xband



A graphical user interface to run band structure programs

Version 6.3

1 Introduction

xband is a graphical user interface (GUI) that supplies a number of basic functionalities to facilitate the use of a band structure program. The menu COMPILE PROGRAMS allows one to edit make, dimension and source files and to compile the available programs. With TIDY UP files needed no more can easily be deleted. One of the most tedious step of a band structure calculation is usually setting up the input file. **xband** simplifies this by creating via CREATE SYSTEM a system file, that contains all information on the atomic configuration and geometry of a system. Various ways of visualisation are supplied to document or check the created atomic configuration that makes use of the program **rasmol**. The system file is independent of the program package used and can be stored and retrieved again later via the SELECT/MODIFY SYSTEM menu. Calling a band structure program package allows one to set up specific input files using the information stored in a system file. In addition program execution can be prepared and initiated in various ways. The resulting output

files can be printed, catenated or edited while data files can be further processed using the program **plot** to create **xmgrace** graphics files. Although **xband** has been developed primarily to support the use of the **SPRKKR** package of H. Ebert et al., it can easily be modified to support other packages as well (see Customisation).

xband has been written in tcl language starting from the LATEX GUI xtem of Lamprecht, Lotz and Weibezahn and can be used, copied, modified and distributed on the basis of the GNU licence rules (see the file copying). **xband** uses auxiliary FORTRAN programs (**plot**, **findsym** and **spheres**) written by H. Ebert and A. Perlov that are part of the **xband** distribution with the GNU licence rules applying. The program **spheres** is based on subroutines that stem from the Stuttgart LMTO-package and that have been developed by G. Krier, O. Jepsen and O.K. Andersen.¹ In addition **xband** uses programs (**emacs**, **xmgrace**, **rasmol** and **dataexplorer**) that are not part of the **xband** distribution, but can be obtained free (e.g. as part of a Linux distribution). For high quality 3D plotting of Bloch spectral functions the **DISLIN** library can optionally be used. It is a plotting library free of charge for academic use and has to be downloaded from http://www.dislin.de and installed as described there.

2 Installation

xband can be obtained from the web-page: http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/ To install **xband** create a directory (in the following ~ /band) and copy the package xband_DATE.tar.gz to that directory. Execute gunzip xband_DATE.tar.gz tar -xvf xband_DATE.tar

This step supplies all tcl-files and creates the subdirectory ~/band/locals that contains all default settings in various files (*.vst) as well as three data files (*.dat). You may modify all files apart from ITXC_spacegroups.dat.

When you call **xband** it checks whether the programs **findsym**, **plot**, **spheres** and **glbox** are available. If not, it will try to create the executables. To supply **findsym** (**plot**, **spheres**, **glbox**) yourself, go to ~/band/symmetry (~/band/graphics, ~/band/spheres, ~/band/glbox) and call make. If the compilation failed, adapting the compiler name and options to your system in the makefile should remove the problems. You have to use Fortran 95 compatible compiler. We suggest to use Intel fortran compiler.In all makefiles variable FC is set to ifort. If necessery, please change it to your favor compiler.

Note that the executable **findsym** (**plot**, **spheres**, **glbox**) will be copied automatically upwards to ~/band and named findsym_\$(OSTYPE) (plot_\$(OSTYPE), sphere_\$(OSTYPE), glbox_\$(OSTYPE)), i.e. for example findsym_linux or findsym_OSF1. This allows one to work with **xband** simultaneously under several operating systems.

If the **DISLIN** library is available on your computer and you want to use it for plotting, please edit the makefile in ~ /band/graphics and change the line USEDISLIN=0 to USEDISLIN=1.

¹We thank these colleagues for the permission to use these subroutines.

xband is started by calling the Unix script **xband** that you'll find in ~ /band. Edit this script and specify the directory where the **xband** tcl-files can be found. E.g.: test XBANDPATH || \$XBANDPATH=\$HOME/band.

To use the script **xband** add the directory ~ /band to your PATH or copy **xband** to a directory that is included in your PATH (e.g. ~/bin or ~/com).

3 Calling xbond

Call **xband** by

xband

or

xband &

If **xband** is called from a xterm window it will write some output to that window used for checking.

4 Main Menu



Figure 1: Screenshot main window

Starting **xband** the main window shown in Fig. 1 will be opened. The top button list supplies the following functionality:

exit : exit xband.

exit + store settings : store present settings for **xband** in */*.xband.vst and exit **xband**.

help: print help information to the text field at the bottom.

clear text field : clear the text field at the bottom.

unlock: if a button like TIDY UP is pressed all others will be locked as long as the corresponding menu is in use. unlock allows one to unlock the buttons, e.g. if the TIDY UP menu was not left properly.

The text field at the bottom will be used for help information. It is also used by other menu windows if these have no own text field. Check this field for hints if something seems to go wrong.

The central field of the main menu shows the **xband** logo and supplies two columns of menu buttons that will be described below. In addition the field displays on its right hand side the names of the working directory and system files after these have been set.

The field between the central one and the text field allows one to call the plot menu via PLOT. In addition it gives access to the program packages that are available to the user. The settings for this field are specified in the file ~ /band/locals/packages.vst. Pressing one of the program package buttons activates the RUN PROGRAM PACKAGE menu that has the same structure for all packages. For that reason only that for the SPRKKR package of H. Ebert et al. will be described below.

5 The SET PREFERENCES menu

X + SET P	REFERENCES • 🗖 ×
colors 🛛 🔶	colored 🕹 grey
geometry 🔶	standard 🕹 small
debugging 🔷	NO info 🔶 print info
fonts settings	modify
editor settings	modify
print-command for ps-files	lpr -Plp
rasmol-version	rasmol
dataexplorer-version	dx
gopenbox-version	box
PRO	DGRAM CALLS
TB-LMTO	tbimto < inputfile
LMTO-AP	Imtoap < inputfile
KKR-AKAI	size2 < inputfile
SPR-KKR	kkrscf < inputfile
PROG_PATH0 - default path	/home/he/bin/
grep string 1	ETOT
grep string 2	ERR
grep string 3	CPA
CLOSE	STORE

Figure 2: Screenshot SET PREFERENCES menu

When starting, **xband** presets all parameters with internal defaults. It then tries to read *~*/.xband.vst if this is available. With SET PREFERENCES (see Fig. 2) you may specify the name of a program (e.g. **rasmol**) if it deviates from the default name.

In case of problems with the size of some menu windows one may reduce their size by changing the geometry setting. By default **xband** uses colours, that may be suppressed. All settings can be modified by editing the files ~ /band/locals/geometry.vst and ~ /band/locals/colors.vst.

The switch **debugging** controls whether debugging information is written to the xterm to start **xband**.

The button **modify** in the field **fonts settings** invokes a menu that allows one to select fonts. After you made your choice for all fonts in use, **xband** writes these to the file

[~] /band/locals/fonts.vst. You can edit this file any time and replace a font by another one. Calling the unix command xlsfonts gives you a list of all fonts available on your machine. Note: if **xband** is called the first time and it cannot find the fonts that have been preset, the font select menu will also be invoked to replace those fonts which are not available.

The button modify in the field **editor settings** invokes a menu that allows one to select an editor. If your favorite editor is not in the list you may add its specifications in ~ /band/locals/editor.vst.

For every program package used one may specify how a program is invoked. This may be program < inputfile

if the input is read from standard input, or

program inputfile options

if the program gets the name and options from the command line.

All settings will be stored in ~ /.xband.vst using the button **STORE** to exit. The content of this file is shown in the info region at the bottom of the main window.

6 The COMPILE PROGRAMS menu

This menu is invoked by **COMPILE PROGRAMS** used to edit make, dimension and source files and to compile programs (see Fig. 3).

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

Makefile, dimension and source file lists: use left mouse click to select. Edit selected files using the edit buttons. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~/band/locals.

Selecting a source file automatically starts **emacs** for editing. Selecting a makefile gives a list of possible calls of make in the makefile window (top region). Use left mouse click to select a make call and execute the compilation.

[X +		COMPILE PROGRAMS	• • X
close help clear text	t field		
current directory <i>T</i> home makefile NONE			
select and run			
	M-FILE SELECTED edit		
source file NO SO	OURCE FILE SELECTED edit		
select directory \$HOME graphics help locals spheres symmetry	select makefile file list (make*): alphabetical AKI AkKI Make	* 🔳 🔶 alphabetical 🛛 .dim 🔳	select and edit source file source file suffx i alphabetical last access
directory:	makefile: (make*)	dim-file: (.dim):	source-file: (.f):

Figure 3: Screenshot COMPILE PROGRAMS menu





7 The TIDY UP menu

The left column of the menu (see Fig. 4) invoked with TIDY UP gives a list of suffixes (edit ~/.xband.vst to modify). Activate/deactivate the suffixes as needed and delete the files with activated suffixes by pressing the button remove all files shown here (right). The names of the deleted files are given in the text field at the bottom of the window.

8 The DIRECTORIES menu



Figure 5: Screenshot DIRECTORY menu

The DIRECTORIES menu (see Fig. 5) invoked via DIRECTORIES allows one to create and remove directories.

Directory list (centre region left): use left mouse click to change the directory.

File list (centre): use left/middle mouse click to select/edit a file.

The column on the right hand side allows one to create and remove directories. To create a new directory modify the entry field at the top of the column and press the appropriate create button. To remove a directory press **REMOVE CURRENT DIRECTORY**. **xband** will take care that you remove only empty directories. Leaving the menu via the button **close+create system** invokes the create system menu without going via the main menu.

9 The CREATE SYSTEM menu

(+				CRE	ATE SYSTEM				- 0
lose h	elp clear te	xt field							
	system	name of syste	m-file		ci	OSE	DO	DNE - RE	TURN
pecify s	structure via:	Structure	type Spa	ice group	Per pedes	multi layers	unlock		edit database
ttice pa	arameters	A =	5.4	[a.u.]		number of sites	NQ	1	
-	5.4	b =	5.4	C =	5.4	inequivalent site:	s NCL	1	
	0.4					atom types	NT	0	
		b/a =	1.0	c/a =	1.0	space group		229	
-	90	β =	90	γ =	90	cubic body-c	entered m3m	O_h	
10	CL WS	X	to specify occu Y	Z	en R_W	ipty spheres	structure	NC	
1		0.000000	0.000000						

Figure 6: Screenshot CREATE SYSTEM menu

This menu (see Fig. 6) is used to create a system file that contains all geometrical information on a system. Leaving the menu activated by CREATE SYSTEM using the button DONE - RETURN writes the system file, while selecting a system using

SELECT/MODIFY SYSTEM rereads it again (see below).

By default the CREATE SYSTEM menu allows one to set up 3D-structures. In addition one can set up 2D- and 0D-structures calling the corresponding menus via the buttons

 Create 2D-system
 and
 Create 0D-system
 (the 0D-feature will come in the next release), respectively.

There are four ways to specify a 3D-system:

Structure type supplies a list of predefined structure types that are specified in

[~]/band/locals/ITXC_structure.dat (see edit database). Select by left mouse click. Specify the lattice parameters as requested. The next window lists all crystallographically inequivalent sites of the selected structure. If these have fixed coordinates, the button line is deactivated. If not, click line and specify coordinates as requested.

Space group supplies a list with all 230 crystallographic space groups. Some space groups are listed twice allowing to use a different choice of the basis vectors, orientation of the unique axis or origin. In doubt, select the space group with the c-axis as the unique axis or the second origin, respectively, because this will include the inversion as symmetry operation. Specify the lattice parameters as requested. The convention for the basis vectors

X	+ St	ructure s	et-up via structure table 🛛 🔹 🗖 🗙	n í	X	+ S1	ructure set-up via space group	×
	A9	hP4	C (Graphite)	Î l	$\overline{\Delta}$	1	P1	C1^1
	A4	cF8	C (Diamond)			2	P-1	Ci^1
	C1	cF12	CaF2 (Fluorite)			3	P2:b	C2^1
	E2_1	cP5	CaTiO3 (cubic-Perovskit			3	P2:c	C2^1
	???	oP2	CdTe			4	P21:b	C2^2
	в2	cP2	CsCl			4	P21:c	C2^2
	C15	cF24	Cu2Mg (cubic laves phas			5	C2:b	C2^3
	L1_2	cP4	Cu3Au			5	C2:c	C2^3
	L1_0	tP2	CuAu			6	PM:b	Cs^1
	L1_1	hR32	CuPt			6	PM:c	Cs^1
	A1	cF4	FCC			7	PC	Cs^2
	???	cP5	Fe4C			7	PA	Cs^2
	C2	cP12	FeS2 (Pyrite)			8	CM:b	Cs^3
	???	oC16	Ga3Pt5			8	CM:C	Cs^3
	A3	hP2	HCP			9	CC:b	Cs^4
	A6	t12	In			9	CC:c	Cs^4
	???	c116	Li (high pressure)			10	Р2/М:b	C2h^1
	B31	oP8	MnP			10	P2/M:c	C2h^1
	???	016	MoPt2			11	P21/M:b	C2h^2
∇	B1	cF8	NaCl (Rock Salt)		∇	11	P21/M:c	C2h^2
				l li				
			CLOSE				CLOSE	

Figure 7: Screenshot structure type (left) and space group (right) listbox

and specification of the atomic positions are summarised in Table I. The next window lists all crystallographic inequivalent sites of the space group. Select a site by clicking the corresponding line. If the site has fixed coordinates, the button line will be deactivated afterwards. If not, specify the missing coordinates as requested. After specifying all sites of the system return pressing DONE - RETURN.

Per pedes allows one to specify a system from scratch. Select the Bravais lattice or click the first line if it is unknown. The basis vectors, that are assumed by **xband**, are summarised in Table II. Give the total numbers of sites in the system and proceed. Supply the lattice parameters in the following window. Alternatively, you may skip this window and specify the primitive lattice vectors yourself in the next window. For all lattice sites the coordinates have to be given first. This can be done in Cartesian or crystallographic units. A radio button allows one to switch between these modes. You can use the **Copy** button to copy the input from any line to the next empty line. **reset** will delete the input of a line. **Occupy** calls the **Specify occupation** menu that is described below.

multi layers allows one to specify the structure for a number of frequently studied multi layer structures. Specify the common lattice parameter first and then select the multilayer system from the menu. Use the scales to specify the number of atom sites within the repeat unit. The restrictions due to three dimensional periodicity are automatically accounted for.

The left column of the menu allows one to create multilayer-systems with a homogeneous lattice, while the right column is used to create multilayers with the repeat unit consisting of two different but matching sublattices. In the latter case the inter-system distance can

X +	Struct	ture set-up per pedes		• 🗆 🗙			
		Bravais lattice					
◇ t	triclinic	primitive	-1	C_i			
\diamond n	monoclinic	primitive	2/m	C_2h			
\diamond n	monoclinic	base centered	2/m	C_2h			
\diamond c	orthorombic	primitive	ານານານ	D_2h			
\diamond c	orthorombic	base-centered	mm	D_2h			
\diamond c	orthorombic	body-centered	mm	D_2h			
\diamond c	orthorombic	face-centered	ານານານ	D_2h			
♦ t	tetragonal	primitive	4/mm	D_4h			
♦ t	tetragonal	body-centered	4/mm	D_4h			
♦ t	trigonal	primitive	– 3m	D_3d			
◇ ł	nexagonal	primitive	6/mm	D_6h			
\diamond c	cubic	primitive	m3m	0_h			
\diamond c	cubic	face-centered	m3m	0_h			
\diamond c	cubic	body-centered	m3m	0_h			
Number of sites NQ:							
input OK GO ON CLOSE							

Figure 8: Screenshot per pedes dialog



Figure 9: Screenshot set lattice parameter menu

be scaled in addition to the layer distance c of the sublattices. You may modify/extend the multilayer menu by editing the file ~ /band/locals/multilayer.vst.

When leaving one of the submenus described above, the program **findsym** is called automatically. **findsym** uses the input file struc.ini and can also be run separately. In any case the result will be written to struc.out and standard output. After the automatic run of **findsym** the structure menu will be extended giving at the bottom a list of all the atomic sites in the system. Apart from specifying the system via Per pedes, these have to be occupied by left mouse clicking a line calling the Specify occupation menu. If there are more than one atoms present on a lattice site (in a substitutional disordered system) click button 2, 3 etc. in the header line to allow for 2, 3 etc. occupants. For every occupant specify its chemical symbol via specify occupant and its concentration using the scale. The corresponding Wigner-Seitz radius is taken from a table that is set up via the file *~*/band/locals/rws.vst, if available. If no value for the Wigner-Seitz radius is predefined, this has to be supplied by the user. In case of

X +			Structure set-up for multi	layers				• 🗆 ×
lattice parame	ter A	Angstroer if nece					CLOSI	
scale c (%)	0.0		ALAT refers to sub s scale inter-system (◆ 1 ◇ 2	of heterog 0.0	jeneous lattice	
bcc (001) I	2	ок	scale c (%)	instance (76)	0.0		0.0	
bcc (001) II	4	ок	fcc(001) / bcc(001)	2		2		ок
bcc (110)	4	ок	fcc(001) / bcc(001)	1		1		ок
bcc (111)	6	ок		2		2		
fcc (001)	4	ок	bcc(001) / NaCl(001)	1		1		ок
fcc (110)	4	ок	bcc(001) / NaCl(001)	2		2		ОК
fcc (111)	6	ок	NaCl(001) / bcc(001)					ок
hcp (001)	4	ок	NaCl(001) / bcc(001)	1				ок
	8		start with sublayer	1				
ZnS (001) + ES	4	ОК	ZnS(001) + ES / bcc(001)	1		1		ок
NaCl (001)	4	ОК						

Figure 10: Screenshot multilayer menu

more than 1 occupant, the average Wigner-Seitz radius will be used that is obtained by summing up the concentration weighted individual radii. The name of an atomic type will be modified by **xband** if a chemical element occupies several crystallographically inequivalent lattice sites.

The Specify occupation menu occupies all equivalent sites simultaneously. After all sites have been occupied, or after setting up the system via Per pedes, the show structure and DONE - RETURN buttons get unlocked. Nevertheless, one may still modify the atomic configuration. When leaving via DONE - RETURN the atomic configuration is stored in the system file whose name is automatically generated and updated after every change of the configuration. Before leaving, however, the system file name may be modified using the entry in the top region of the window. The edit database button gives the possibility to add a structure to the database ~ /band/locals/ITXC_structure.dat. Left mouse click invokes the editor for the top region of the set of the instructure.

editor for the two ITXC-database files. Follow the instructions given in ITXC_structure.dat to add a new structure.

xband sets the Wigner-Seitz radii of the atoms according to the table in [~]/band/locals/rws.vst. Alternatively one may set the Wigner-Seitz-radii by pressing the button

adjust R₋WS + empty spheres. This will invoke the program **spheres** that sets the values according to a guess for the charge density. In addition one may add empty spheres. For these a lower and upper limit of their radii may be fixed. The program **spheres** should be invoked only after the structure has been completely specified. The symmetry of the system will not be modified by a run of **spheres**.

To check the generated configuration, input files for several visualizers can be created via show structure.

The menu (see Fig. 11) called that way allows one to display the atomic structure in four different ways by left mouse click on the corresponding buttons in the top row of the run visualizer menu window.

X +				run visualiz	er				• 🗆 ×			
unit cell r	epeated along primitive axes	unit cell rep	peated within m	ectangular box	cluster arou	nd selected atomic site	surface incl	uding selecte	ed atomic site			
N1	1	LX	1.0		IQCNTR	1	IQSURF	1				
N2		LY	1.0		NSHCLUS	2	h					
N3		LZ	1.0		CLURAD	0.0	k	0				
							Т	1				
							u	1.0				
	L3 4.0											
							orient	🔶 up	🔷 down			
	Visualizer: rasmol dataexplorer gopenbox (generic structure) scale Wigner-Seitz radius											
	scale object 1.0											
show :	🔄 show site labels 👅 show unit cell 👅 show cube 👅 show axis 👅 show empty spheres 💿 color of atomic spheres 💠 atomic number 🔶 atom type											
			run visualiz	er (set up of inp	out may take	a while)						
				CLOSI	E							

Figure 11: Screenshot run visualizer menu

unit cell repeated along primitive axes shows the lattice sites with the basis repeated along the three directions of the primitive basis vectors. The number of repetitions can be specified.

unit cell repeated within rectangular box displays the lattice sites with the basis repeated to fill a rectangular box. The side length of the box (in units of ALAT) can be specified.

cluster around selected atomic site sets up an atomic cluster centred at a specified lattice site IQ. The size of the cluster may be fixed by the number of neighbouring atomic shells or its radius (in units of ALAT).

surface including selected atomic site sets up a surface fragment for the Miller indices (h,k,l) going through site IQ with its width and lateral extensions specified in units of ALAT.

The current system can be visualized using three different programs, which have to be choosen in the visualizer-line: **rasmol dataexplorer** and A. Perlov's **gOpenBox**. Unavailabe parameters are grayed out correspondingly.

The button gOpenBox (generic structure) creates a generic input file for the gOpenBox program. None of the parameters set in the menu are therefore taken into account.



Figure 12: Screenshot rasmol as visualizer



Figure 13: Screenshot dataexplorer as visualizer

The radius of a sphere representing an atom may be scaled up using the scale object parameter. The value 1 corresponds to the proper Wigner-Seitz radius. The checkbuttons at the bottom allow one to add labels to the lattice sites giving the atom type name TXTT, atom type number IT, and lattice site number IQ. A cube with side length ALAT, the crystallographic unit cell and the Cartesian axes may be shown as well.



Figure 14: Screenshot **gOpenBox** as visualizer

Because **rasmol** was designed for molecules a number of geometrical restrictions are imposed. These can be circumvented in most cases by scaling the dimensions of the system up or down by the supplied scale (default value is 1).

After setting the mode and the required parameters the inputfiles for the chosen visualizer are created and the corresponding program is executed by clicking on the run visualizer button.

rasmol is using the data file X_xband.pdb together with the script file X_xband.ras. These can be used later on Unix level calling rasmol -script X_xband.ras.

dataexplorer is using the data file X_xband.dx together with the network file X_xband.net. These can be used if calling **dataexplorer** standalone.

gOpenBox is using the file X_xband.gopenbox or in generic structure mode the file X_xband.structure. Both can be used later on Unix level calling glbox X_xband.gopenbox or glbox X_xband.structure.

10 The CREATE 2D-SYSTEM menu

Calling the CREATE 2D-SYSTEM menu via the button Create 2D-system opens the window shown in Fig. 15. There are 4 ways to create a 2D-system.

homogeneous extended lattice : The corresponding menu shown in Fig. 16 allows one to set up extended 2d-systems with a homogeneous underlaying lattice. The system is assumed to consist of a periodic left (L) and right (R) bulk (specified by a corresponding unit cell), and a spacer in between. The occupation of all layers may be symmetric or not and bulk (L) may be identical to bulk (R) (symmetric systems need less input from user). The unit cells may be enlarged along the in plane a and b axis (e.g. to simulate disordered systems). The bulk unit cells may be larger than the structure unit. The interlayer distance may

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$\begin{array}{c c c c c c c c c c c c c c c c c c c $		edit database		nlock	un														via:	ure v	truct	ify sl	Spec
adjust R WS by scaling Calculate R WS + empty splieres show structure I Q CL WS X Y Z R_WS NLQ NOQ IT TXTT CONC 1 1 - 0.250000 0.250000 2.662000 3 1 1 Fe_a 1.00 2 2 - 1.250000 0.250000 0.250000 2.662000 3 1 2 Fe_b 1.00 3 3 - 0.750000 0.750000 0.750000 2.669000 3 1 3 cu 1.00		. 3 3 bcc (001) logeneous	NCL NT 2D hon		ites	dent s pes e type	quiva m ty uctur ice ty	ineq ator stru latti		508	7320		:/a =		4 5	5. 0.	b = b/a =		. 8	10.		:e pa	a =
4 3 - 1.750000 0.750000 2.669000 3 1 3 cu 1.00 5 3 - 1.250000 1.250000 2.669000 3 1 3 cu 1.00 6 3 - 2.250000 1.250000 2.669000 3 1 3 cu 1.00 6 3 - 2.50000 1.250000 2.669000 3 1 3 cu 1.00 7 2 - 1.750000 1.750000 2.662000 3 1 2 Ye_b 1.00 8 3 - 2.750000 1.750000 1.750000 2.662000 3 1 3 cu 1.00		1.00 1.00 1.00 1.00 1.00 1.00 1.00	∍_a ≥_b u u u u s_b	1 Fe 2 Fe 3 Cu 3 Cu 3 Cu 3 Cu 2 Fe		1 1 1 1 1 1 1	NLQ 3 3 3 3 3 3 3 3 3	N)))))	L_WS 62000 62000 69000 69000 69000 69000	1 2.1 2.1 2.1 2.1 2.1 2.1 2.1		ty spi 2 0000 0000 0000 0000 0000 0000	2 5 2 5 2 5 7 5 7 5 2 5 2 5 7 5	0. 0. 0. 1. 1. 1.	caling 000 000 000 000 000 000 000	by so 2 500 2 500 2 500 2 500 1 7 500 1 2 500 1 2 500 1 7 500	50000 50000 50000 50000 50000 50000 50000	0.25 1.25 0.75 1.75 1.25 2.25 1.75	1 0 1 1 2 1		1 2 3 3 3 3 2	Ĩ 2 3 4 5 6 7	X

Figure 15: Screenshot create 2D system menu

χ +	Structure set-up for layered system		s extended lattice	
lattice parameter A 5.	4 Angstroem to a if necessar			CLOSE
	repeat structure unit along a	layers in basic structure unit	total number of layers including bulk(L) and bulk(R)	select
specify layer system bulk(L) bulk(R)	2	1	2	bcc (001) I
occupation of layers	repeat structure unit along b 2	2	4	bcc (001) II
 ♦ symmetric ♦ NON-symmetric 		2	4	bcc (110)
bulk(L) = bulk(R)	repeat structure unit along c to generate unit cell of bulk(L)	3	6	bcc (111)
◆ YES ◇ NO	repeat structure unit along c	2	4	fcc (001)
	to generate unit cell of bulk(R)	2	4	fcc (110)
		3	6	fcc (111)
	scale lattice parameter c (%) 0.0	2	4	hcp (001)
		4	8	ZnS (001) + ES
		2	4	NaCl (001)

Figure 16: Screenshot structure set-up menu for layered system with homogeneous extended lattice

be scaled by scaling the parameter c. The right column of the menu allows one to select among various predefined structures (see 2D_structure.dat For each 2D-structure the number of layers in the basic structure unit (that will be repeated) is given and the total number of layers can be chosen consistently with a scale. The following occupation menu called by

X + Stru	cture set-up for layered system with I	heterogeneous exter	nded lattice 🔹 🗖 🗙
lattice parameter A 5.4	Angstroem to a.u. if necessary	ALAT refers to s	♦ 2 CLOSE
specify layer system bulk(L) bulk(R)	repeat structure unit along a	layers in basic structure units	select
occupation of layers ◆ symmetric	repeat structure unit along b 1	2 / 2	fcc(001) / bcc(001) ZnS(001) + ES / bcc(001)
♦ NON-symmetric bulk(L) = bulk(R)	repeat structure unit 1 along c to generate unit cell of bulk(L)	2 / 2	bcc(001) / NaCl(001)
 YES NO 	1 repeat structure unit 1 along c	2 / 2	NaCl(001) / bcc(001)
struc(L) = struc(R) ♦ ¥ES ♦ NO	to generate unit cell of bulk(R) 1		
number of sub systems 3	scale inter-system distance (%) 0,0		
sequence of structure units ◆ 1 2 1 ◇ 2 1 2	scale c of structure unit 1 (%) 0.0 scale c of structure unit 2 (%) 0.0		

Figure 17: Screenshot structure set-up menu for layered system with heterogeneous extended lattice

[X +	Structure set-up for layered syste	m with homogen	eous slab lattice	• 🗆 ×
lattice parameter A 5.	4 Angstroem to if necessar			CLOSE
	repeat structure unit along a	layers in basic structure unit	total number of layers	select
specify layer system vac vac	2	1	2	bcc (001) I
occupation of layers	repeat structure unit along b 1	2	4	bcc (001) II
 ♦ symmetric ♦ NON-symmetric 		2	4	- bcc (110)
	scale lattice parameter c (%) 0.0	3	6	bcc (111)
	,	2	4	fcc (001)
		2	4	- fcc (110)
		3	6	fcc (111)
		2	4	hcp (001)
		4	8	ZnS (001) + ES
		Z	4	NaCl (001)

Figure 18: Screenshot structure set-up menu for layered system with homogeneous slab lattice

the right hand button is desribed below.

heterogenous extended lattice : The menu invoked by this button is very similar to the



Figure 19: Screenshot structure set-up menu for layered system with heterogeneous slab lattice



Figure 20: Screenshot structure set-up menu for layered system with heterogeneous slab lattice

previous one (shown in Fig. 17) but allows one to set up layered systems set up of two different structure units. Accordingly the structure of bulk (L) and bulk (R) (struc (L) and struc (R), respectively) may be the same or different. The total structure may consist of many subsystems having alternating structure unit 1 and 2, starting with unit 1 or 2. All relevant interlayer distances may be scaled seperately. The right hand column gives the various

+		Str	ucture set-up	o for 2D layere	d systems: Coor	rdinates o	f sites	• 🗆 :
						2	D all done RETURN	CLOSE
			lattice p	arameter A	5.4	[a.u	J	
			a1 [A]	2	0	0		
			a2 [A])	1	0		
			a3 [A]	2.0	2.0	2.0		
str	uct	x [A]	у [А] z [3	A]			
bulk(L)	site 1:	0.25	0.25	0.25	оссиру	сору	Fe 1.00	
	site 2:	1.25	0.25	0.25	occupy	сору	Fe 1.00	
	site 3:	0.75	0.75	0.75	occupy	сору	Cu 1.00	
spacer	site 4:	1.75	0.75	0.75	occupy	сору	Cu 1.00	
	site 5:	1.25	1.25	1.25	occupy	сору	Cu 1.00	
	site 6:	2.25	1.25	1.25	оссиру	сору	Cu 1.00	
	site 7:	1.75	1.75	1.75	оссиру	сору	Fe 1.00	
bulk(R)	site 8:	2.75	1.75	1.75	occupy	сору	Fe 1.00	

Figure 21: Screenshot coordinates of sites set-up menu for layered system

+		Sta	ucture set-u	ıp for 2D layer	ed systems: Cool	dinates of	sites		
						2	D all done	RETURN	CLOSE
			lattice	parameter A	5.4	[a.u.]		
			a1 [A]	2	0	0	_		
			a2 [A]	0	2	0			
			a3 [A]	10.0	10.0	10.0			
switch lat	ttice site display	top	f	orward	backward	ba	ttom	displayin	g 16 out of 80 sites
	struct	x [A]	y [#	4] z	[A]				
bulk(L)	site 1:	0.25	0.25	0.25	occupy	copy	Fe 1	. 00	
	site 2:	0.25	1.25	0.25	occupy	copy	Fe 1	. 00	
	site 3:	1.25	0.25	0.25	occupy	copy	Fe 1	. 00	
	site 4:	1.25	1.25	0.25	occupy	сору	Fe 1	. 00	
	site 5:	0.75	0.75	0.75	occupy	copy	Fe 1	. 00	
	site 6:	0.75	1.75	0.75	occupy	copy	Fe 1	. 00	
	site 7:	1.75	0.75	0.75	оссиру	copy	Fe 1	. 00	
	site 8:	1.75	1.75	0.75	оссиру	copy	Fe 1	. 00	
spacer	site 9:	1.25	1.25	1.25	occupy	copy	Fe 1	. 00	
	site 10:	1.25	2.25	1.25	оссиру	copy	Fe 1	. 00	
	site 11:	2.25	1.25	1.25	оссиру	copy	Fe 1	. 00	
	site 12:	2.25	2.25	1.25	occupy	copy	Cu 1	. 00	
	site 13:	1.75	1.75	1.75	occupy	сору	Cu 1	. 00	
	site 14:	1.75	2.75	1.75	оссиру	copy	Cu 1	. 00	
	site 15:	2.75	1.75	1.75	occupy	copy	Cu 1	. 00	
	site 16:	2.75	2.75	1.75	occupy	copy	Cu 1	. 00	

Figure 22: Screenshot coordinates of sites set-up menu for layered system

structures available (see 2D_structure.dat) together with the number of layers in the two basic structure units (left). Selecting a 2D-structure invokes the menu shown in Fig. 20. The two columns to the left (with different coloured background) give a projection from top and side of the two basic structure unit. The following menu following to the right allows one to specify the various numbers of layers in the subsystems (In Fig. 20 there are 3 subsystems having - from top - structure 1, 2 and 1 as indicated by the background color). The number of layers in the subsystem can be chosen together with the index of the starting layer. The latter option is necessary to have a proper matching of the subsystems. This can be visualised on

the right hand side by a projection pressing the view interface button. Alternatively the 4 layers around the interface can be viewed via rasmol using the use rasmol button. The following occupation menu described below is called by the Settings OK - GO ON button.

homogeneous slab lattice: The corresponding menu is completely analogous to the one for extended systems and is shown in Fig. 18. The only difference is that bulk (L) and bulk (R) is missing now; i.e. the slab has a finite extension perpendicular to the layers and is surrounded by vacuum.

heterogenous slab lattice: Again the menu shown in Fig. 19 is analogous to its counterpart for extended systems.

Having set up a 2D-structure using one of the various menus, the lattice sites may be occupied via the menu shown in Fig. 21. Go through the table from top to bottom and specify occupation of a site via the <u>OCCUPY</u> button. Pressing one of the <u>COPY</u> button of the occupied sites copies its occupation to the next empty sites. For symmetric systems the occupation is mirrored automatically.

If there are too many sites to be shown on the screen only a subset is displayed. One can go through the list by paging using one of the buttons above the list. This situation applies to the screenshot shown in Fig. 22 that shows 16 sites for an extended 2D-system with 80 sites in total (including bulk (L) and bulk (R)).

11 The CREATE 0D-SYSTEM menu

0D-systems, i. e. impurities and deposited clusters are set up via the CREATE 0D-SYSTEM button. Before pressing this button, one has to select the system file of the underlying structure (e. g. 3D bulk or 2D surface) first. One will be prompted to choose an existing system file or to create a new one if no system is currently selected. Otherwise the create 0D-system step A menu (see Fig. 23) will open. Here one can specify how big the underlying structure is chosen to later modify it with the 0D system, and around which site the system should be centered. Specify how many unit cells the system is expected to be. Click Occupy to continue. This brings up the create 0D-system step B menu (see Fig. 24). There are three views of the underlying sysems, one for a view along each axis. The view on the right is the one for the z-axis and only shows three different layers of the system. Small atoms represent atoms with the lowest z-value of these three layers. On the right hand one can adjust which layers are shown with the prev layer and next layer buttons.

Now one or more additional occupation types have to be created in the usual way. These appear in the list of occupation types together with the types of the underlying lattice. If a occupation type is selected, atoms of the underlying lattice can be set to this type by clicking on the atom in the z-axis view. The atom is also selected. To select an atom without changing the type or to unselect an atom, use the middle or right mouse button, respectively. At any time one can check the structure by pressing the Show 3D button. Selected atoms have a bigger radius than unselected lattice sites in this visualization. One can easily select all atoms surrounding the so far selected atoms by using the add relaxation zone button. Either the number of surrounding shells or a radius has to be supplied to do so.



Figure 23: Screenshot Create 0D-structure, step A

If the system is set up, click **Done** and enter a new filename to save the system.

12 The SELECT/MODIFY SYSTEM menu

The button **SELECT/MODIFY SYSTEM** invokes a menu to select and possibly to modify a system file that has been created earlier.

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

System and potential file lists: use left mouse click to select and middle mouse click to select and quit. Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~ /band/locals.

Having selected a system file one may quit or modify the system pressing the modify button. This step invokes the menu shown in Fig. 26. In the top region the old settings for the lattice parameter and primitive vectors are given followed by the present or new settings. To the right a number of buttons are available that allow to scale the primitive vectors or to stretch or compress the system along the Cartesian axes. The bottom table gives the old and new coordinates of the lattice sites. This can be given in Cartesian or crystallographic units. This table allows one to modify the basis vectors individually. Leaving the modify menu



Figure 24: Screenshot Create 0D-structure, step B

displays the resulting system data via the window shown in Fig. 27. If the modifications influence the symmetry of the system this will be automatically accounted for.

13 The RUN PROGRAM PACKAGE menu

If the button SPR-KKR or any other program button is pressed the corresponding RUN PROGRAM PACKAGE menu is activated.

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

Input, job and output file lists: use left mouse click to select and middle mouse click to select and edit using **emacs**. Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. The filter allows one to select certain subsets of the files to be listed. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in [~]/band/locals.

With an input, job or output file selected or created the corresponding pull down menu (column of buttons in the middle of the top region) gets unlocked. This menu allows one to

[X +	SELECT SYSTEM	• • ×
close help clear text field current directory /home/he/band sysfile Fe.sys potential file Fe.pot select directory \$HOME \$HOME/band3 \$HOME/band	edit modify edit sysfile: select select + quit sysfile list (.sys): alphabetical last access Fe.sys NaCl.sys myFe.sys xband_tmp.sys	pot-file: select select + quit pot-file suffix file list (.pot): alphabetical last access Fe.pot NaCl.pot myFe.pot
directory:	sysfile: (.sys)	pot-file: (.pot):
new pot-file selected: Fe.pot		

Figure 25: Screenshot SELECT SYSTEM menu



Figure 26: Screenshot modify system menu step 1

edit, copy, move, delete, catenate or print the files and supplies some more functionality.

Selecting an input file allows one to run the various programs of the package. A new input file can be created via **create input**. For this purpose, the system information has to be available. This is the case if a system was selected or created via **SELECT/MODIFY SYSTEM** or **CREATE SYSTEM** before calling **SPR-KKR**. If **create input** is pressed without a system specified, the user will be asked to select or create a system file. The next call of **create input** should be successful and activate the input menu, that is of course dependent on the package.

$\frac{1}{1} \frac{1}{1} - 0,000000 $	(+	MODIFY 3D-SYS	TEM FILE Fe STEP 2	- 0
Fe DONE - RETURN CLOSE The symmetry of the system might be lowered by modifications made the program <findsym> tried to find out new symmetry attice parameters $A = 5.4$ [a.u.] a = 4.67653718043 b = 4.67653718043 c = 4.67653718043 inequivalent sites NCL 1 b/a = 1.0 c/a = 1.0 atom types NT 1 b/a = 109.4712206 $\beta = 109.4712206$ $\gamma = 109.4712206$ adding t R W3 by scaling Close Close attice parameters $A = 5.4$ [a.u.] b/a = 1.0 c/a = 1.0 atom types NT 1 atom types NT 1 b/a = 109.4712206 $\gamma = 109.4712206$ Todulate R W3 * onply spinors atom types NT 1 Close Done result of find out new symmetry Close Done result of find out new symmetry Close NO 1 b/a = 1.0 c/a = 1.0 Structure type BCC Close Prove the system of sites th</findsym>	clear text field			
the program <fridsym> tried to find out new symmetry the program <fridsym> tried to find out new symmetry lattice parameters A = 5.4 [a.u.] number of sites NQ 1 a = 4.67653718043 b = 4.67653718043 c = 4.67653718043 inequivalent sites NL 1 b/a = 1.0 c/a = 1.0 atom types NT 1 c = 109.4712206 β = 109.4712206 γ = 109.4712206 BCC adjust R WS by scaling calculate R WS + empty spineres show structure I Q CL WS X Y Z R_WS NLQ NOQ IT TXTT CONC</fridsym></fridsym>	· · · ·	em-file	DONE - RETURN	CLOSE
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				de
by scaling empty spheres snow structure IQ CL WS X Y Z R_WS NLQ NOQ IT TXTT CONC	= 4.67653718043 b = b/a =	4.67653718043 c = 1.0 c/a =	4.67653718043 inequivalent sit 1.0 atom types structure type	tes NCL 1 NT 1
		bý scaling en Y Z	R_WS NLQ NOQ	

Figure 27: Screenshot modify system menu step 2



Figure 28: Screenshot RUN SPRKKR PACKAGE menu

X +		Cre	ate input file			• 🗆 ×
SELE	CT SYSTEM	input file n	ame		CLOSE	write inpfile quit
S	edit stem file	Fe_DOS.inp	Fe_DOS.inp		CLUBE	write+edit inpfile quit
DATASET	Fe		TAU CALC	POINTS		
ADSI	DOS		P NKTAB	250		
POTFIL	Fe.pot		TAU CALC	♦ CLUSTER		
TASK	\Rightarrow DOS \diamond S	SCF	IQCNTR		1	
NE	50		NSHCLUS	0	◆ NSH	
EMIN	-0.2	Ry				EXPERT MODE
EMAX	1.0	Ry	CLURAD	1.5		
lm (E)	0.01	Ry	CLUNAD		🔶 RAD	
EF		Ry				
	🔟 search EF					

Figure 29: Screenshot SPRKKR create input menu

For the **SPRKKR** package **create input** allows one to create input files to run **kkrscf** and **kkr-gen** to calculate the potential self-consistently and the DOS, respectively. The menu automatically creates the name of the input and potential files according to the system name and TASK. Before leaving the menu you may change these names as you like. Using the menu go through step by step by first selecting the TASK. This will in general create suggestions for the remaining entries.

X +			Create	input file				• 🗆 ×
	SELECT SYSTEM		input file name	•	CL	DSE	write inpfile quit	
	edit system file	Fe_DOS.in	p				write+edit inpfil quit	e
DATASET ADSI POTFIL TASK	System me Fe DOS Fe.pot • DOS ◇ SCF • EKREL ◇ BLOCHSI ◇ VBXPS ◇ CLXPS ◇ AES ◇ NRAES ◇ A ◇ XAS ◇ XMO ◇ COMPTON ◇ CREAL ◇ RECTANG	aps Sigma 🔷 Moke	ETA RMAX GMAX TAU CALC	♦ WEYL ♦ POIL 400 900 250 250 250 250 250 250 250 250 250 2			quit PARA > NREL ◇ SRE REL ◇ Brook > Sole-c ◇ sci > SOC-xy ◇ Si > z-axis ◇ com > non-collinear 0 ◇ 1 ◇ 2 ◇ > NOWRDOS WRLMLDOS WRKAPDOS	s-OP 🗞 LDA+U ale-SOC DC-zz mon orientation 2 3 < 4 < 5
E-GHID	♦ RECT-LOG ♦ ARC		IQCNTR		1		U WRPOLAR	🗆 EFG
ne Emin Emax	50 -0.2 1.0	Ry Ry	NSHCLUS CLURAD NLOUT	0	♦ NSH ◇ RAD	TAU-MAT WRITE READ POTFILE	 ◆ AUTO ◆ WRTAUMQ ◆ RDTAUMQ □ OVERWRITE 	♦ WRTAU♦ RDTAU
lm (E) EF	0.01	Ry Ry		nentum expansion M	NL = I_max + 1		STANDARD MODI	=

Figure 30: Screenshot **SPRKKR** expert create input menu

If you change to the **EXPERT MODE** you will have a long list of possible tasks. For several of them you will be asked to set specific parametrs, e.g. to select an atom type for which the

X-ray absorption spectrum has to be calculated. If necessery you can modify the parameters fixing the energy grid (left bottom). The top part of the middle column allows one to select the mode how the τ -matrix is calculated - either via Brillouin zone integration or in the cluster mode. This implies you later using either **kkrgen** (**kkrscf**) or **kkrclu**. The right hand column of the menu offers a lot of ways to control the calculations and the output. A detailed description of the many parameters can be found in the **SPRKKR** manual.

With an input file selected or created the program buttons get unlocked. The corresponding pull down menu allows among others to run the programs interactively, to submit a local batch job, to submit a job to the queue system (using **qsub**) and to create a job file, that can be executed or submitted later in an Unix window. Interactive execution of the program is done in a Unix xterm window with the output appended to X.out. A message will be given on the screen after the run has been completed.

When running a program or creating a job file connected with this, **xband** checks whether the executable is available. If it cannot be found in the default directory PROG_PATH0 **xband** will give a warning and stop execution. To enable execution of the program the user can copy the executable to PROG_PATH0, change PROG_DIR0 via SET PREFERENCES or set the program directory explicitly via PROG PATH.

The RUN PROGRAM PACKAGE menu supplies in its top right corner two columns of buttons. Those on the left column allow one to call other **xband** menus and services while those on the right hand side supply a shortcut to some Unix commands. The button files alows to handle files in many different and specific ways.

14 The PLOT DATA menu

The PLOT DATA menu invoked via PLOT is meant to simplify data handling when plotting the results of a band structure program. The menu uses the program **plot** that supplies an interface between the **SPRKKR**-program package of H. Ebert et al. and **xmgrace**. If you use another band structure package you have to supply your own version of **plot** or modify the one supplied. The file ~ /band/graphics/xmgr.f contains all necessary routines to create a **xmgrace** file with the most important parameters, i.e. label, legends and so on, set starting from an arbitrary data table.

Directory list (centre region left): use left mouse click to change the directory. You can also type the name of the new directory in the entry field below the list for this purpose.

data, pin and xmgrace file lists: use left mouse click to select and invoke corresponding program execution.

Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in [~]/band/locals.

Left mouse click on a data file selects the file and invokes **plot** that creates the corresponding **xmgrace** file(s).

[X +		PLOT DATA	• • ×
	ar text field		
· · ·	/home/he/band		
datafile	Fe_SCF_SCFSTART.dosedit	sort mode 🛛 🔷 alphabetical	
pin-file	NO PIN-FILE SELECTED edit	🕹 last access	
xmgr-file	Fe_SCF_SCFSTART.dos_Fe.agredit	Filter *	
select directory	select and run datafile	select and run pin-file	select and run xmgr file
\$HOME \$HOME/band	*.dos suffix *.rat *.bsf	suffix	suffix
directory:	Fe_DOS.dos Fe_SCF_SCFSTART.dos		Fe_DOS.dos_Fe.agr Fe_SCF_SCFSTART.dos_Fe.agr
new xmgr-file s 1437	elected: Fe_SCF_SCFSTART.dom_Fe.agr		

Figure 31: Screenshot PLOT DATA menu

Left mouse click on (one of) the new file(s) in the right file list calls **xmgrace**.

All other files listed in the rightmost listbox could also be displayed by left mouse click. The appropriate programm, like **xmatrix** or **ghostview** which is bound to the extension is executed automatically.

plot allows one to supply an additional **plot** input file (*.pin) that is read prior to the data file. Middle mouse click on a data file invokes a menu that allows one to give additional parameters for plotting and broadening. A corresponding **plot** input file is created when leaving the menu. This file is fed to **plot** by left mouse click in the pin-file list. The subsequently created **xmgrace** file can be viewed by invoking **xmgrace** via left mouse click in the **xmgrace** file list.

The Bloch spectral function is plotted using the **xmatrix** program from the **MATHPACK** library or by utilizing the **DISLIN** library. Using the latter opens either a view-only window which could be closed as indicated in the window title or creates a postscript file which can be displayed using **ghostview**. The required input for **xmatrix** is a pair of files with the extensions mpk (datafile) and xmv (visualisation). Due to limited capabilities of **xmatrix**, labeling is incomplete.

15 Customisation

Customisation of **xband** can be done on three different levels.

Use **SET PREFERENCES** to switch between supplied default settings and specify your print command, default program directory and program names. All settings made will be stored in ~/.xband.vst.

xband sets all parameters first using internally stored defaults and then tries to read updates from ~/.xband.vst and additional default files in the directory ~/band/locals. While ~/.xband.vst may be updated via SET PREFERENCES the other files remain always untouched. The only exception is the file ~/band/locals/ITXC_structure.dat that may be modified via edit database within the CREATE SYSTEM menu by the user.

If **xband** should deal with a new program package, this can be done by editing the file [~]/band/locals/packages.vst. Follow the description given there to add the new program package to the main menu. Alternatively, you may modify ~/.xband.vst after it has been created. If no further action is made **xband** will not be able to write a specific input file but will just copy the content of the selected system file X.sys to the input file X.inp. To enable creation of a specific input file supply in ~/band a corresponding tcl-file create_input_NEWPACK.tcl with NEWPACK the name of the new program package. Copy for example create_input_KKR-AKAI.tcl to create_input_NEWPACK.tcl and use it as a template. There are two procedures in this file to be adapted. The first one has to be called create_input_NEWPACK and supplies the input mask for all additional variables to be transferred to the input file. Writing of the input file is done by the second procedure that has to be called write_input_NEWPACK and which is invoked by pressing one of the various quit buttons in the create input menu. Thus, creating your own specific input file via write_input_NEWPACK, you may use all information stored in a system file. The various variables are tabulated in Table III. All other information needed to run the new package can be supplied via an appropriate input mask setup in the procedure create_input_NEWPACK.

H. Ebert

Munich, June 2012

Table I

Conditional basis and atomic position vectors according to the convention of the International Tables of X-ray crystallography.

Conditional vectors (Natural coordinate system):

Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic:

$\vec{T}_1 = ($	1	0	0)
$\vec{T}_{2}=($	$b/a \cos \gamma$	$b/a \sin \gamma$	0)
$\vec{T}_{3}=($	$c/a(\cos\beta - \cos\alpha\cos\gamma)/\sin\gamma$	$-c/a * \cos \alpha$	$\sqrt{(c/a)^2 - T_{3,x}^2 - T_{3,y}^2}$

Hexagonal and trigonal (in hexagonal axes):

 $\vec{T}_1 = (\sin \gamma \ \cos \gamma \ 0) \\ \vec{T}_2 = (0 \ 1 \ 0) \\ \vec{T}_3 = (0 \ 0 \ c/a)$

Rhombohedric:

 $\cos \theta = \sqrt{\frac{2}{3}}(1 - \cos \alpha),$

 α : angle between vectors.

$\vec{T}_1 = ($	$\frac{1}{2}\cos\theta$	$-\frac{\sqrt{3}}{2}\cos\theta$	$\sin \theta$)
$\vec{T}_2 = ($	$\frac{1}{2}\cos\theta$	$\frac{\sqrt{3}}{2}\cos\theta$	$\sin \theta$)
$\vec{T}_{3} = ($	$-\cos\theta$	0	$\sin \theta$)

All atomic position vectors must be given in multiples of $\vec{T_1}$, $\vec{T_2}$ and $\vec{T_3}$

Basis vectors:

For space groups, where the first letter is P (primitive) (Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic, Hexagonal, Rhombohedric)

 $\vec{a}_1 = \vec{T}_1$ $\vec{a}_{2} = \vec{T}_{2}$ $\vec{a}_3 = \vec{T}_3$ first letter is I (body centered) (Orthorhombic, Tetragonal, Cubic) $\vec{a}_1 = -\frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_2 + \frac{1}{2}\vec{T}_3$ $\vec{a}_2 = \frac{1}{2}\vec{T}_1 - \frac{1}{2}\vec{T}_2 + \frac{1}{2}\vec{T}_3$ $\vec{a}_3 = \frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_2 - \frac{1}{2}\vec{T}_3$ first letter is F (face centered) (Orthorhombic, Cubic) $\vec{a}_1 = \frac{1}{2}\vec{T}_2 + \frac{1}{2}\vec{T}_3$ $\vec{a}_2 = \frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_3$ $\vec{a}_3 = \frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_2$ first letter is **B** (base (AC) centered) (Monoclinic, Orthorhombic) $\vec{a}_1 = \frac{1}{2}\vec{T}_1 - \frac{1}{2}\vec{T}_3$ $\vec{a}_{2} = \vec{T}_{2}$ $\vec{a}_3 = \frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_3$ first letter is C (base (AB) centered) (Monoclinic,Orthorhombic) $\vec{a}_1 = \frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_2$ $\vec{a}_2 = -\frac{1}{2}\vec{T}_1 + \frac{1}{2}\vec{T}_2$ $\vec{a}_{3} = \vec{T}_{3}$ first letter is **R** (rhombohedric in hexagonal axes) $\vec{a}_1 = \frac{2}{3}\vec{T}_1 + \frac{1}{3}\vec{T}_2 + \frac{1}{3}\vec{T}_3$ $\vec{a}_2 = -\frac{1}{3}\vec{T}_1 + \frac{1}{3}\vec{T}_2 + \frac{1}{3}\vec{T}_3$ $\vec{a}_3 = -\frac{1}{3}\vec{T}_1 - \frac{2}{3}\vec{T}_2 + \frac{1}{3}\vec{T}_3$

Table II

Basis vectors \vec{a}_1 , \vec{a}_2 and \vec{a}_3 assumed by **xband** for the input mode **Per Pedes** according to the user selected Bravais lattice. Note that the International Tables of X-ray crystallography allows for some Bravais lattices more than one choice of the basis vectors.

Bravais lattice	basis vectors used by xband
1) triclinic primitive	(a, 0, 0)
	$(b\cos\gamma,b\sin\gamma,0)$
	$\left(c(\cos\beta - \cos\alpha\cos\gamma)/\sin\gamma, -c\cos\alpha, a\sqrt{(c/a)^2 - a_{3,x}^2 - a_{3,y}^2}\right)$
2) monoclinic primitive	(a,0,0)
	$(b\cos\gamma,b\sin\gamma,0)$
	(0,0,c)
3) monoclinic base-centered	$\frac{\frac{1}{2}(a+b\cos\gamma,b\sin\gamma,0)}{\frac{1}{2}(-a+b\cos\gamma,b\sin\gamma,0)}$
	$\frac{1}{2}(-a+b\cos\gamma,b\sin\gamma,0)$
	(0,0,c)
4) orthorombic primitive	(a,0,0)
	(0, b, 0)
	(0,0,c)
5) orthorombic base-centered	$\frac{1}{2}(a,b,0)$
	$\frac{1}{2}(-a,b,0)$
	(0,0,c)
6) orthorombic body-centered	$rac{1}{2}(-a,b,c) \ rac{1}{2}(a,-b,c) \ rac{1}{2}(a,b,-c)$
	$\frac{1}{2}(a,-b,c)$
	$\frac{1}{2}(a,b,-c)$
7) orthorombic face-centered	$\frac{\frac{1}{2}(0,b,c)}{\frac{1}{2}(a,0,c)}$
	$\frac{1}{2}(a,0,c)$
	$\frac{1}{2}(a,b,0)$
8) tetragonal primitive	(a,0,0)
	(0, a, 0)
	(0,0,c)
9) tetragonal body-centered	$\overline{\frac{1}{2}}(-a,a,c)$
	$\frac{1}{2}(a,-a,c)$
	$ \frac{\frac{1}{2}(-a,a,c)}{\frac{1}{2}(a,-a,c)} \\ \frac{\frac{1}{2}(a,a,-c)}{\frac{1}{2}(a,a,-c)} \\ a(\frac{1}{2}\cos\theta,-\frac{\sqrt{3}}{2}\cos\theta,\sin\theta) $
10) trigonal primitive	$a(\frac{1}{2}\cos\theta, -\frac{\sqrt{3}}{2}\cos\theta, \sin\theta)$
$\cos\theta = \sqrt{\frac{2}{3}(1 - \cos\alpha)}$	$a(\frac{1}{2}\cos\theta, \frac{\sqrt{3}}{2}\cos\theta, \sin\theta)$
V C	
11) hexagonal primitive	$\frac{a(-\cos\theta, 0, \sin\theta)}{\frac{1}{2}(a\sqrt{3}, -a, 0)}$
	(0, a, 0)
	(0,0,c)
12) cubic primitive	(a,0,0)
	(0,a,0)
	(0,0,a)
13) cubic face-centered	$\frac{\frac{1}{2}(0, a, a)}{\frac{1}{2}(a, 0, a)}$ $\frac{\frac{1}{2}(a, a, 0)}{\frac{1}{2}(a, a, 0)}$
	$\frac{1}{2}(a,0,a)$
	$\frac{1}{2}(a,a,0)$
14) cubic body-centered	$\frac{1}{2}(-a,a,a)$
	$\frac{1}{2}(a,-a,a)$
	$rac{1}{2}(a,a,-a)$

Table III

Variables stored in and supplied by any 3D system file, respectively. For additional information used to deal with 2D-structures: see the file write_read_system.tcl.

Variable	Description
BRAVAIS	number specifying the Bravais lattice (see table II)
TABBRAVAIS(\$BRAVAIS)	name of the Bravais lattice with number BRAVAIS
SPACEGROUP	ITXC space group number
SPACEGROUP_AP	space group number in A. Perlov's table
STRUCTURE_TYPE	name of structure type
ALAT	lattice parameter A [a.u.]
воа	ratio of lattice parameters b/a
COA	ratio of lattice parameters c/a
LATPAR(\$i)	lattice parameters a, b, c for \$i=1,,3 [a.u.]
LATANG(\$i)	lattice angles α , β , and γ [deg]
RBASX(\$i)	x-component of primitive basis vectors for \$i=1,,3 [A]
RBASY(\$i)	y-component of primitive basis vectors for \$i=1,,3 [A]
RBASZ(\$i)	z-component of primitive basis vectors for \$i=1,,3 [A]
NQ	number of lattice sites
RQX(\$IQ)	x-component of atomic position \$IQ=1,,\$NQ [A]
RQY(\$IQ)	y-component of atomic position \$IQ=1,,\$NQ [A]
RQZ(\$IQ)	z-component of atomic position \$IQ=1,,\$NQ [A]
RWS(\$IQ)	Wigner-Seitz-radius for atomic position \$IQ=1,,\$NQ [A]
NLQ(\$IQ)	angular momentum expansion l_{max} + 1 for atomic position \$IQ=1,,\$NQ
NOQ(\$IQ)	number of occupants on site \$IQ for disordered systems
ITOQ(\$IO,\$IQ)	number of atomic type of occupant \$IQ on site \$IQ
NCL	number of inequivalent lattice sites, i.e. classes
WYCKOFFCL(\$ICL)	Wyckoff symbol for lattice sites of class \$ICL
NQCL(\$ICL)	number of lattice sites in class \$ICL
IQECL(\$IE,\$ICL)	lattice site number of \$IE-th site in class \$ICL; \$IE=1,,\$NQCL
NT	number of atomic types
ZT(\$IT)	atomic number of atomic type \$IT
TXTT(\$IT)	chemical symbol of atomic type \$IT; eventually extended
CONC(\$IT)	concentration c of atomic type \$IT ($0 \le c \le 1$);
	i.e. probability to find it on a site \$IQAT (see below)
NAT(\$IT)	number of lattice sites occupied by atomic types \$IT
IQAT(\$IA,\$IT)	lattice site number of \$IA-th site occupied by atom type \$IT;
	\$IA=1,,\$NAT