}$. PreV: Smoothening parameter/instrumental broadening: σ corresponding to a Gaussian function ($\sigma = \frac{FWHM}{2{,}35}$).

line 7 free format

Energy	Energy E0 of the incident electrons (in keV)

line 8 free format

ThetaX, ThetaY	ThetaX (mrad): angle between 000 and the EELS aperture in the direction of the second excited spot. ThetaY: angle in the orthogonal direction.

line 9 free format

TwoThetaB	$\vec{Q}_x - \vec{Q}_{x'}$ in mrad; usually the default value of 0 is not changed. It is only necessary when calculating off diagonal terms of the mixed dynamic form factor.

line 10 free format

DeltaThX, DeltaThY, NStep	Simulation of a series with different Bragg angles: increments $\Delta\theta_x$, $\Delta\theta_y$; number of cases - 1. NSTEP is usually set to 0 to simulate only one case

line 11 free format

LambdaMax	λ_{max} in the $3j$ Symbol (must be less than LAMBMAX). To restrict the calculation to the Dipole-Selection rule, set $\lambda_{max} = 1$

line 12 free format

Choice	Choice can either be L to simulate along a line or P to simulate in two dimensions

line 13 free format

Formula	Formula can either be N (normal: use l' DOS), F (fine: user $l'm'$ DOS) or H (hyperfine: use cross-DOS). Choice selects which formula is used to simulate the EELS spectra. **N** is normally used to simulate polycrystalline samples and gives an integral over 4π. **H** and **F** are required for the simulation of angular resolved spectra; in cases with a symmetry lower than orthorombic **H** is required.

line 14 free format

AAlpha, ABeta, AGamma	Euler angles between observer and crystal basis (only used if formula = F or H)

line 15 free format

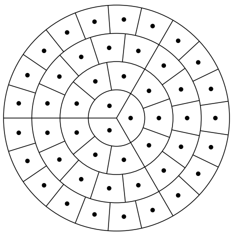
SpecAp	spectrometer aperture (mrad) (only used if formula = F or H)

line 16 free format

CoAng	collection angle (mrad) (only used if formula = F or H)

line 17 free format

NR, NT — integration parameters; set if SpecAp or CoAng $\neq 0$, integration scheme for NR=3 and NT=4 has the following grid:



8.12 OPTIMIZE (Volume and c/a Optimization)

This program generates a series of new struct files corresponding to different volumes or c/a ratios (depending on your input choice) from an existing struct file (either **`case_initial.struct`** or **`case.struct`**) and writes a shell script **`optimize.job`**. You may modify this script and execute it to find the equilibrium volume or c/a ratio (see Sec.5.3.1). When **`case_initial.struct`** is not present, it will be generated from the original **`case.struct`**.

8.12.1 Execution

The program **`optimize`** is executed by invoking the command:

`optimize optimize.def` or **`x optimize`**

8.12.2 Input

You have to specify interactively whether volume or c/a optimization should be carried out, how many cases you want to do and how large the change (+/- xx %) should be for each case.

8.13 ELAST (Elastic constants for cubic cases)

This program was contributed by:

Thomas Charpin
Lab. Geomateriaux de l'IPGP, Paris, France
(In September 2001 we received the sad notice that Thomas Charpin died in a car accident).
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

This package calculates elastic constants for cubic crystals. It is described in detail by the author in Charpin 2001.

8.13.1 Execution

The package is driven by three scrips:

- **init_elast**:
  It prepares the whole calculation and should be run in a directory with a valid **case.struct** and **case.inst** file. It creates the necessary subdirectories **elast**, **elast/eos**, **elast/tetra**, **elast/rhomb**, **elast/result**, the templates for tetragonal and rhombohedral distortion and initializes the calculations using **init_lapw**.
- **elast_setup**:
  It should be run in the **elast** directory, generates the distorted struct-files and **eos.job**, **rhomb.job** and **tetra.job**. These scripts must be adapted to your needs (spin-polarization, convergence,...) and run. **elast_setup** can be run several times (for different distortions,...).
- **ana_elast**:
  Once all calculations are done, change into **elastresult** and run this script. The final results are stored in **elastresultoutputs**.
- **genetempl, setelast, anaelast**:
  These three small programs are called by the above scripts.

8.14 MINI (Geometry minimization)

This program is usually called from the script **min_lapw** and performs movements of the atomic positions according to the calculated forces. It generates a new **case.struct** file which can be used in the next geometry/time step. Depending on the input options, **mini** helps to find the equilibrium positions of the atoms -using a damped Newton dynamics or a Broyden-Fletcher-Goldfarb-Shanno (BFGS) variable metric method- (see Kohler et al. 1996) or performs a molecular dynamics simulation. The forces are read from a file **case.finM**, while the "history" of the geometry optimization or MD is stored in **case.tmpM**

Note: We also tried several charge density extrapolation schemes, so that the new scf-run can be performed with a better starting density. However, they are currently not activated.

8.14.1 Execution

The program **mini** is executed by invoking the command:

mini mini.def or **x mini**

8.14.2 Dimensioning parameters

The following dimensioning parameters are collected in the file **param.inc**:

MAXIT	maximum number of geometry steps
NRAD	number of radial mesh points
NCOM	number of LM terms in density
NNN	number of neighboring atoms for nn
NSYM	order of pointgroup

8.14.3 Input

Two examples are given below; one for molecular dynamics using a NOSE thermostat and one for a Newton geometry optimization:

Input for Molecular dynamics:

```
---------------- top of file: nbc.inM --------------------
NOSE                      (NOSE/MOLD (a4))
58.9332 400. 1273. 5.0    (Masse, delta t, T, nose-frequency)
58.9332 400. 1273. 5.0
58.9332 400. 1273. 5.0
58.9332 400. 1273. 5.0
58.9332 400. 1273. 5.0
58.9332 400. 1273. 5.0
------------------- bottom of file -----------------------
```

Interpretive comments on this file are as follows.

line 1: format(a4,f5.2)

MINMOD		Modus of the calculation
	MOLD	Performs next molecular dynamics timestep
	NOSE	Performs next molecular dynamics timestep using a NOSE thermostat

line 2: free format

MASS	Atomic mass of i^{th} atom
TIMESTEP	Time step of MD (in atomic units, depends on highest vibrational frequencies)
TEMP	Simulation Temperature (K)
NOSF	Nose-frequency

>>>**line 2:** must be repeated for every atom

Input for geometry optimization:

```
---------------- top of file: nbc.inM --------------------
NEWT 2.0               (NEWT/BFGS   tolf (a4,f5.2))
0.3 0.3 0.3 0.8        ( 1..3:delta, 4:eta(1=friction zero))
0.3 0.3 0.3 0.8        ( 1..3=0 constraint)
------------------- bottom of file -----------------------
```

Interpretive comments on this file are as follows.

line 1: format(a4,f5.2)

MINMOD		Modus of the calculation
	NEWT	Performs geometry optimization with damped Newton scheme according to $R_m^{\tau+1} = R_m^\tau + \eta_m(R_m^\tau - R_m^{\tau-1}) + \delta_m F_m^\tau$ where R_m^τ and F_m^τ are the coordinate and force at time step τ. When the force has changed its direction from the last to the present timestep (or is within the tolerance TOLF), η_m will be set to $1 - \eta_m$.

BFGS	Performs geometry optimization with the variable metric method of BFGS. This option works well when a quadratic approximation is a good approximation to the specific potential surface
TOLF	Force tolerance, determines when geometry optimization stops

line 2: free format

DELTA(1-3)	x,y,z-delta parameters for damped Newton scheme. Determines speed of motion. Good values must be found for each individual system. They depend on the atomic mass, the vibrational frequencies and the starting point. DELTA(i) = 0 constrains the corresponding i-th coordinate (both in NEWT and BFGS)
ETA	damping (friction) parameter for damped Newton scheme. ETA=1 means no friction, ETA=0 means no speed from previous time steps

>>> **line 2:** must be repeated for every atom

8.15 OPTIC (calculating optical properties)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

The calculation of optical properties requires a dense mesh of eigenvalues and the corresponding eigenvectors. For that purpose start **kgen** and generate a fine k-mesh (with many k-points). Run **lapw1** and then **lapw2** with the option FERMI (*Note: You must also put TETRA / value=101. or ROOT/ALL in* ***case.in2***) in order to generate the weight-file. After the vector-file has been generated by **lapw1** run **optic** in order to produce the momentum matrix elements. Then the program **joint** carries out the BZ integration and computes the imaginary part of the complex dielectric tensor. In order to obtain the real part of the dielectric tensor **kram** may be executed which uses the Kramers-Kronig relations.

The program **optic** generates the momentum matrix elements

$\mathbf{M}_i = < n'\vec{k}|\vec{p}.\vec{e}_i|\, n\vec{k} >$

between all band combinations for each k-point given in the vector-file. For the orthogonal lattices the squared diagonal components can be found in the file **case.outmat**. For non-orthogonal systems all 6 components $(M_j)^* M_k$ can be calculated according to the symmetry of the crystal. In systems without inversion symmetry the complex version **opticc** must be executed.

The dielectric tensor components (and other quantities) are given per spin in case of the spin-polarized calculation and as a sum of both spin directions if the calculation is non-spinpolarized.

Due to spin-orbit coupling imaginary parts of the nondiagonal elements may occur. This in general, up to 9 components can be calculated at the same time.

8.15.1 Execution

The program **optic** is executed by invoking the command:

> **optic(c) optic.def** or **x optic [-c -up|dn -so]**

Recommended procedure for spin-orbit coupling:

In order to get the correct matrix elements, the files **case.vectorso[up|dn]** have to be used. For that purpose the following procedure is recommended:

- run SCF cycle: **run[sp]_lapw -so**
- generate a fine k-mesh for the optics part: **x kgen**
- change TOT to FERMI in **case.in2c**
- execute **run[sp]_lapw -so -s lapw1 -e lcore** with this fine k-mesh
- run optic: **x opticc -so [-up]**
- run joint: **x joint [-up]**
- run kram: **x kram [-up]**

Note: Also in the spin-polarized case only one call to ***optic****,* ***joint*** *and/or* ***kram*** *(either up or down) is necessary, since the spins are not independent any more and both vector-files are used at the same time.*

8.15.2 Dimensioning parameters

The following dimensioning parameters (listed in **param.inc_r** and **param.inc_c**) are used:

LMAX	highest l+1 in basis function inside sphere (consistent with input in case.in1)
LOMAX	highest l for local orbital basis (consistent with input in case.in1)
NRAD	number of radial mesh points
NSYM	order of point group

8.15.3 Input

An example is given below:

```
---------------- top of file: case.inop --------------------
256 1            : NKMAX, NKFIRST
-5.0 2.0         : EMIN, EMAX
2                : number of choices (columns in *outmat)
1                : Re xx
3                : Re zz
------------------- bottom of file ------------------------
```

Interpretive comments on this file are as follows:

line 1: free format

nkmax, nkfirst	maximal number of k-points , number of k-point to start calculation

line 2: free format

emin, emax	absolute energy range (Ry) for which matrix elements should be calculated

line 3: free format

ncol	number of choices (columns in case.outmat)

line 4+: free format

icol	column to select. Choices are: 1 ... Re $< x >< x >$ 2 ... Re $< y >< y >$ 3 ... Re $< z >< z >$ 4 ... Re $< x >< y >$ 5 ... Re $< x >< z >$ 6 ... Re $< y >< z >$ 7 ... Im $< x >< y >$ 8 ... Im $< x >< z >$ 9 ... Im $< y >< z >$ Options 7-9 apply only in presence of SO, options 4-6 only in non-orthogonal cases.

8.16 JOINT (Joint Density of States)

This program was contributed by:

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Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

This program carries out the BZ integration using the momentum matrix elements calculated before by **`optic`**. The interband or the intraband contributions to the imaginary part of the dielectric tensor can be computed. Alternatively, the DOS or the joint DOS can be derived.

The output in **`case.joint`** can be plotted with an xy-plotting package.

Warning: Negative values for ϵ_2 may occur due to negative weights in Blöchl's tetrahedron method.

8.16.1 Execution

The program **`joint`** is executed by invoking the command:

`joint joint.def` or **`x joint [-up|dn]`**

8.16.2 Dimensioning parameters

The following parameter is listend in files **`param.inc`**:

NSYM	order of point group
MG	number of columns

Note: The program might become very large if MG is set to a large value!

8.16.3 Input

An example is given below:

```
---------------- top of file: case.injoint -----------------------
    1    40                   : LOWER AND UPPER BANDINDEX
  -0.0000    0.00100   2.0000 : EMIN DE EMAX FOR ENERGYGRID IN ryd
eV                            : output units  eV / ryd
    4                         : SWITCH
    2                         : NUMBER OF COLUMNS
   0.1  0.1  0.3              : BROADENING (FOR DRUDE MODEL - switch 6,7)
------------------- bottom of file ------------------------------
```

Interpretive comments on this file are as follows:

line 1: free format

b1, b2		lower and upper band index

line 2: free format

emin, de, emax		Energy window and increment in Ry

line 3: free format

units	eV	output in units of eV
	Ry	output in units of Ry

line 4: free format

switch	0	joint DOS for each band combination
	1	joint DOS as sum over all band combinations
	2	DOS for each band
	3	DOS as sum over all bands
	4	imaginary part of the dielectric tensor (ϵ_2)
	5	imaginary part of the dielectric tensor for each band combination
	6	intraband contributions: number of “free“ electrons per unit cell assuming bare electron mass (calculated around $E_F \pm 10 * de$ as defined in input line 4), plasma-frequency
	7	in addition to switch 6 the contributions from different bands to the plasma frequency are analyzed.

line 5: free format

ncol		number of columns

line 6: free format
broadening

x,y,z		broadening parameters (in units defined in line 3) for Drude-model

The band analysis for all options (switches 0, 2, 5, and 7) has been improved: For each tensor component additional files are created, where each column contains the contributions from a single band or band combination. The file names are e.g. **`case.Im_eps_xx_1`**, **`case.Im_eps_xx_1`**, or **`case.jdos_1`** etc. where the number of files depend on the number of bands/band combinations.

Warning: The number of band combinations might be quite large!

8.17 KRAM (Kramers-Kronig transformation)

This program was contributed by:

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email: claudia.ambrosch@uni-graz.at
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

The Kramers-Kronig analysis is carried out for the actual number of columns contained in the **`case.joint[up|dn]`** file. For each real component its imaginary counterpart is created and vice versa. All dielectric tensor components can be found in file **`case.epsilon[up|dn]`**. The real and imaginary parts of the optical conductivity (in $10^{15}/s$) are written to file **`case.sigmak[up|dn]`**. In addition, file **`case.absorp`** contains the real parts of the optical conductivity (in $1/(\Omega cm)$ and the absorption coefficients. The loss function is also calculated (**`case.eloss`**), where for the previously calculated Plasma-frequency the intraband contributions can be added. The 3 sumrules are checked and written to **`case.sumrules`**.

The output in **`case.epsilon[up|dn]`** and **`case.sigmak[up|dn]`** can be plotted with an xy-plotting package.

8.17.1 Execution

The program **`kram`** is executed by invoking the command:

`kram kram.def` or **`x kram [-up|dn]`**

8.17.2 Dimensioning parameters

The following parameters are listed in files **`param.inc`**:

MAXDE	maximum number of points in energy mesh
MPOL	fixed at 6

8.17.3 Input

An example is given below:

```
--------------- top of file: case.inkram ----------------------
```

```
 0.0    gamma for Lorentz broadening (in units selected in joint)
 0.0    energy shift (scissors operator) (in units selected in joint)
  1      add intraband contributions? yes/no: 1/0
 12.60   plasma frequencies
  0.20   Gammas for Drude terms
------------------- bottom of file ------------------------------
```

Interpretive comments on this file are as follows:

line 1: free format

EGAMM		Lorentz broadening (in energy units selected in joint)

line 2: free format

ESHIFT		Energy shift (scissors operator) (in energy units selected in joint)

line 3: free format

INTRA	0	Intraband contributions are not added
	1	Intraband contributions are added (requires plasma-frequency)

line 4: free format

EPL		Plasma-frequency (calculated by **`joint`** using SWITCH=6)

line 5: free format

EDRU		Broadening for Drude terms

8.18 FSGEN (Fermi-surface generation)

Unfortunately there is no really versatile tool for Fermi surface generation or analyzing FS properties. We have collected here a series of small programs together with some description on how to proceed to generate 2D-Fermisurfaces within WIEN.

- As usually, you have to run an scf cycle and determine a good Fermi-energy. "Good" means here a Fermi-energy coming from a calculation with a dense k-mesh.
- You should than create a mesh within a plane of the BZ, where you want to plot the FS. Some utility programs like **`sc_fs_mesh`**, (fcc, bcc and hex are also available) may help you here, but only some planes of the BZ have been implemented so far. Please check these simple programs and modify them according to your needs. Insert the generated k-mesh **`fort.2`** into **`case.in1`**.
- Run **`lapw1`** with this k-mesh.
- Run **`spaghetti`** with input-options such that it prints the bands which intersect EF to **`case.spaghetti_ene`** (line 6, see sec. 8.3)
- Edit **`case.spaghetti_ene`** and insert a line at the top:
  NX, NY, x-len, y-len, NXinter, NYinter, Invers, Flip
  where
  NX, NY are the number of points in the two directions
  x-len, y-len are the length of the two directions of the plane (in bohr^{-1}, you can find this in **`case.spaghetti_ene`**)
  NXinter, NYinter: interpolated mesh, e.g. 2*NX-1

Invers: 0/1: mirrors x,y
FLIP: 0/1: flips x,y to y,x

- Run **spagh2rho < case.spaghetti_ene** to convert from this format into a format which is compatible with the **case.rho** file used for charge density plotting. It generates files **fort.11**, **fort.12**, ... (for each band separately) and you should use your favorite plotting program to generate a contourplot of the FS (by using a contourlevel = 0).

9 Utility Programs

Contents

9.1 symmetso

This program helps to setup spin-orbit calculations in magnetic systems. Since SO may break symmetry in certain spacegroups, it classifies your symmetry operations into operations **A**, which do not invert the magnetization (identity, inversion, rotations with the rotation axis parallel to magnetization), **B**, which invert it (mirror planes) and **C**, which change the magnetisation in some other way. (Note: magnetization is a result of a circular current, or equivalently, an axial vector resulting from a vector product $\hat{z} \sim \hat{x} \times \hat{y}$). **symmetso** will keep all A-type and throw away all C-type symmetry operations. Depending on the presence of inversion symmetry it will keep (inversion is present) or remove the B-type operations. Finally, **symmetso** uses the remaining symmetry operations to check/generate equivalent atomic positions (it can happen that some equivalent atoms become non-equivalent after inclusion of SO interaction).

In essence, it reads your **case.struct** and **case.inso** (for the direction of magnetization) files and creates an ordered **case.struct_orb** file with proper symmetry and equivalent atoms. It also generates a file **case.ksym**, which is a struct file with valid operations to generate a proper k-mesh using **''x kgen -so''**. In addition proper input files **case.in1, case.in2, case.inc, case.vspup/dn, case.vnsup/dn, case.clmsum, case.clmup/dn** are generated, so that you can continue with **runsp -so** without any further changes.

9.1.1 Execution

The program **symmetso** is executed by invoking the command:

symmetso symmetso.def or **x symmetso [-c]**

Usually it is called from the script **initso_lapw** and thus needs not to be invoked manually.

9.2 afminput

This program helps to determine an input for **clmcopy**, which is a program which copies spin-up densities of atom 1 to spin-down densities of atom 2 and vice versa in an anti-ferromagnetic arrangement. It uses **case.clmup** and **case.clmdn** to find out how and which atoms (and Fourier coefficients) must be interchanged. Therefore "exact" antiferromagnetic densities are necessary, generated either by using the appropriate starting densities from **dstart** (after you put AFM configuration in **case.inst**) or after a very well converged SCF calculation. Please see the comments in sect. 4.5.4 on how to proceed in detail for AFM calculations.

There is no other input file, but you may be ask to decide, whether two densities are "equal" or not.

9.2.1 Execution

The program **afminput** is executed by invoking the command:

afminput afminput.def or **x afminput**

9.2.2 Dimensioning parameters

The following parameters are used:

NCOM	number of LM components in the density (in **param.inc**)
NDIG	number of significant digits for "equivalency" of density components
NDIG1	as above for Fouriercoefficients
EMIN	exponent of a density component, which will be considered as "zero" in the program

9.3 clmcopy

This program generates the spin-dn density (**case.clmdn**) from a given spin-up density (**case.clmup**) according to rules in **case.inclmcopy** (generated earlier by **afminput**) for an AFM calculation. It works only for certain cases and it is well possible, that certain AFM structures will need code-extensions (as implemented for MnF_2 and $FeCO_3$), since there is not only a simple sign change of an up/dn Fouriercoefficient, but they may be swaped to a different K-vector too. Please see the comments in sect. 4.5.4 on how to proceed in detail for AFM calculations.

9.3.1 Execution

The program **clmcopy** is executed by invoking the command:

clmcopy clmcopy.def or **x clmcopy**

9.3.2 Dimensioning parameters

The following parameters are used in **`param.inc`**:

NCOM	number of LM components in the density
NRAD	number of radial mesh points
NSYM	number of symmetryoperations

9.3.3 Input

An example is given below:

```
---------------- top of file: case.inclmcopy -----------------------
   3                   NUMBER of ATOMS to CHANGE
   1   2               INTERCHANGE these ATOMS
   0                   NUMBER of LM to CHANGE SIGN
                       LM list
   3   3               INTERCHANGE these ATOMS
   4                   NUMBER of LM to CHANGE SIGN
 2 2 4 2 6 2 6 6       LM list
   4   4               INTERCHANGE these ATOMS
   6                   NUMBER of LM to CHANGE SIGN
 1 0 3 0 3 2 5 0 5 2 5 4    LM list
   3                   NUMBER of K-VECTOR-types to change sign
NORMAL                 (COMPLEX, MNF2, FECO3)
odd 0   0   -1.0
odd 0   odd -1.0
evenodd 0   -1.0
```

Interpretive comments on this file are as follows:

line 1: free format

NATOM	Number of atoms for which rules for copying the density will be defined

line 2: free format

N1, N2	Interchange spin-up and dn densities of atoms N1 and N2

line 3: free format

NLM	Number of LM values, for which you have to change the sign when swapping up and dn-densities

line 4: free format

L,M	NLM pairs of L and M, for which you have to change the sign when swapping up and dn-densities

Lines 2-4 have to be repeated NATOM times.

line 5: free format

NKK	number of K-vector types, for which you have to change the sign when swapping up and dn-densities

line 6: A10

CASE		defines how to treat the Fourier-coefficients
	MNF2	AFM Rutile structure (lines 7ff not used)
	FECO3	AFM $FeCO_3$ structure (lines 7ff not used)
	COMPLEX	uses all of lines 7ff
	NORMAL	uses x,y,z of lines 7ff and multiplies them with -1.d0

line 7: (3a4,2f4.1)

x,y,z,factor,factorc		
	x,y,z	character of the K-vector component. Can be “arb “, “even”, “odd “ or “0 “
	factor	factor with which one multiplies the real part of the up Fouriercomponents (CASE=COMPLEX, usually -1.)
	factorc	factor with which one multiplies the imaginary part of the up Fourier-components (CASE=COMPLEX, usually -1.)

Line 7 has to be repeated NKK times.

9.4 reformat

To produce a surface plot of the electron density using **`rhoplot_lapw`** (which is an interface to **`gnuplot`**), data from the file **`case.rho`** created by **`lapw5`** must be converted using **`reformat`**

The sources of the program **`reformat.c`** are supplied in **`SRC_reformat`**.

9.5 hex2rhomb and rhomb_in5

hex2rhomb interactively converts the positions of an atom from hexagonal to rhombohedral coordinates (needed in **case.struct**).

rhomb_in5 interactively helps to generate input **case.in5** for rhombohedral systems. It defines a plane as needed in the input file when you specify 3 atoms of that plane.

The sources of these programs are supplied in **SRC_trig**.

9.6 eosfit

Small program to calculate the Equation of States (EOS; Equilibrium volume V_0, Bulk modulus B_0 and it's derivative B_0', see Murnaghan 1944). It relies on the file **case.analysis** created from **w2web** using Total Energy and Volume.

The sources are supplied in **SRC_eosfit**.

9.7 spacegroup

This program was contributed by:

Vaclav Petricek
Institute of Physics
Academy of Sciences of the Czech Republic
Na Slovance 2
182 21 Praha (Prague) 8
Czech Republic
petricek@fzu.cz
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

Interactive program to generate equivalent positions for a given spacegroup and lattice. The program is also used internally from **w2web** to generate positions when selecting spacegroups in the **StructGen^{TM}**.

9.8 analyse

This program was contributed by:

Hartmut Enkisch
Institute of Physics E1b
University of Dortmund
Dortmund, Germany
enkisch@pop.uni-dortmund.de
Please make comments or report problems with this program to the WIEN-mailinglist. If necessary, we will communicate the problem to the authors.

analyse reads data from **case.scf** and writes them into **analyse.dat**. For each iteration it writes one line containing the parameters specified in the command line. **analyse** is meant to work in conjunction with the **scfmonitor** script (see 5.2.5).

9.9 xyz2struct

xyz2struct reads x,y,z-data from **case.xyz** and writes them into **case.struct_xyz**. You may have to adapt the read-format in the line with the label 10 in SRC_trig/xyz2struct.f. Since xyz data contain no symmetry information, all atoms with the same "label" will be treated as equivalent. The nuclear charges ZZ will not be given and you have to insert them manually.

(I recommend this program only for cases with many non-equivalent atoms and (almost) no symmetry. If you have spacegroup-information it is probably easier to use **StructGen™** and copy/paste of the positions).

9.10 StructGen™ of w2web

The new **StructGen™** helps to generate the master input file **case.struct**. It has the following additional features:

- automatic conversion from/to Å and Bohr
- Use spacegroup information (in conjunction with the **spacegroup** program (see 9.7 to generate equivalent positions)
- built in calculator to carry out simple arithmetic operations to specify the position parameters (of the equivalent atoms). Each position of equivalent atoms can be entered as a number, a fraction (e.g. $1/3$) or a simple expression (e.g. $0.21 + 1/3$). The first position defines the variables x, y and z, which can be using in expression defining the other positions (e.g. $-y$, x, $-z + 1/2$).

9.11 Visualization

9.11.1 BALSAC

balsac (Build and Analyze Lattices, Surfaces and Clusters) was written by Klaus Hermann (Fritz-Haber Institut, Berlin). It provides high quality postscript files. In SRC_balsac-utils we provide the following interface programs to convert from **WIEN2k** to **balsac**:

- **str2lat** to convert **case.struct** to **case.lat** (the BALSAC "lat" file).
- **str2plt** to convert **case.struct** to **case.plt** (the BALSAC "plt" file for one unit cell).
- **outnn2plt** to convert **case.outputnn** to **case.plt** (the BALSAC "plt" file for one unit cell). You have to select one atom (central atom) and than all nn-atoms are converted into the plt file.
- In addition converters to the xyz-format (**str2xyz, outnn2xyz**) for other plotting programs are also available.

For an example see figure 3.1 For scientific questions concerning BALSAC please contact Klaus Hermann at hermann@FHI-Berlin.MPG.DE

Balsac is available from:

Garching Innovation GmbH, Mrs. M. Pasecky Hofgartenstr. 8, D-80539 Munich, Germany
Tel.: +49 89 2909190, Fax.: +49 89 29091999
e-mail: gi@ipp.mpg.de
web: http://www.fhi-berlin.mpg.de/th/personal/hermann/balpam.html

9.11.2 XCrysDen

XCrysDen (Kokalj 1999) is a render and analysis package. It has the following features:

- render and analyze (distances, angles) the crystal structure
- generate k-mesh for bandstructure plots
- generate input and render 2D charge densities
- generate input and render 3D charge densities
- generate input and render Fermi surfaces

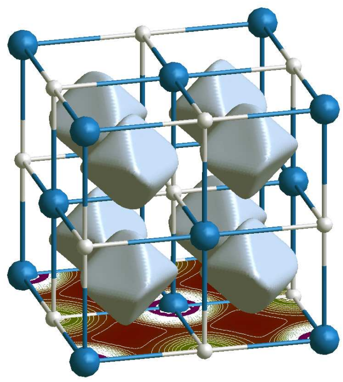

Figure 9.1: 3D electron density in TiC generated with XCrysDen

XCrysDen is available from:

Tone Kokalj
Jozef Stefan Institute, Dept. of Physical and Organic Chemistry
Jamova 39, SI-1000 Ljubljana, Slovenia
Tel.: +386 61 177 3520, Fax: +386 61 177 3811
Tone.Kokalj@ijs.si

10 How to run WIEN2k for selected samples

Three test cases are provided in the **WIEN2k** package. They contain the two starting files **`case.struct`** and **`case.inst`** and all the output so that you can compare your results with them.

The test cases are the following (where the names correspond to what was called CASE in the rest of this User's Guide)

```
TiC
Fccni
TiO2
```

We recommend to run these test cases (in a different directory) and compare the output to the provided one. All test cases are setup such that the CPU-time remains small (seconds). For real production runs the value of RKMAX in **`case.in1`** must be increased and a better (denser) k-mesh should be used.

In addition we provide a subdirectory **`example_struct_files`** were various more complicated struct files can be found.

10.1 TiC

The TiC example is described in detail in chapter 3 (**Quickstart**).

10.2 Fcc Nickel (spin polarized)

Ferromagnetic Nickel is a test case for a spin-polarized calculation. Ni has the atomic configuration $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^8$, $4s^2$ or [Ar] $3d^8$, $4s^2$. We treat the $1s$, $2s$, $2p$ and $3s$ as core states, and $3p$ (as local orbital), $3d$, $4s$ and $4p$ are handled as valence states. In a spin-polarized calculation the file structure and the sequence of programs is different from the non-spin-polarized case (see 4.5.2).

Create a new session and its corresponding directory. Generate the structure with the following data (we can use a large sphere as you will see from the output of **nn**):

Title	fcc Ni
Lattice	F
a	6.7 bohr
b	6.7 bohr
c	6.7 bohr
α, β, γ	90
Atom	Ni, enter position (0,0,0) and RMT = 2.3

Initialize the calculation using the default RKmax and use 3000 k-points (a ferromagnetic metal needs many k-points to yield reasonably converged magnetic moments). Allow for spin-polarization.

Start the scf cycle (**runsp_lapw**). At the bottom of the converged scf-file (**Fccni.scf**) you find the magnetic moments in the interstital region, inside the sphere and the total moment per cell (only the latter is an "observable", the others depend on the sphere size).

```
:MMINT: MAGNETIC MOMENT IN INTERSTITIAL =   -0.03266
:MMI01: MAGNETIC MOMENT IN SPHERE  1    =    0.65679
:MMTOT: TOTAL MAGNETIC MOMENT IN CELL   =    0.62413
```

10.3 Rutile (TiO_2)

This example shows you how to "optimize internal parameters".

Create a new session and its corresponding directory. Generate the structure with the following data (we use a smaller O sphere because Ti-d states are harder to converge then O-p):

Title	TiO2
Spacegroup	$P4_2/mnm$ (136)
a	8.682 bohr
b	8.682 bohr
c	5.592 bohr
α, β, γ	90
Atom	Ti, enter position (0,0,0) and RMT = 2.0
Atom	O, enter position (0.3,0.3,0) and RMT = 1.6

StructGen™should automatically add the equivalent positions.

Initialize the calculation using RKmax=6.5 in **tio2.in1_st** and use 100 k-points and a "shift" in **kgen**.

If you have a parallel machine, create a **.machine** file (possibly with 9 (or 3) processors since we have 9 k-points, for details see 5.4). You can use "*Execution* ⇓ Run scf", activate the "parallel" button" and "start scf" in **w2web**, or the UNIX command

cp $WIENROOT/SRC_templates/.machine .

Then start the structure minimization in **w2web** using "*Execution* ⇓ mini.positions". This will generate **TiO2.inM**, which you should edit and change the "stepsize" from 5.0 to 3.0. For execution you can either use the defaults or put

run_lapw -I -p -fc 1.0

as job (for parallel execution).

Alternatively you can use

cp $WIENROOT/SRC_templates/case.inM TiO2.inM
emacs TiO2.inM (and change all 5.0 to 3.0)
min_lapw -j ''run_lapw -I -fc 1 -p''

This will start an scf cycle, call the program **min**, which generates a new struct file using the calculated forces, and continues with the next scf cycle. It will continue until the forces are below 1 mRy/bohr (TiO2.inM) and the final results are not "saved" automatically but can be found in the "current" calculation.

You can watch the minimization using the file **TiO2.scf_mini**, which contains the final iteration of each geometry step. If the forces in this file oscillate from plus to minus and seem to diverge, or if they change very little, you can edit **TiO2.inM** (reduce or increase the stepsize), and remove **TiO2.tmpM** (contains the "history" of the minimization and is used to calculate the velocities of the moving atoms).

The final structural parameter of the O-atom should be close to x=0.304, which compares well with the experimental x=0.305.

Part III

Installation of the WIEN2k package and Dimensioning of programs

11 Installation and Dimensioning

Contents

11.1 Requirements

WIEN2k is written in FORTRAN 90 and requires a UNIX operating system since the programs are linked together via C-shell scripts. It has been implemented successfully on the following computer systems: Intel Pentium PCs running under Linux, IBM RS6000, HP, SGI, DEC Alpha and SUN. Hardware requirements will change from case to case (small cases with 10 atoms per unit cell can be run on a Pentium-II PC with 128 MB under Linux), but we recommend a more powerful PC or workstation with at least 256 MB (better 512 MM or more) memory and plenty of disk space (a few Gb).

For coarse grain parallization on the k-point level, a cluster of PCs with a 100 Mb/s network is sufficient. Faster communication is recommended for the fine grain (single k-point) parallel version.

In order to use all options and features (such as the new graphical user interface **w2web** or some of its plotting tools) the following public domain program packages in addition to a F90 compiler must be installed:

- perl 5 or higher (for **w2web** only)
- emacs or another editor of your choice
- ghostscript (with jpg support)
- gnuplot (with png support)
- www-browser
- pdf-reader, acroread
- MPI+SCALAPACK (for fine grain parallelization only)
- Tcl/Tk-Toolkit (for Xcrysden only)

Usually these packages should be available on modern systems. If one of these packages is not available it can either be installed from public domain sources (ask your computing center, use the WWW to search for the nearest location of these packages) or the corresponding configuration may be changed (e.g. using vi instead of emacs). None of the principal components of **WIEN2k** requires these packages, only **w2web** needs them.

11.2 Installation of WIEN2k

11.2.1 Expanding the WIEN2k distribution

The **WIEN2k** package comes as a single tar file (or you can download about 50 individual tar files separately), which should be placed in a subdirectory which will be your **$WIENROOT** directory (e.g. **./WIEN2k**). In addition you can download three examples, namely **TiC.tar.gz, TiO2.tar.gz** and **Fccni.tar.gz**.

Uncompress and expand all files using:

tar -xvf wien2k_00.tar (skip this if you downloaded files separately)
gunzip *.gz
chmod +x ./expand_lapw
./expand_lapw

You should have gotten the following directories:

```
./SRC
  SRC_afminput
  SRC_aim
  SRC_analyse
  SRC_balsac-utils
  SRC_clmcopy
  SRC_dstart
  SRC_elast
  SRC_eosfit
  SRC_filtvec
  SRC_fsgen
  SRC_initelnes
  SRC_initxspec
  SRC_irrep
  SRC_joint
  SRC_kgen
  SRC_kram
  SRC_lapw0
  SRC_lapw1
  SRC_lapw2
  SRC_lapw3
  SRC_lapw5
  SRC_lapw7
  SRC_lapwdm
  SRC_lapwso
  SRC_lcore
  SRC_lib
  SRC_lorentz
  SRC_lstart
  SRC_mini
  SRC_mixer
  SRC_nn
  SRC_optic
  SRC_optimize
  SRC_reformat
  SRC_sgroup
  SRC_spacegroup
  SRC_spaghetti
  SRC_sumpara
  SRC_symmetry
  SRC_telnes
  SRC_templates
  SRC_tetra
  SRC_trig
  SRC_txspec
  SRC_usersguide_html
  example_struct_files
  TiC
  TiO2
  fccni
```

Thus, each program has its source code (split into several files) in its own subdirectory. All programs are written in FORTRAN90 (except SRC_sgroup and SRC_reformat, which are in C).

/SRC contains the users guide (in form of a postscript file **usersguide.ps** and as pdf-file **usersguide.pdf**), all c-shell scripts and some auxiliary files.

/SRC_usersguide_html contains the html version of the UG.

/Fccni, **/TiC** and **/TiO2** contain three example inputs and the respective outputs.

/example_struct_files contains a collection of various struct files, which could be of use especially for the less experienced user.

/SRC_templates contains various input templates.

In addition to the expansion of the tar-files **./expand_lapw** copies also all csh-shell scripts from **/SRC** to the current directory and creates links for some abbreviated commands.

11.2.2 Site configuration for WIEN2k

At the end of **expand_lapw** you will be prompted to start the script

./siteconfig_lapw

When you start this script for the first time (file **INSTALLDATE** not present), you will be guided through the setup process.

Later on you can use **siteconfig_lapw** to redimension parameters, update individual packages and recompile the respective programs.

During the first run, you will be asked to specify:

- your system; at this point system specific files (e.g. **cputim.f** will be installed. If your system is not listed, use the system **generic**, which should compile on any machine.
- your FORTRAN90 and C compilers;
- your compiler and linker options as well as the place for LAPACK and BLAS libraries. Depending on the system you selected, we have included some recommended compiler and linker options, which are known to work on our systems (use **generic** when you have problems here; see also sec. 11.2.4). On some systems it is required to specify LAPACK and BLAS libraries twice (i.e. R_LIBS:-llapack_lapw -lblas_lapw -llapack_lapw -lblas_lapw). This generates Makefiles from the corresponding Makefile.orig in all subdirectories.
- configuration of parallel execution will ask whether your system is shared memory, so that default parameters can be set accordingly (**$WIENROOT/parallel_options** is the file where this information is stored).
- to configure parallel execution for distributed systems, specify the command to open a remote shell, which on most systems is **rsh** or **ssh**.
- You will then be asked wether you want to run fine-grained parallel. This is only possible if MPI and SCALAPACK are installed on your system and requires a fast network (100Mb/s is not very good) or a shared memory machine. It pays off only for big cases (matrixsize > 5000).
- You should define NMATMAX, i.e. the maximum matrixsize (number of basisfunctions). This value should be adjusted according to the memory of your hardware. Rough estimates are:
  NMATMAX= 5000 ==> 256MB (real) or 500MB (complex, without inversion symmetry)
  NMATMAX=10000 ==> 1GB (real) (==> cells with about 80-150 atoms/unitcell) If you choose it too large, **lapw1** will start to "page" leading to inacceptable performance or a crash.
- Now you are prompted to compile all programs (this will be done using **make**) and the executables are copied to the **$WIENROOT** directory.

Compilation might take quite some time. After compilation you will find a file **compile.msg** in each **SRC_*** directory.

Later on you can use **siteconfig_lapw** to change parameters, options or to update a package.

11.2.3 User configuration

Each **WIEN2k** user should run the script **userconfig_lapw**. This will setup a proper environment.

The script **userconfig_lapw** will do the following for you:

- set a path to **WIEN2k** programs
- add aliases, and
- add environment variables (**$WIENROOT**) to your **~/.cshrc** file.

Note: This will work only when the csh, tcsh or bash-shell is your login shell. Depending on your settings you may have to add similar lines also in your ***.login*** *file. If you are using a different login-shell, edit your startup files manually.*

11.2.4 Performance and special considerations

The script **siteconfig_lapw** is provided for general configuration and compilation of the **WIEN2k** package. When you call this script for the first time and follow the suggested answers, **WIEN2k** should run on your system (see 11.2.2).

The codes in the individual subdirectories **/SRC_program** are compiled using make. The file **Makefile** is generated during installation using **Makefile.orig** as template.

In some directories the source files ***.frc, *.F** and **param.inc_r/c** contain both, the real and complex (for systems without inversion symmetry) version of the code. You create the corresponding versions with **make** and **make complex,** respectively. (The ***.frc** and ***.F** files will then be preprocessed automatically).

The fine-grained parallel versions **lapw0_mpi; lapw1_mpi, lapw1c_mpi, lapw2_mpi, lapw2c_mpi** are created using **make para** (lapw0) and **make rp; make cp**.

For timing purposes a subroutine **CPUTIM** is used in several programs and specific routines for IBM-AIX, HP-UX, DEC-OSF1, SGI and SUN are available. On other systems **cputim_generic.c** should work.

On some HP systems you may encounter problems like: "stack growth failure". You may recompile with -K, reconfigure your Unix-kernel (with increased stack-size) or put large arrays in the respective program into COMMONS.

Most of the CPU time will be spent in **lapw1** and (to a smaller extent) in **lapw2 and lapw0**. Therefore we recommend to optimize the performance for these 3 programs:

- Find out which compiler options (**man f90**) make these programs run faster. You could specify a higher optimization (-O3), specify a particular processor architecture (-qarch=pp2 or -R10000, ...) or a preprocessor (like kapp or vast).
- Good performance depends on highly optimized BLAS and LAPACK libraries. Whenever it is possible, replace the supplied libraries (**SRC_lib/blas_lapw** and **SRC_lib/lapack_lapw**), by routines from your vendor (essl on IBM, complib.sgimath on SGI, dxml on DEC, try also blas, nag, or imsl libraries). If such libraries are not available try to optimize them yourself using the "ATLAS" system. (see http://math-atlas.sourceforge.net). We provide an ATLAS-BLAS for a Pentium4 with **WIEN2k**.

11.2.5 Global dimensioning parameters

WIEN2k is written in Fortran 90 and all important arrays are allocated dynamically. The only important parameters left are NMATMAX and NUME, specifying the maximum matrixsize (should be adjusted to the memory of your hardware, see above) and the maximum number of eigenvalues (must be increased for unitcells with large number of electrons)

Some less important parameters are still present and described in chapter "dimensioning parameters" of the respective section in chapter 6.

We recommend to use **siteconfig_lapw** for redimensioning and recompilation. In order to work properly, the parameter XXXX in the respective **param.inc** files must obey the following syntax:

```
PARAMETER(XXXX= ....)
```

Note: between "(", XXXX and "=" there must be no space.

11.3 Installation and Configuration of w2web

11.3.1 General issues

w2web requires **perl**, which should be available on most systems. (If not contact your system administrator or install it yourself from the WWW)

When you start **w2web** for the first time on the computer where you want to execute **WIEN2k** (you may have to telnet, ssh,.. to this machine) with the command **w2web [-p xxxx]**, you will be asked for a username/password (I recommend you use the same as for your UNIX login).

Later on you can add/remove users using "*Configuration* ⇓ edit accounts ".

You must also specify a "port" number (which can be changed the next time you start **w2web**). If the default port (7890) used to serve the interface is already in use by some other process, you will get the error message `w2web failed to bind port 7890 - port already in use!`. Then you will have to choose a different port number (between 1024 and 65536) . Please remember this port number, you need it when connecting to the **w2web** server.

*Note: Only user **root** can specify port numbers below 1024!*

Once **w2web** has been started, use your favorite WWW-browser to connect to **w2web**, specifying the correct portnumber, e.g. **netscape http://hostname_where_w2web_runs:7890**

Using "*Configuration* ⇓ interface configuration" you can further tailor the behaviour according to your wishes. In particular you can define new "execution types" to adjust to your queuing system. For example the line
batch=batch <%f
defines an execution type "batch" using the UNIX batch command. **w2web** collects its commands in a temporary script and you can access it using %f.

w2web saves several variables in startup files which are in the (~/.w2web) directory.

11.3.2 How does w2web work?

w2web acts like a normal web-server - except that it runs on a "user level port" instead of the default http-port 80. It serves html-files and executes perl-scripts or executes system or user commands on the server host.

11.3.3 w2web-files in you home directory

w2web creates on the first run the directory .w2web in your home directory with the following content:

- .w2web/conf
- .w2web/logs
- .w2web/sessions

11.3.4 The configuration file conf/w2web.conf

In this file various configuration parameters are stored by **w2web**. To restrict the access to certain IP addresses you can add lines like:

```
deny=*.*.*.*
allow=128.130.134.* 128.130.142.10
```

11.3.5 The password file conf/w2web.users

This file is created during the first run of **w2web**, and can be managed from within "Session Management ⇓ edit accounts", However now accounts are not activated until the next start of the **w2web**-server.

If you remove this file, the next start of **w2web**will activate the installation procedure again.

11.3.6 Using the https-protocol with w2web

In order to use the https-protocol the perl-library Net::SSLeay in addition to the OpenSSL package must be installed on your system. Both are freely available.

If you run **w2web**-server in ssl-mode you should get a site certificate for your server - in the meantime you can use the supplied certificate in **`$WIENROOT/SRC_w2web/bin/w2web.pem`** (by setting the keyfile=... line in your w2web.conf).

This certificate will not expire until 2015. Usually browsers will complain that they do not know the Certificate Authority who issued this certificate - if you don't like this message, you must buy a certificate from VeriSign, Thawte or a similar CA.

11.4 Environment Variables

WIEN2k uses the following environment variables:

WIENROOT base directory where **WIEN2k** is installed
PDFREADER specifies program to read pdf files (acroread, xpdf,...)
SCRATCH directory where **`case.vector`** and **`case.help??`** are stored.
EDITOR path and name of your prefered editor
XCRYSDEN_TOPDIR if this variable is set **WIEN2k** will activate all interface extensions to XCrysDen.
USE_REMOTE [0|1] determines whether parallel jobs are run in background (on shared memory machines) or using rsh. It is overridden by settings in **`$WIENROOT/parallel_options`**
WIEN_GRANULARITY Default granularity for parallel execution. It is overridden by setting the granularity in the **`.machines`** file or in **`$WIENROOT/parallel_options`**
WIEN_EXTRAFINE if set, the residual k-points are spread one by one over the processors.

12 Trouble shooting

In this chapter hints are given for solving some difficulties that have occurred frequently. This chapter is by no means complete and the authors would appreciate further suggestions which might be useful for other users. Beside the printed version of the users guide, an online pdf version is available using **help_lapw**. You can search for a specific keyword (use ^f keyword) and hopefully find some information.

> There is a mailing list for **WIEN2k** related questions. To subscribe to this list send mail to:
> `majordomo@theochem.tuwien.ac.at`
> with the text "subscribe wien". You will then automatically be added to the mailing list
> `wien@theochem.tuwien.ac.at`
> Please make use of this list!

If an error occurs in one of the SCF programs, a file program.error is created and an error message is printed into these files. The **run_lapw** script checks for these files and will automatically stop if a non-empty error file occurs.

Check the files **case.dayfile** (which is written by **init_lapw** and **run_lapw**), **:log** (where a history of all commands using **x** is given) and ***.error** for possible explanations.

In several places the dimensions are checked. The programs print a descriptive error message and stop.

case.outputnn: This file gives error messages if the atomic spheres overlap. But it should also be used to check the distances between the atoms and the coordination number (same distance). If inconsistencies exists, your **case.struct** file may contain an error. A check for overlapping spheres is also included in **mixer** and **lapw1**.

case.outputd: Possible stops or warnings are:

"NO SYMMETRY OPERATION FOUND IN ROTDEF": This indicates that in your **case.struct** file either the positions of equivalent atoms are not specified correctly (only positive coordinates allowed!!) or the symmetry operations are wrong.

case.output1: Possible stops or warnings are:

- **"NO ENERGY LIMITS FOUND IN SELECT":** This indicates that E_{top} or E_{bottom} could not be found for some $u_l(r, E_l)$. Check your input if it happens in the zeroth iteration. Later, (usually in the second to sixth iteration) it may indicate that in your SCF cycle something went wrong and you are using a crazy potential. Usually it means that mixing was too big and large charge fluctuations occured. Check previous charges for being physically reasonable (grep for labels :NTOxx :CTOxx :DIS). You will probably have to delete **case.broy*** and **case.scf**, rerun **x dstart** and reduce the mixing parameter in **case.inm**. In very difficult (magnetic) cases a PRATT mixing with 0.01 mixing might be necessary at the beginning!

"STOP RDC_22": This indicates that the overlap matrix is not positive definite. This usually happens if your **`case.struct`** file has some error in the structure or if you have an (almost) linear dependent basis, which can happen for large RKMAX values and/or if you are using very different (extremely small and large) sphere radii R_{MT}.

"X EIGENVALUES BELOW THE ENERGY emin": This indicates that X eigenvalues were found below emin. Emin is set in **`case.in1`** (see sec. 7.3.3) or in **`case.klist`** generated by KGEN, see 6.3, 6.5). It may indicate that your value of emin is too high or the possibility of ghostbands, but it can also be intentional to truncate some of the low lying eigenvalues.

If you don't find enough eigenvalues (e.g.: in a cell with 4 oxygens you expect 4 oxygen s bands at roughly -1 Ry) check the energy window (given at the end of the first k-point in **`case.in1`** or in **`case.klist`**) and make sure your energy parameters are found by subroutine SELECT or set them by hand at a reasonable value.

case.output2: Possible stops or warnings are:

"CANNOT BE FOUND": This warning, which could produce a very long output file, indicates that some reciprocal K-vector would be requested (through the k-vector list of lapw1), but was not present in the list of the K generated in lapw2. You may have to increase the NWAV, and/or KMAXx parameters in lapw2 or increase GMAX in **`case.in2`**. The problems could also arise from wrong symmetry operations or a wrong structure in **`case.struct`**.

"QTL-B VALUE": If larger than a few percent, this indicates the appearance of ghost bands, which are discussed below in section 12.1.
The few percent message (e.g up to 10 %) does not indicate a ghost band, but can happen e.g. in narrow d-bands, where the linearization reaches its limits. In these cases one can add a local orbital to improve the flexibility of the basis set. (Put one energy near the top and the other near the bottom of the valence band, see section 7.3.3).

FERMI LEVEL not converged (or similar messages). This can have several reasons: i) Try a different Fermi-Method (change TETRA to GAUSS or TEMP in **`case.in2`**). ii) Count the number of eigenvalues in **`case.output1`** and compare it with the number of valence electrons. If there are too few eigenvalues, either increase EMAX in **`case.klist`** (from 1.5 to e.g. 2.5) or check if your scf cycle had large charge oszillations (see **SELECT** error above)

If the SCF cycle stops somewhere (especially in the first few iterations), it is quite possible, that the source of the error is actually in a previous part of the cycle or even in a previous (e.g. the zeroth) iteration. Check in the **`case.scf`** file previous charges, eigenvalues, ... whether they are **physically reasonable** (see **SELECT** error above).

12.1 Ghost bands

Approximate linear dependence of the basis set or the linearization of the energy dependence of the radial wave functions (see section 2.2) can lead to spurious eigenvalues, termed "ghost bands".

The first case may occur in a system which has atoms with very different atomic sphere radii. Suppose you calculate a hydroxide with very short O-H bonds so that you select small R_{MT} radii for O and H such as e.g. 1.0 and 0.6 a.u., respectively. The cation may be large and thus you could choose a large R_{MT} of e.g. 2.4 a.u. However, this gives a four time larger effective RKmax for the cation than for H, (e.g. 16.0 when you select RKmax=4.0 in **`case.in1`**). This enormous difference in the convergence may lead to unphysical eigenvalues. In such cases choose lmax=12 in **`case.in1`** (in order to get a very good re-expansion of the plane waves) and reduce R_{MT} for the cation to e.g. 1.8 a.u.

The second case can occur when you don't use a proper set of local orbitals. In this situation the energy region of interest (valence bands) falls about midway between two states with different principle quantum numbers, but with the same l-value (for one atom).

Take for example Ti with its $3p$ states being occupied as (semi-core) states, while the $4p$ states remain mostly unoccupied. In the valence band region neither of those two states (Ti $3p$, $4p$) should appear. If one uses 0.2 Ry for the expansion energy E(1) for the p states of Ti, then Ti-p states do appear as ghost bands. Such a run is shown below for TiO_2 (rutile).

The lowest six eigenvalues at GAMMA fall between about -1.30 and -1.28 Ry. They are ghost bands derived from fictitious Ti-p states. The next four eigenvalues between -0.94 and -0.78 Ry correspond to states derived from O 2s states, which are ok, since there are four O's per unit cell, four states are found.

The occurrence of such unphysical (indeed, unchemical!) ghostbands is the first warning that something went wrong. A more definite warning comes upon running LAPW2, where the corresponding charge densities are calculated. If the contribution to the charge density from the energy derivative of the basis function [the B_{lm} coefficient in equ. 2.4,2.7] is significant (i.e. much more than 5 per cent) then a warning is issued in LAPW2.

In the present example it reads:

```
QTL-B VALUE .EQ. 40.35396 !!!!!!
```

This message is found in both the **case.scf** file and in **case.output2**.

When such a message appears, one can also look at the partial charges (QTL), which are printed under these conditions to OUTPUT2, and always appear in the files **case.helpXX**, etc., where the last digit refers to the atomic index.

In the file below, note the E(1) energy parameter as well as the 6 ghost band energies around -1.29.

```
-------------- top of file:tio2.scf ----------------------------
          ATOMIC SPHERE DEPENDENT PARAMETERS FOR ATOM  Titanium
          OVERALL ENERGY PARAMETER IS     .2000
          E( 0)=     .2000
--->      E( 1)=     .2000
          E( 2)=     .2000   E(BOTTOM)=    -.140   E(TOP)= -200.000


          ATOMIC SPHERE DEPENDENT PARAMETERS FOR ATOM  Oxygen
          OVERALL ENERGY PARAMETER IS     .2000
          E( 0)=    -.7100   E(BOTTOM)=   -2.090   E(TOP)=     .670

       K=    .00000    .00000    .00000           1
:RKM  : MATRIX SIZE= 599  RKM= 6.99  WEIGHT= 8.00  PGR:
       EIGENVALUES ARE:
        -1.2970782   -1.2970782   -1.2948747   -1.2897193  -1.2897193
        -1.2882306    -.9389111    -.8484857    -.7880729   -.7880729
         -.0484830    -.0162982     .0121181     .0976534    .0976534
          .1914068     .1914068     .2341991     .3286919    .3477629
          .3477629     .3809219     .5143729     .5356211    .5550735
          .5617155     .5617155     .7087550     .7197110    .8736991
          .8736991     .9428865     .9533619    1.2224570   1.2224570
         1.4285169
       ********************************************************
       NUMBER OF K-POINTS:          1

:NOE  : NUMBER OF ELECTRONS          =  48.000
:FER  : F E R M I - ENERGY           =    .53562

:POS01: AT.NR. -1  POSITION =  .00000  .00000  .00000  MULTIPLICITY=  2
       LMMAX=10
       LM=  0 0 2 0 2 2 4 0 4 2 4 4 6 0 6 2 6 4 6 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0
:CHA01: TOTAL CHARGE INSIDE SPHERE   1 =     8.802166
:PCS01: PARTIAL CHARGES SPHERE =  1 S,P,D,F,PX,PY,PZ,D-Z2,D-X2Y2,D-XY,D-XZ,D-YZ
:QTL01:  .127 6.080 2.518  .067 2.011 2.047 2.022 1.090  .760 .155  .480  .034
                    VXX         VYY         VZZ       UP TO R
:VZZ01:            -4.96856     8.48379    -3.51524       2.000
```

```
:POS02: AT.NR. -2  POSITION =  .30500  .30500  .00000  MULTIPLICITY=  4
       LMMAX=16
       LM=  0 0 1 0 2 0 2 2 3 0 3 2 4 0 4 2 4 4 5 0 5 2 5 4 6 0 6 2 6 4 6 6 0 0
:CHA02: TOTAL CHARGE INSIDE SPHERE   2 =     5.486185
:PCS02: PARTIAL CHARGES SPHERE =  2 S,P,D,F,PX,PY,PZ,D-Z2,D-X2Y2,D-XY,D-XZ,D-YZ
:QTL02: 1.559 3.902  .022  .002 1.296 1.306 1.300  .014  .004 .000  .003  .001
                      VXX         VYY         VZZ        UP TO R
:VZZ02:              .25199     -.55091      .29892       1.600

:CHA  : TOTAL CHARGE INSIDE CELL =      48.000000
:SUM  : SUM OF EIGENVALUES =            -15.810906

   QTL-B VALUE .EQ.   40.35396   !!!!!!
      NBAND in QTL-file:         24
----------------end of truncated file tio2.scf----------------------
```

Next we show **`tio2.output2`** for the first of the ghost bands at -1.297 Ry. One sees that it corresponds mainly to a p-like charge, which originates from the energy derivative part Q(UE) of the Kohn-Sham orbital. Q(UE) contributes 40.1% compared with 8.5% from the main component Q(U). Q(UE) greater than Q(U) is a good indication for a ghost band.

```
----------------part of file tio2.output2 -------------------------
   QTL-B VALUE .EQ.   40.35396   !!!!!!
  K-POINT:   .0000   .0000   .0000   599  36           1
  BAND #  1  E= -1.29708  WEIGHT= 2.0000000
         L= 0     L= 1      PX:      PY:      PZ:    L= 2    DZ2:  DX2Y2:    DXY:     DXZ:     DYZ:    L= 3
 QINSID:    .0000  48.6035  35.0996  13.5039   .0000   .0000   .0000   .0000   .0000   .0000   .0000   .0030
 Q(U)  :    .0000   8.4902   6.0125   2.4777   .0000   .0000   .0000   .0000   .0000   .0000   .0000   .0026
 Q(UE) :    .0000  40.1132  29.0871  11.0261   .0000   .0000   .0000   .0000   .0000   .0000   .0000   .0005
         L= 0     L= 1      PX:      PY:      PZ:    L= 2     DZ2:  DX2Y2:    DXY:     DXZ:     DYZ:    L= 3
 QINSID:    .1294    .0707    .0000    .0055   .0653   .0088   .0038   .0049   .0000   .0000   .0000   .0022
 Q(U)  :    .1279    .0627    .0000    .0052   .0575   .0087   .0038   .0049   .0000   .0000   .0000   .0020
 Q(UE) :    .0016    .0081    .0000    .0003   .0077   .0001   .0000   .0000   .0000   .0000   .0000   .0002
 QOUT  : 1.9265
---------------------bottom of truncated file ---------------------
```

Another file in which the same information can be found is **`tio2.help31`**, since the ghost band is caused by a bad choice for the Ti-p energy parameter:

```
----------------------Top of file tio2.help31 ---------------------
  K-POINT:   .0000   .0000   .0000   599  36           1
  BAND #  1  E= -1.29708  WEIGHT= 2.0000000
  L= 0     .00000      .00000    .00000    .00000    .00000    .00000
  L= 1   48.60346     8.49022  40.11324    .00000    .00000    .00000
    PX:  35.09960     6.01247  29.08712    .00000    .00000    .00000
    PY:  13.50386     2.47774  11.02612    .00000    .00000    .00000
    PZ:    .00000      .00000    .00000    .00000    .00000    .00000
  L= 2     .00000      .00000    .00000    .00000    .00000    .00000
   DZ2:    .00000      .00000    .00000    .00000    .00000    .00000
 DX2Y2:    .00000      .00000    .00000    .00000    .00000    .00000
   DXY:    .00000      .00000    .00000    .00000    .00000    .00000
   DXZ:    .00000      .00000    .00000    .00000    .00000    .00000
   DYZ:    .00000      .00000    .00000    .00000    .00000    .00000
  L= 3     .00304      .00255    .00050    .00000    .00000    .00000
  L= 4     .00000      .00000    .00000    .00000    .00000    .00000
  L= 5     .00096      .00082    .00014    .00000    .00000    .00000
  L= 6     .00000      .00000    .00000    .00000    .00000    .00000
-------------------bottom of truncated file--------------------------
```

Note again for L=1 the percentage of charge associated with the primary (APW) basis functions ul (8.5%) versus that coming from the energy derivative component (40.1%).

If a ghost band appears, one should first analyze its origin as indicated above, then use appropriate local orbitals to improve the calculation and get rid of these unphysical states.

Do not perform calculations with "ghost-bands", even when the calculation converges.

Good luck !

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Part IV

Appendix

A Local rotation matrices

Local rotation matrices are used to rotate the global coordinate system (given by the definition of the Bravais matrix) to a local coordinate system for each atomic site. They are used in the program for two reasons:

- to minimize the number of LM combinations in the lattice harmonics expansion (of potential and charge density according to equ. 2.10). For example for point group mm2 one needs for L=1 just LM=1,0 if the coordinate system is chosen such that the z-axis coincides with the 2-fold rotation axis, while in an arbitrary coordinate system the three terms 1,0; 1,1 and -1,1 are needed (and so on for higher L).
- The interpretation e.g. of the partial charges requires a proper orientation of the coordinate system. In the example given above, the p orbitals split into 2 irreducible representations, but they can be attributed to p_z and p_x, p_y only if the z-axis is the 2-fold rotation axis.

It is of course possible to perform calculations without "local rotation matrices", but in such a case the LM combinations given in Table 7.40 (and by SYMMETRY) may not be correct. (A program SYM written by G. Vielsack determines the LM values for arbitrary orientations.)

Fortunately, the "local rotation matrices" are usually fairly simple and are now **automatically inserted** into your **`case.struct`** file. Nevertheless we recommend to check them in order to be sure.

The most common coordinate transformations are

- interchanging of two axes (e.g. x and z)
- rotation by $45°$ (e.g. in the xy-plane)
- rotation of z into the (111) direction

Inspection of the output of SYMMETRY tells you if the local rotation matrix is the unit matrix or it gives you a clear indication how to find the proper matrix.

The local rotation matrix $\mathbf{R}$, which transforms the global coordinates r to the rotated ones r', is defined by $\mathbf{R}r = r'$.

There are two simple ways to check the local rotation matrixes together with the selected LM combinations:

- charge density plots generated with LAPW5 must be continuous across the atomic sphere boundary (especially valence or difference density plots are very sensitive, see 8.6)
- Perform a run of LAPW1 and LAPW2 using the GAMMA-point only (or a complete star of another k point). In such a case, "wrong" LM combinations must vanish. Note that the latter is true only in this case. For a k mesh in the IBZ "wrong" LM combinations do not vanish and thus must be omitted!!

A first example for "local rotation matrices" is given for the rutile TiO2, which has already been described as an example in section 10.3. Also two other examples will be given (see below).

A.1 Rutile (TiO_2)

Examine the output from symmetry. It should be obvious that you need local rotation matrices for both, Ti and O:

```
....
Titanium   operation #  1     1
Titanium   operation #  2     -1
Titanium   operation #  5     2 || z
Titanium   operation #  6     m n z
Titanium   operation # 12     m n 110
Titanium   operation # 13     m n -110
Titanium   operation # 18     2 || 110
Titanium   operation # 19     2 || -110
  pointgroup is mmm (neg. iatnr!!)
  axes should be: m n z, m n y, m n x
```

This output tells you, that for Ti a mirror plan normal to z is present, but the mirror planes normal to x and y are missing. Instead, they are normal to the (110) plane and thus you need to rotate x, y by $45°$ around the z axis. (The required choice of the coordinate system for mmm symmetry is also given in Table 7.40)

```
....
Oxygen     operation #  1     1
Oxygen     operation #  6     m n z
Oxygen     operation # 13     m n -110
Oxygen     operation # 18     2 || 110
  pointgroup is mm2 (neg. iatnr!!)
  axes should be: 2 || z, m n y
```

For O the 2-fold symmetry axes points into the (110) direction instead of z. The appropriate rotation matrices for Ti and O are:

$$\begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix}$$

A.2 Si Γ-phonon

Si possesses a face-centered cubic structure with two equivalent atoms per unit cell, at (±0.125, ±0.125, ±0.125). The site symmetry is -43m. For the Γ-phnon the two atoms are displaced in opposite direction along the (111) direction and cubic symmetry is lost. The output of SYMMETRY gives the following information:

```
Si         operation #  1     1
Si         operation # 13     m n -110
Si         operation # 16     m n -101
Si         operation # 17     m n 0-11
Si         operation # 24     3 || 111
Si         operation # 38     3 || 111
  pointgroup is 3m (neg. iatnr!!)
     axis should be: 3 || z, m n y
lm: 0 0  1 0  2 0  3 0  3 3  4 0  4 3  5 0  5 3  6 0  6 3  6
```

Therefore the required local rotation matrix should rotate z into the (111) direction and thus the matrix in the "struct" file should be:

0.4082483	-.7071068	0.5773503	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{3}$
0.4082483	0.7071068	0.5773503	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{3}$
-.8164966	0.0000000	0.5773503	$-2\frac{\sqrt{6}}{6}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{3}$

A.3 Trigonal Selenium

Selenium possesses space group P3121 with the following struct file:

```
H    LATTICE,NONEQUIV.ATOMS: 1
MODE OF CALC=RELA  POINTGROUP:32
 8.2500000 8.2500000  9.369000
ATOM= -1: X= .7746000  Y= .7746000  Z= 0.0000000
          MULT= 3          ISPLIT= 8
ATOM= -1: X= .2254000  Y= .0000000  Z= 0.3333333
ATOM= -1: X= .0000000  Y= .2254000  Z= 0.6666667
Se         NPT=  381  R0=.000100000 RMT=2.100000000  Z:34.0
LOCAL ROT.MATRIX:    0.0       0.5000000 0.8660254
                     0.0000000 -.8660254 0.5000000
                     1.0000000 0.0000000 0.0
   6    IORD OF GROUP G0
......
```

The output of SYMMETRY reads:

```
Se         operation #  1     1
Se         operation #  9     2 $|$$|$ 110
  pointgroup is 2 (neg. iatnr!!)
  axis should be: 2 || z
lm: 0 0  1 0  2 0  2 2 -2 2  3 0  3 2 -3 2  4 0  4 2 -4 2 ......
```

Point group 2 should have its 2-fold rotation axis along z, so the local rotation matrix can be constructed in two steps: firstly interchange x and z (that leads to z || (011)) and secondly rotate from (011) into (001) (see the struct file given above). Since this is a hexagonal lattice, SYMMETRY uses the hexagonal axes, but the local rotation matrix must be given in cartesian coordinates.

B Periodic Table

Periodic Table of the Elements

1**H** $\mathrm{1s}$																	2**He** $\mathrm{1s^{2}}$
3**Li** $\mathrm{He2s}$	4**Be** $\mathrm{He2s^{2}}$											5**B** $\mathrm{He2s^{2}2p}$	6**C** $\mathrm{He2s^{2}2p^{2}}$	7**N** $\mathrm{He2s^{2}2p^{3}}$	8**O** $\mathrm{He2s^{2}2p^{4}}$	9**F** $\mathrm{He2s^{2}2p^{5}}$	10**Ne** $\mathrm{He2s^{2}2p^{6}}$
11**Na** $\mathrm{Ne3s}$	12**Mg** $\mathrm{Ne3s^{2}}$											13**Al** $\mathrm{Ne3s^{2}3p}$	14**Si** $\mathrm{Ne3s^{2}3p^{2}}$	15**P** $\mathrm{Ne3s^{2}3p^{3}}$	16**S** $\mathrm{Ne3s^{2}3p^{4}}$	17**Cl** $\mathrm{Ne3s^{2}3p^{5}}$	18**Ar** $\mathrm{Ne3s^{2}3p^{6}}$
19**K** $\mathrm{Ar4s}$	20**Ca** $\mathrm{Ar4s^{2}}$	21**Sc** $\mathrm{Ar3d^{1}4s^{2}}$	22**Ti** $\mathrm{Ar3d^{2}4s^{2}}$	23**V** $\mathrm{Ar3d^{3}4s^{2}}$	24**Cr** $\mathrm{Ar3d^{5}4s^{1}}$	25**Mn** $\mathrm{Ar3d^{5}4s^{2}}$	26**Fe** $\mathrm{Ar3d^{6}4s^{2}}$	27**Co** $\mathrm{Ar3d^{7}4s^{2}}$	28**Ni** $\mathrm{Ar3d^{8}4s^{2}}$	29**Cu** $\mathrm{Ar3d^{10}4s^{1}}$	30**Zn** $\mathrm{Ar3d^{10}4s^{2}}$	31**Ga** $\mathrm{Ar3d^{10}4s^{2}4p}$	32**Ge** $\mathrm{Ar3d^{10}4s^{2}4p^{2}}$	33**As** $\mathrm{Ar3d^{10}4s^{2}4p^{3}}$	34**Se** $\mathrm{Ar3d^{10}4s^{2}4p^{4}}$	35**Br** $\mathrm{Ar3d^{10}4s^{2}4p^{5}}$	36**Kr** $\mathrm{Ar3d^{10}4s^{2}4p^{6}}$
37**Rb** $\mathrm{Kr5s}$	38**Sr** $\mathrm{Kr5s^{2}}$	39**Y** $\mathrm{Kr4d^{1}5s^{2}}$	40**Zr** $\mathrm{Kr4d^{2}5s^{2}}$	41**Nb** $\mathrm{Kr4d^{3}5s^{2}}$	42**Mo** $\mathrm{Kr4d^{5}5s^{1}}$	43**Tc** $\mathrm{Kr4d^{5}5s^{2}}$	44**Ru** $\mathrm{Kr4d^{6}5s^{2}}$	45**Rh** $\mathrm{Kr4d^{7}5s^{2}}$	46**Pd** $\mathrm{Kr4d^{8}5s^{2}}$	47**Ag** $\mathrm{Kr4d^{10}5s^{1}}$	48**Cd** $\mathrm{Kr4d^{10}5s^{2}}$	49**In** $\mathrm{Kr4d^{10}5s^{2}5p}$	50**Sn** $\mathrm{Kr4d^{10}5s^{2}5p^{2}}$	51**Sb** $\mathrm{Kr4d^{10}5s^{2}5p^{3}}$	52**Te** $\mathrm{Kr3d^{10}5s^{2}5p^{4}}$	53**I** $\mathrm{Kr4d^{10}5s^{2}5p^{5}}$	54**Xe** $\mathrm{Kr4d^{10}5s^{2}5p^{6}}$
55**Cs** $\mathrm{Xe6s}$	56**Ba** $\mathrm{Xe6s^{2}}$	57-71 **La-Lu**	72**Hf** $\mathrm{Xe4f^{14}5d^{2}6s^{2}}$	73**Ta** $\mathrm{Xe4f^{14}5d^{3}6s^{2}}$	74**W** $\mathrm{Xe4f^{14}5d^{5}6s^{1}}$	75**Re** $\mathrm{Xe4f^{14}5d^{5}6s^{2}}$	76**Os** $\mathrm{Xe4f^{14}5d^{6}6s^{2}}$	77**Ir** $\mathrm{Xe4f^{14}5d^{7}6s^{2}}$	78**Pt** $\mathrm{Xe4f^{14}5d^{8}6s^{2}}$	79**Au** $\mathrm{Xe4f^{14}5d^{10}6s^{1}}$	80**Hg** $\mathrm{Xe4f^{14}5d^{10}6s^{2}}$	81**Tl** $\mathrm{Xe4f^{14}5d^{10}6s^{2}6p}$	82**Pb** $\mathrm{Xe4f^{14}5d^{10}6s^{2}6p^{2}}$	83**Bi** $\mathrm{Xe4f^{14}5d^{10}6s^{2}6p^{3}}$	84**Po** $\mathrm{Xe4f^{14}3d^{10}6s^{2}6p^{4}}$	85**At** $\mathrm{Xe4f^{14}5d^{10}6s^{2}6p^{5}}$	86**Rn** $\mathrm{Xe4f^{14}5d^{10}6s^{2}6p^{6}}$
87**Fr** $\mathrm{Rn7s}$	88**Ra** $\mathrm{Rn7s^{2}}$	89-103 **Ac-Lr**															

57**La** $\mathrm{Xe5d6s^{2}}$	58**Ce** $\mathrm{Xe4f^{2}6s^{2}}$	59**Pr** $\mathrm{Xe4f^{3}6s^{2}}$	60**Nd** $\mathrm{Xe4f^{4}6s^{2}}$	61**Pm** $\mathrm{Xe4f^{5}6s^{2}}$	62**Sm** $\mathrm{Xe4f^{6}6s^{2}}$	63**Eu** $\mathrm{Xe4f^{7}6s^{2}}$	64**Gd** $\mathrm{Xe4f^{7}5d6s^{2}}$	65**Tb** $\mathrm{Xe4f^{9}6s^{2}}$	66**Dy** $\mathrm{Xe4f^{10}6s^{2}}$	67**Ho** $\mathrm{Xe4f^{11}6s^{2}}$	68**Er** $\mathrm{Xe4f^{12}6s^{2}}$	69**Tm** $\mathrm{Xe4f^{13}6s^{2}}$	70**Yb** $\mathrm{Xe4f^{14}6s^{2}}$	71**Lu** $\mathrm{Xe4f^{14}5d6s^{2}}$
89**Ac** $\mathrm{Rn6d7s^{2}}$	90**Th** $\mathrm{Rn6d^{2}7s^{2}}$	91**Pa** $\mathrm{Rn5f^{2}6d^{1}7s^{2}}$	92**U** $\mathrm{Rn5f^{3}6d^{1}7s^{2}}$	93**Np** $\mathrm{Rn5f^{4}6d^{1}7s^{2}}$	94**Pu** $\mathrm{Rn5f^{6}7s^{2}}$	95**Am** $\mathrm{Rn5f^{7}7s^{2}}$	96**Cm** $\mathrm{Rn5f^{7}6d7s^{2}}$	97**Bk** $\mathrm{Rn5f^{9}7s^{2}}$	98**Cf** $\mathrm{Rn5f^{10}7s^{2}}$	99**Es** $\mathrm{Rn5f^{11}7s^{2}}$	100**Fm** $\mathrm{Rn5f^{12}7s^{2}}$	101**Md** $\mathrm{Rn5f^{13}7s^{2}}$	102**No** $\mathrm{Rn5f^{14}7s^{2}}$	103**Lr** $\mathrm{Rn5f^{14}6d7s^{2}}$

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