# lmf – Questaal's Full Potential LMTO Code

**Part 1:**

1. setting up a basic ctrl file
2. the atomic calculations and **lmf** basis setup
3. running **lmf**
4. plotting LDA band structures
5. adding local orbitals and plane waves
6. using the **blm** setup utility

**Part 2:**
practical tutorial on Se relaxation

# Ctrl file for SrTiO3

- Pm-3m (space group 221); ICSD ref 80872: $a = 3.8996(5)$Å

| spec | Wyckoff | positions |
|---|---|---|
| Sr | (1a) | $(0, 0, 0)$ |
| Ti | (1b) | $(1/2, 1/2, 1/2)$ |
| O | (3c) | $(0, 1/2, 1/2)$ |

```
# cubic perovskite SrTiO3
STRUC
 NSPEC=3      # number of different species
 NBAS=5       # number of occupied sites
 ALAT=7.3692  # expt lattice constant (bohr) (3.8996AA)
 PLAT=1 0 0
      0 1 0
      0 0 1   # lattice vectors

SITE
 ATOM=Sr XPOS=0 0 0
 ATOM=Ti XPOS=1/2 1/2 1/2
 ATOM=O  XPOS=0 1/2 1/2
 ATOM=O  XPOS=1/2 1/2 0
 ATOM=O  XPOS=1/2 0 1/2

SPEC          # definitions for individual species
 ATOM=Sr Z=38 R=2.6 LMX=2 # R_mt and LMX key in LMTO
 ATOM=Ti Z=22 R=2.2 LMX=2
 ATOM=O  Z=8  R=1.6 LMX=2

VERS          # ctrl file format version
 LMF=7 FP=7 LM=7
```

# SrTiO3 – lmchk output

*great! Can we check that it makes sense?*

```
run > ls -l
total 8
-rw-r--r--  1 jerome  staff  571 May 12 11:32 ctrl.srtio3
run > lmchk ctrl.srtio3
 ----------------------  START LMCHK ----------------------

 LMCHK:    nbas = 5  nspec = 3  vn 7.11.i  verb 35
 special
 pot:      XC:BH
 float:    float P LDA-style
 autoread: none

                Plat                                  Qlat
   1.000000   0.000000   0.000000        1.000000   0.000000   0.000000
   0.000000   1.000000   0.000000        0.000000   1.000000   0.000000
   0.000000   0.000000   1.000000        0.000000   0.000000   1.000000
   alat = 7.3692  Cell vol = 400.185207

 LATTC:  as= 2.000   tol=1.00E-08   alat= 7.36920   awald= 0.271
         r1=  2.885   nkd= 93       q1=  3.426   nkg= 171

 SGROUP: 1 symmetry operations from 0 generators
 SYMLAT: Bravais system is cubic with 48 symmetry operations.
 SYMCRY: crystal invariant under 48 symmetry operations for tol=1e-5
 GROUPG: the following are sufficient to generate the space group:
         i*r3d r2(0,1,1)
         i*r3d r2(0,1,1)
 MKSYM:  found 48 space group operations ... includes inversion
 Use default rmaxs = 7.218 a.u. = 2.7*avw = 0.98*alat
```

# SrTiO3 – lmchk output

```
   Site     Class            Rmax        Hcr                 Position
    1       1  Sr          2.600000    1.820000    0.00000    0.00000    0.00000
    2       2  Ti          2.200000    1.540000    0.50000    0.50000    0.50000
    3       3  O           1.600000    1.120000    0.00000    0.50000    0.50000
    4       3  O           1.600000    1.120000    0.50000    0.50000    0.00000
    5       3  O           1.600000    1.120000    0.50000    0.00000    0.50000

 Cell volume= 400.18521   Sum of sphere volumes= 169.69627 (0.42404)

 ib jb  cl1     cl2        Pos(jb)-Pos(ib)      Dist  sumrs   Ovlp    %    summt   Ovlp   %
  2  3  Ti      O        -3.685  0.000  0.000   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8
  2  4  Ti      O         0.000  0.000 -3.685   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8
  2  5  Ti      O         0.000 -3.685  0.000   3.685  3.800   0.12   3.1*  2.660  -1.02 -27.8

 OVMIN, 81 pairs:  fovl = 9.43828e-10   <ovlp> = 3.1%   max ovlp = 3.1%
 Exit 0 LMCHK
 CPU time:    0.031s   Wall clock    0.062s   11:33:00 12.05.2017        on

 Wall-clock time: 0.063s. Resolution 0.000001s

run >
```

- overlap $\sim 3\%$ is maybe ok: we will learn later how to improve upon this using **blm**
- for more information, increase the verbosity from the command line, eg:

  **`lmchk --pr50 srtio3`**
- lots of information: also neighbour tables, bond angles, ... (see Se example)

# Ctrl file for SrTiO3

Before running a DFT calculation we must:

1. specify the exchange-correlation functional
2. run the atom solver **lmfa** to setup basis
3. identify any semicore states
4. specify the smooth grid (plane-wave cut-off) for representing $n$ and $V$
5. specify the $\vec{k}$-sampling
6. specify the maximum number of iterations to self-consistency

# SrTiO3 – Basis

specify the exchange-correlation functional and LMTO basis:

```
VERS          # ctrl file format version
 LMF=7 FP=7 LM=7

HAM           # options relating to the Hamiltonian
  XCFUN=1     # LDA (VWN)
# XCFUN=0 101 130 #PBE-GGA using LibXC interface
  AUTOBAS[MTO=2 LMTO=5] # MTO=2: read from "basp" file
                        # LMTO=5: use BIG basis
  GMAX=0      # smooth grid cut-off
              # use the recommendation from lmfa
```

`AUTOBAS` introduces options for automatic basis:

**lmfa**: (radial) atom solver, *provides* core density, atomic eigenfunctions and basis definitions

**lmf**: (full potential) band program, *requires* atom density and basis definitions

# SrTiO3 – lmfa output (1)

output of running **lmfa**:

```
 Species Sr:  Z=38  Qc=36  R=2.600000  Q=0
 mesh:   rmt=2.600000  rmax=49.676653  a=0.025  nr=425  nr(rmax)=543
  Pl=  5.5     5.5     4.5     4.5
  Ql=  2.0     0.0     0.0     0.0

  iter      qint         drho          vh0          rho0          vsum      beta
    1    38.000000   6.880E+03      190.0000    0.1890E+03     -76.3617   0.30
   52    38.000000   4.253E-05      403.4924    0.8727E+05    -286.9181   0.30


 sumev=-0.535008  etot=-6351.658531  eref=0.000000

 Free-atom wavefunctions:
 valence:       eval        node at       max at        c.t.p.    rho(r>rmt)
   5s        -0.26750          1.649        3.616        5.425      0.892875
   5p        -0.09680          1.962        4.862        8.333      0.965189
   4d        -0.10320          0.652        2.151        8.148      0.611161
   4f         0.01876          0.000       35.936       49.677*     1.000000

 core:          ecore        node at       max at        c.t.p.    rho(r>rmt)
   1s     -1169.16523          0.000        0.026        0.052      0.000000
   2s      -158.32529          0.052        0.145        0.227      0.000000
   2p      -140.77626          0.000        0.116        0.244      0.000000
   3s       -24.44466          0.210        0.436        0.632      0.000000
   3p       -18.78747          0.188        0.431        0.721      0.000000
   3d        -9.42158          0.000        0.376        1.008      0.000003
   4s        -3.00733          0.594        1.187        1.701      0.017430
   4p        -1.68003          0.613        1.324        2.193      0.059807
```

occupancy and eigenvalues for each state of each species

# SrTiO3 – lmfa output (2)

```
Optimise free-atom basis for species Sr, rmt=2.6
l  it     Rsm       Eh      stiffR    stiffE       Eval       Exact      Pnu     Ql
0  50    5.014   -1.324       34.7       1.2    -0.25087   -0.26750     5.32    2.00
... rsm exceeded rmt .. repeat with rsm=rmt
0  14    2.600   -0.100       34.7    2365.1    -0.21210   -0.26750     5.32    2.00
1  21    3.783   -0.100       32.7    1011.9    -0.10503   -0.09680     5.12    0.00
... rsm exceeded rmt .. repeat with rsm=rmt
1   1    2.600   -0.100       32.7    -612.9    -0.07161   -0.09680     5.12    0.00
2  11    1.658   -0.100      576.5    -114.9    -0.08060   -0.10320     4.79    0.00
eigenvalue sum:  exact   -0.53501    opt basis   -0.42419    error 0.11081

Make LMTO basis parms for species Sr to lmxb=3, rmt=2.6  vbar=0
l  it     Rsm        Eh         Eval       Exact      Pnu     Ql    Gmax
0  11    1.733*   -0.100*    -0.13053   -0.26750     5.32    2.00    4.0
1  42    0.300    -5.000     -1.01117   -0.09680     5.12    0.00   26.2
... l=1  fit parms out of range ... revert to defaults
1  42    1.733+   -0.100+    -0.05603   -0.09680     5.12    0.00
2  11    1.658    -0.100*    -0.08060   -0.10320     4.79    0.00    4.7
3   1    1.733+   -0.100+     0.30532    0.01876     4.19    0.00
```

basis construction ... for all species. Lastly:

```
   rho: r>rmt   1.368046   r<rmt   4.631954   qtot   6.000000

FREEAT:  writing file basp0

FREEAT:  estimate HAM_GMAX from RSMH:  GMAX=9.4

Sum of reference energies: 0
Exit 0 LMFA
CPU time:    0.177s   Wall clock    0.205s   13:27:25 12.05.2017        on

Wall-clock time: 0.206s. Resolution 0.000001s
```

we use this recommendation for the smooth mesh grid

# SrTiO3 – lmfa output (3)

**lmfa** also generates the "basp" file, containing the automatically fitted basis:

```
BASIS:
 Sr RSMH= 1.733 1.733 1.658 1.733 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.733 1.733 1.658 EH2= -0.9 -0.9 -0.9
 Ti RSMH= 1.467 1.467 1.091 1.467 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.467 1.467 1.091 EH2= -0.9 -0.9 -0.9
 O RSMH= 0.851 0.813 1.067 1.067 EH= -0.465 -0.1 -0.1 -0.1 RSMH2= 0.851 0.813 1.067 EH2= -1.265 -0.9 -0.9
```

- this is a large *spdf,spd* basis (but, remember `LMX`)
- the generated basis definition is written to **`basp0.ext`**
- `EH` and `EH2`: Hankel energies, here in "LDA" style
- `RSMH` and `RSMH2`: smoothing radii optimised by **lmfa**
- to use the basis, we **need to copy** **`basp0.ext`** to **`basp.ext`**

# SrTiO3 – ready to go

```
# cubic perovskite SrTiO3
STRUC
 NSPEC=3       # number of different species
 NBAS=5        # number of occupied sites
 ALAT=7.3692   # expt lattice constant (bohr) (3.8996AA)
 PLAT=1 0 0
      0 1 0
      0 0 1    # lattice vectors

SITE
 ATOM=Sr XPOS=0 0 0
 ATOM=Ti XPOS=1/2 1/2 1/2
 ATOM=O  XPOS=0 1/2 1/2
 ATOM=O  XPOS=1/2 1/2 0
 ATOM=O  XPOS=1/2 0 1/2

SPEC           # definitions for individual species
 ATOM=Sr Z=38 R=2.6 LMX=2 # R_mt and LMX key in LMTO
 ATOM=Ti Z=22 R=2.2 LMX=2
 ATOM=O  Z=8  R=1.6 LMX=2

VERS           # ctrl file format version
 LMF=7 FP=7 LM=7

HAM            # options relating to the Hamiltonian
 XCFUN=1       # LDA (VWN)
# XCFUN=0 101 130 #PBE-GGA using LibXC interface
 AUTOBAS[MTO=2 LMTO=5] # MTO=2: read from "basp" file
                       # LMTO=5: use BIG basis
 GMAX=9.5      # smooth grid cut-off from LMFA

BZ
 NKABC=10 10 10 # k-mesh divisions

ITER
 NIT=50        # max scf iterations
```

# SrTiO3 – run lmf (1)

```
run > clear
run > ls
ctrl.srtio3
run > lmfa srtio3 > atomlog
run > mv basp0.srtio3 basp.srtio3
run > mpirun -np 4 lmf srtio3 > scflog
run > cat save.srtio3
h ehf=-8505.8980933 ehk=-8504.4915374
i ehf=-8507.0104948 ehk=-8492.1939833
i ehf=-8505.7239925 ehk=-8504.9668352
i ehf=-8505.5817481 ehk=-8505.2006142
i ehf=-8505.4880124 ehk=-8505.417938
i ehf=-8505.4825994 ehk=-8505.4432019
i ehf=-8505.4728415 ehk=-8505.4631945
i ehf=-8505.4721799 ehk=-8505.4721639
i ehf=-8505.47202 ehk=-8505.4720064
c ehf=-8505.4720245 ehk=-8505.4720211
run > tail scflog

   it 10  of 50    ehf=   -8505.472024   ehk=   -8505.472021
 From last iter    ehf=   -8505.472020   ehk=   -8505.472006
 diffe(q)= -0.000004 (0.000026)    tol= 0.000010 (0.000030)   more=F
c ehf=-8505.4720245 ehk=-8505.4720211
 Exit 0 LMF      on vpn-3-063
 CPU time:   63.127s   Wall clock   63.196s   14:38:46 12.05.2017        on

 Wall-clock time: 63.195s. Resolution 0.000001s

run >
```

- great!
- remember: energies in Rydberg

# SrTiO3 – run lmf (2)

**main reporting via stdout:**

- version, special features
- header, lattice, symmetry, BZ sampling, species data
- Hamiltonian info, charges
- for each scf step:
  - average potentials ($V_{mtz}$)
  - local orbital setup
  - $E_f$, VBM/CBM/$E_g$
  - eigenvalues at selected $\vec{k}$
  - update logarithmic derivatives `P`
  - energy contributions
  - info on (charge) mixing
  - scf progress, total energy (moment)

**varies depending upon setup/code**

**verbosity can be changed:** `lmf --pr10` **(spartan) or** `--pr60` **(hefty)**

# SrTiO3 – run lmf (3)

| | |
|---|---|
| `atm.srtio3` | core and valence density and potential for atom (ASCII) |
| `atomlog` | stdout from **lmfa** (worth recording) |
| `basp.srtio3` | basis definition (essentially ctrl file data) |
| `ctrl.srtio3` | |
| `log.srtio3` | slightly cryptic log infos |
| `mixm.srtio3` | scf mixing history (binary) |
| `moms.srtio3` | weights of overlap matrix (binary) |
| `rst.srtio3` | full restart information (binary, can ask for ASCII) |
| `save.srtio3` | energy (and possibly total spin) during scf cycle (ASCII) |
| `scflog` | stdout from **lmf** (really worth recording!) |
| `wkp.srtio3` | $\vec{k}$-point weights (binary) |

*plus many more files generated for different tasks/outputs!*

# SrTiO3 – run lmf (4)

**`lmf --input|less`** very useful quick-reference for input tokens!

```
run > lmf --input
...

 DYN_MD                 opt    ---
   Parameters for molecular dynamics
 DYN_MD_MODE            reqd   i4       1,  1     default = 0
   0: no MD 1: NVE 2: NVT 3: NPT
 DYN_MD_TSTEP           opt    r8       1,  1     default = 20.671
   Time step (a.u.)
 DYN_MD_TEMP            opt    r8       1,  1     default = 0.00189999
   Temperature (a.u.)
 DYN_MD_TAUP            opt    r8       1,  1     default = 206.71
   Thermostat relaxation time (a.u.)
 DYN_MD_TIME            reqd   r8       1,  1     default = 20671000
   Total MD time (a.u.)
 DYN_MD_TAUB            opt    r8       1,  1     default = 2067.1
   Barostat relaxation time (a.u.)
 DYN_MD_P               opt    r8       1,  1     default = 0
   External pressure
 NB: 1 deg.K = 6.3333e-6 a.u.; 1 fs = 20.67098 a.u.

 --- Parameters for GW ---
 GW_NKABC               opt    i4v      3,  1
   No. qp along each of 3 lattice vectors.
   Supply one number for all vectors or a separate number for each vector.
 GW_BZJOB               opt    i4v      3,  1     default = 0
   0 centers BZ mesh at origin, 1 centers off origin
   Supply one number for all vectors or a separate number for each vector.
run >
```

each of the codes **lmf**,**blm**,**lmgf**,**lmfgwd**, etc ... provide this

# SrTiO3 – run lmf (5)

**`lmf --help`** print quick information about command line arguments

```
run > lm --help
 usage:  lm [--OPTION] [-var-assign] [ext]

 --h
 --help          Print this message, and quit
 --input         List categories, tokens, and data program expects, and quit
 --show          Print control file after parsing by preprocessor,
                 and echo input data as read from the control file
 --showp         Same as --show, but quit after input parsed
 --iactiv        (--no-iactiv) Turn on (off) interactive mode
                 This switch overrides input file setting
 --pr#1[,#2...] Set the verbosity (stack) to values #1,#2, ...
 --time=#1[,#2] Print timing info to # levels (#1=summary; #2=on-the-fly)

 -vnam=expr      Define numerical variable "nam"; set to result of 'expr'
 -cnam=strn      Define character variable "nam"; set to 'strn'

 --rpos=filnam  After reading input file, read site positions from "filnam"
 --fixlat        Adjust lattice vectors and point group ops, attempt to
                 render them internally consistent
 --fixpos[:tol=#] Adjust positions slightly, rendering them
                 as consistent as possible with the symmetry group
 --nosym         Suppress symmetry operations

 lm-specific options:

 --rs=#1,#2 --band[~option...] --pdos[~option...] -mix=#1[,#2] --onesp --weula --rsedit --efrnge
 For --band mode options, see doc/generating-energy-bands.html

 lm v 7.11.i

 Wall-clock time: 0.001s. Resolution 0.000001s

run >
```

# SrTiO3 – a little ctrl file magic

```
1  -vnam=expr      Define numerical variable "nam"; set to result of 'expr'
```

- access from the command line to variables defined in the ctrl file!
- preprocessor variables in **`ctrl`** file introduced by "% const var=exp"
- evaluated before being passed to the code
- variables which are changed from their defaults are echoed in the **`save.ext`** file
- quite a rich syntax/grammar with many features
- used extensively by **blm** and demo cases

# SrTiO3 – a little ctrl file magic

- example: converging the $\vec{k}$ mesh:

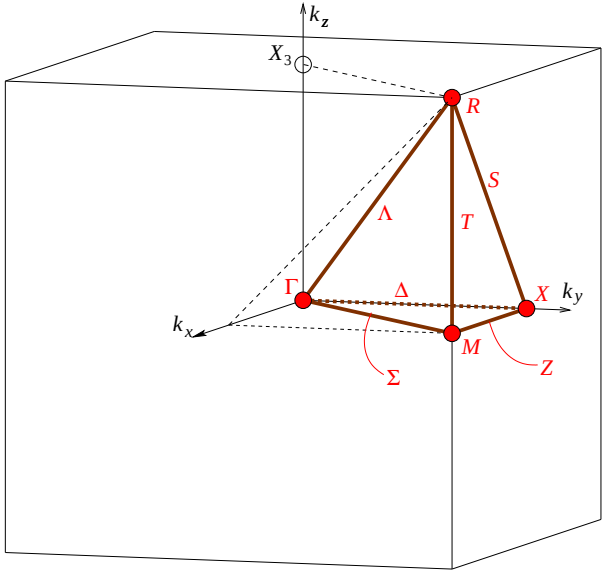
```
 GMAX=9.5      # smooth grid cut-off from LMFA

% const nk=10
BZ
 NKABC={nk} # k-mesh divisions

ITER
 NIT=50        # max scf iterations
```

- **NKABC**: can take three argments $(a,b,c)$ or one (all the same)
- **NKABC**: when one negative value given, value relates to full BZ, $(a,b,c)$ are scaled according to reciprocal cell vector lengths

```
run > vi ctrl.srtio3
run > for i in -50 -100 -200 -500 -1000 -1e4
> do
> lmf -vnk=$i srtio3 >scflog_$i
> done
run > grep ^c save.srtio3
c nk=-50 ehf=-8505.4706686 ehk=-8505.4706653
c nk=-100 ehf=-8505.4717582 ehk=-8505.4717562
c nk=-200 ehf=-8505.4719586 ehk=-8505.471957
c nk=-500 ehf=-8505.4720141 ehk=-8505.4720126
c nk=-1e3 ehf=-8505.4720129 ehk=-8505.4720116
c nk=-1e4 ehf=-8505.4720128 ehk=-8505.4720116
run >
```

# SrTiO3 – plot the band structure (simple)

- require path in $\vec{k}$

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http://www.cryst.ehu.es

setup a file **qp.srtio3** describing the path...

```
68   0.5 0.0 0.0   0.0 0.0 0.0 # X--G
96   0.0 0.0 0.0   0.5 0.5 0.0 # G--M
68   0.5 0.5 0.0   0.5 0.5 0.5 # M--R
118  0.5 0.5 0.5   0.0 0.0 0.0 # R--G
0    0.0 0.0 0.0   0.0 0.0 0.0 # terminates
```

Cartesian $\vec{k}$ coordinates

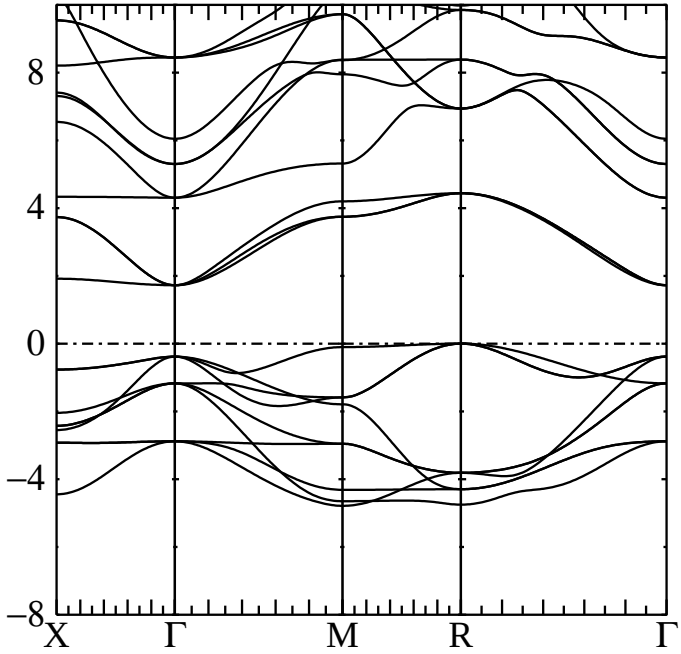
try to get reasonably equal spacing

rerun: **`lmf --band srtio3`**
(using converged potential contained in **rst** file)

gives new file: **bnds.srtio3** (ASCII $\varepsilon_{i,\vec{k}}$)

# SrTiO3 – plot the band structure (simple)

- `echo -8,10,8,6 | plbnds -fplot -ef=0 -scl=13.6 -lbl=X,G,M,R,G bnds.srtio3`
- **`fplot`** – general plotting utility
- **`plbnds`** – bnds to plot tool
- options: emin, emax, width(cm), height(cm)
- **`fplot -disp -f plot.plbnds`**
  – gives you a .ps figure:
- lots of information:
  https://www.questaal.org/docs/misc/fplot/

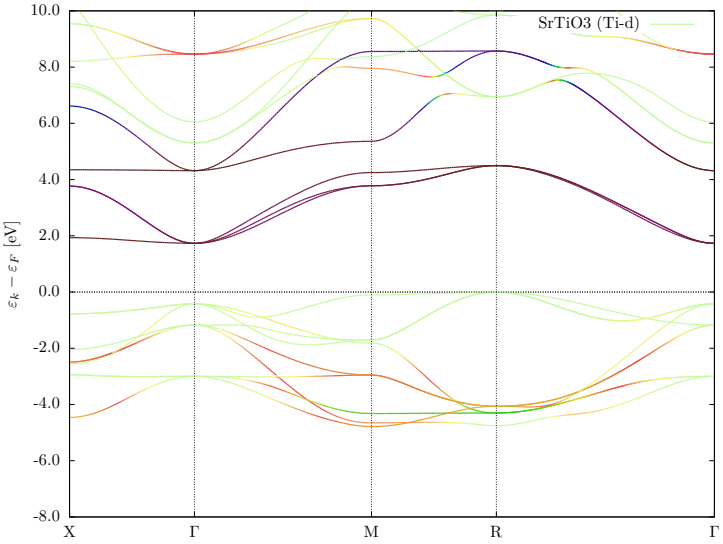


# SrTiO3 – band structure with character

- first ask **lmf** for details of the order of the basis:
  `lmf --quit=ham --pr60 srtio3`

```
Orbital positions in hamiltonian, resolved by l:
 Site  Spec  Total    By l ...
   1    Sr     1:18   1:1(s)   2:4(p)   5:9(d)   10:10(s) 11:13(p) 14:18(d)
   2    Ti    19:36   19:19(s) 20:22(p) 23:27(d) 28:28(s) 29:31(p) 32:36(d)
   3    O     37:54   37:37(s) 38:40(p) 41:45(d) 46:46(s) 47:49(p) 50:54(d)
   4    O     55:72   55:55(s) 56:58(p) 59:63(d) 64:64(s) 65:67(p) 68:72(d)
   5    O     73:90   73:73(s) 74:76(p) 77:81(d) 82:82(s) 83:85(p) 86:90(d)
suham :  80 augmentation channels, 80 local potential channels  Maximum lmxa=3
```

- want the 10 Ti-d components (2-$\kappa$ basis)
- run **lmf** again with options to the –band flag:
  `lmf --band col=23:27,32:36 srtio3`
- fplot does colouring well, also!



# SrTiO3 – using local orbitals (1)

- **lmf** offers several ways of including semicore states in the valence: traditional local orbitals and extended local orbitals (their own $h(z)$)
- generally qualitative difference, sometimes significant
- when to include semicore-states?
  - reasonably shallow atomic states ($\varepsilon_i > -2.5 Ryd$)
  - atomic states that leak ($Q(r > r_{mt}) > 0.002e$)
- this is a change in the basis: re-run the atom solver **lmfa**
- a couple of new ctrl parameters

```
1
2  HAM            # options relating to the Hamiltonian
3   XCFUN=1       # LDA (VWN)
4  # XCFUN=0 101 130 #PBE-GGA using LibXC interface
5   AUTOBAS[MTO=2 LMTO=5 LOC=1 ELOC=-2.5 QLOC=0.002]
6                           # MTO=2: read from "basp" file
7                           # LMTO=5: use BIG basis
8                           # LOC=1: search for semicore states
9               # ELOC: atomic eigenvalue condition
10              # QLOC: semicore leakage condition
11  GMAX=9.5      # smooth grid cut-off from LMFA
```

# SrTiO3 – using local orbitals (2)

```
HAM            # options relating to the Hamiltonian
 XCFUN=1       # LDA (VWN)
# XCFUN=0 101 130 #PBE-GGA using LibXC interface
 AUTOBAS[MTO=2 LMTO=5 LOC=1 ELOC=-2.5 QLOC=0.002]
                          # MTO=2: read from "basp" file
                          # LMTO=5: use BIG basis
                          # LOC=1: search for semicore states
             # ELOC: atomic eigenvalue condition
             # QLOC: semicore leakage condition
 GMAX=9.5      # smooth grid cut-off from LMFA
```

- **lmfa** finds Sr 4p ($-1.680 Ryd$) and Ti 3p ($Q(r > r_{mt}) = 0.0220$)

```
run > ls
ctrl.srtio3_5
run > lmfa ctrl.srtio3_5 >atomlog
run > grep -A5 "Find local" atomlog
 Find local orbitals which satisfy E > -2.5 Ry  or  q(r>rmt) > 2e-3
 l=1   eval=-1.680  Q(r>rmt)=0.0598  PZ=4.915  Use: PZ=14.915
 l=2   eval=-9.422  Q(r>rmt)=3e-6  PZ=3.964  Use: PZ=0.000

 tailsm: fit tails to 6 smoothed hankels, rmt= 2.60000, rsm= 1.30000
 HNSMFT: 103 points in interval  2.60000  33.29923;  q=  1.785753
--
 Find local orbitals which satisfy E > -2.5 Ry  or  q(r>rmt) > 2e-3
 l=1   eval=-2.851  Q(r>rmt)=0.0220  PZ=3.926  Use: PZ=13.926
```

- syntax for local orbitals: `PZ` (l)
- +10 for extended local orbital (default and best)

# SrTiO3 – using local orbitals (3)

- new basis file:

```
BASIS:
 Sr RSMH= 1.733 1.733 1.658 1.733 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.733 1.733 1.658 EH2= -0.9 -0.9 -0.9
     PZ= 0 14.915
 Ti RSMH= 1.467 1.467 1.091 1.467 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.467 1.467 1.091 EH2= -0.9 -0.9 -0.9
     PZ= 0 13.926
 O RSMH= 0.851 0.813 1.067 1.067 EH= -0.465 -0.1 -0.1 -0.1 RSMH2= 0.851 0.813 1.067 EH2= -1.265 -0.9 -0.9
```

- after running **lmfa**, copy `basp0.ext`→`basp.ext`

- the core Q has now changed as we move the semicore into the valence: **must rerun lmfa**

- (otherwise: "Exit -1 problem in locpot – possibly low LMXA, or orbital mismatch, species Sr")

- transition elements, high-lying (higher $n$ than occupied) local orbitals are useful, too:
  - for Ti: `PZ= 0 13.926` becomes `PZ= 0 13.926 4.3`
  - high-lying local orbitals are of conventional type

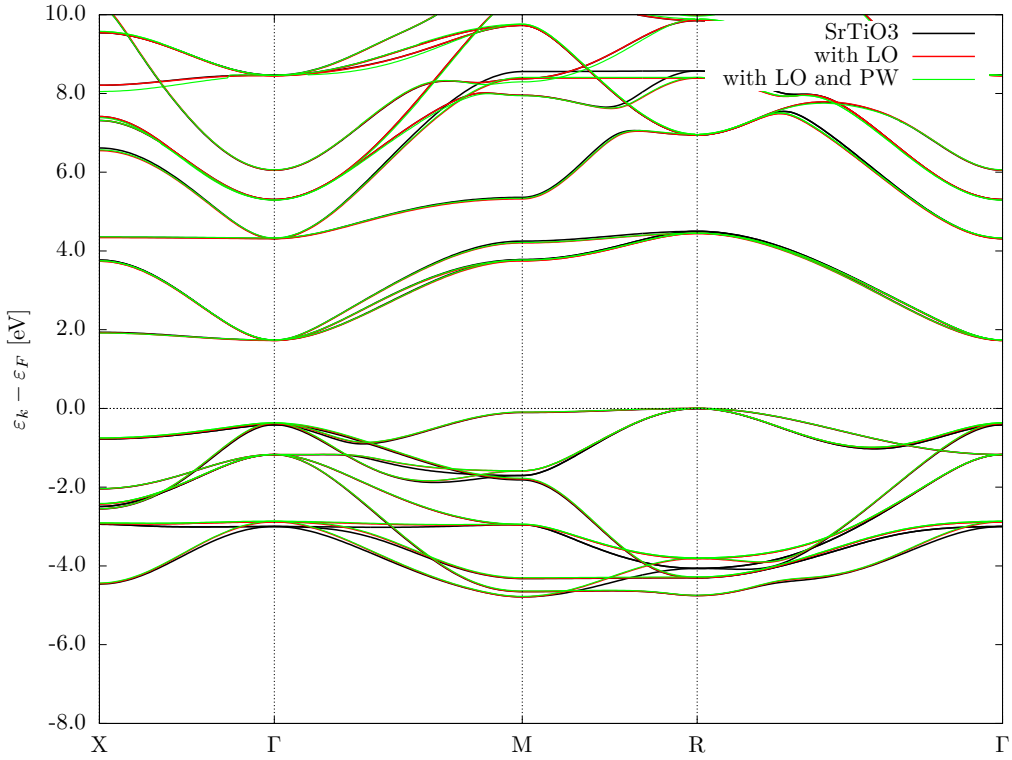
# SrTiO3 – improving the basis with plane waves

- pretty easy to specify: cut-off energy
- necessary for more open structures
- remedies LMTO deficiencies

```
                        # LMTO=5: use BIG basis
                        # LOC=1: search for semicore states
             # ELOC: atomic eigenvalue condition
             # QLOC: semicore leakage condition
 GMAX=9.5      # smooth grid cut-off from LMFA
 PWMODE=11 PWEMIN=0.0 PWEMAX=2.0

BZ
 NKABC=10 10 10 # k-mesh divisions
```

- prefer **PWMODE=11**: cut-off relates to $(\vec{k} + \vec{G})$
- reduce $r_{mt}$ if a large PW set is desired
- avoid over-completeness in difficult cases with **HAM_OVEPS=1e-10**
- beware that expense increases with **PWEMAX**
  (here, 2Ryd amounts to $\sim 30$ extra basis functions)

# SrTiO3 – improving the basis with plane waves




- LMTO basis is already excellent (PW are not needed)
- the semi-core states are significant

# automatic ctrl generator: blm (1)

- a lot of options and settings in the control file
- basis choices, particularly $r_{mt}$, can be difficult
- different variables needed for different kinds of calculations
- **blm** provides easy atomated interface
- common choices represented by command line flags (see: `blm --help`)
- higher level interface to the code

# automatic ctrl generator: blm (2)

workflow: **cif→init** using **cif2cell** (community python utility)

**init→ctrl** using **blm**

```
run > ls
MyBaseFileName_80872.cif
run > /opt/cif2cell-1.2.10/cif2cell MyBaseFileName_80872.cif > cif2cell.stdout
run > ls
MyBaseFileName_80872.cif cif2cell.stdout
run > cif2init cif2cell.stdout >cif2init.stdout
run > ls
MyBaseFileName_80872.cif cif2cell.stdout          cif2init.stdout          init
run > mv init init.srtio3
run > cat init.srtio3
HEADER Sr (Ti O3) (Strontium titanate)
LATTICE
#        SPCGRP=221
#        A=3.8996  B=3.8996  C=3.8996   ALPHA=90  BETA=90  GAMMA=90
% const a=3.8996
         ALAT={a}  UNITS=A
         PLAT=     1.0000000     0.0000000     0.0000000
                   0.0000000     1.0000000     0.0000000
                   0.0000000     0.0000000     1.0000000
SITE
      ATOM=Sr        X=      0.0000000     0.0000000     0.0000000
      ATOM=Ti        X=      0.5000000     0.5000000     0.5000000
      ATOM=O         X=      0.0000000     0.5000000     0.5000000
      ATOM=O         X=      0.5000000     0.5000000     0.0000000
      ATOM=O         X=      0.5000000     0.0000000     0.5000000
run > blm init.srtio3 >blmlog
run > ls
MyBaseFileName_80872.cif blmlog                   cif2init.stdout          log.srtio3
actrl.srtio3             cif2cell.stdout          init.srtio3              site.srtio3
```

# automatic ctrl generator: blm (3)

output from **blm**:

```
makrm0: initial MT radii from first estat potential maximum
 site    spec             rmt       rmt-       rmt-       rold    lock
                                   <spec avg>  spec-min
   1     1:Sr            3.1085      0.0000     0.0000     0.0000
   2     2:Ti            2.0893      0.0000     0.0000     0.0000
   3     3:O             1.5945      0.0000     0.0000     0.0000
   4     3:O             1.5945      0.0000     0.0000     0.0000
   5     3:O             1.5945      0.0000     0.0000     0.0000
SCLWSR:  mode = 0  vol = 400.182 a.u.   Initial sphere packing = 53.7%  scaled to 71.8%
constr omax1=   0.0   0.0   0.0 %    omax2= 100.0 100.0 100.0 %
actual omax1=   0.0   0.0   0.0 %    omax2=   0.0   0.0   0.0 %

... Create input file actrl.dat (express mode 3)
IOSITE: wrote to file 'site', 5 sites

Wall-clock time: 0.148s. Resolution 0.000001s
```

- automatic scheme for finding $r_{mt}$ based on potential landscape
- structure is placed in "site.dat" file – separates structure from ctrl variables
- EXPRESS category provides alias to common options

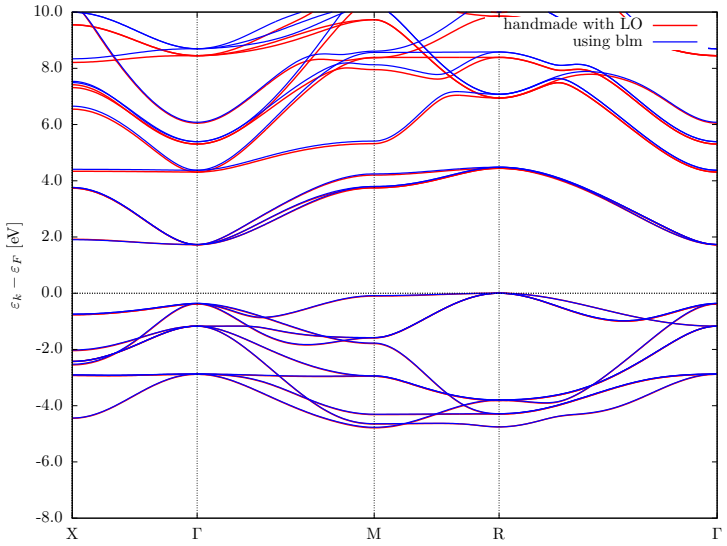
# automatic ctrl generator: blm (4)

the generated **ctrl** file:

```
# Autogenerated from init.dat using:
# blm

# Variables entering into expressions parsed by input
% const nit=10
% const met=5
% const so=0 nsp=so?2:1
% const lxcf=2 lxcf1=0 lxcf2=0      # for PBE use: lxcf=0 lxcf1=101 lxcf2=130
% const pwmode=0 pwemax=3           # Use pwmode=1 or 11 to add APWs
% const nkabc=0 gmax=0

VERS  LM:7 FP:7 # ASA:7
IO    SHOW=f HELP=f IACTIV=f VERBOS=35,35  OUTPUT=*
EXPRESS
# Lattice vectors and site positions
  file=   site

# Basis set
  gmax=   {gmax}                   # PW cutoff for charge density
  autobas[pnu=1 loc=1 lmto=5 mto=4 gw=0]

# Self-consistency
  nit=    {nit}                    # Maximum number of iterations
  mix=    B2,b=.3,k=7              # Charge density mixing parameters
  conv=   1e-5                     # Convergence tolerance (energy)
  convc=  3e-5                     # tolerance in RMS (output-input) density

# Brillouin zone
  nkabc=  {nkabc}                  # 1 to 3 values
  metal=  {met}                    # Management of k-point integration weights in metals

# Potential
  nspin=  {nsp}                    # 2 for spin polarized calculations
```

# automatic ctrl generator: blm (5)

```
  nspin=  {nsp}                    # 2 for spin polarized calculations
  so=     {so}                     # 1 turns on spin-orbit coupling
  xcfun=  {lxcf},{lxcf1},{lxcf2}   # set lxcf=0 for libxc functionals

#SYMGRP i*r3d r2(0,1,1)
HAM
      PWMODE={pwmode} PWEMIN=0 PWEMAX={pwemax} OVEPS=0 # For APW addition to basis
      FORCES={so==0} ELIND=-0.7
SPEC
  ATOM=Sr        Z= 38  R= 3.615925  LMX=3  LMXA=3
  ATOM=Ti        Z= 22  R= 2.089718  LMX=2  LMXA=4
  ATOM=O         Z=  8  R= 1.594872  LMX=2  LMXA=3
```




- very good agreement (eg, $\Delta E_g = 8$meV)
- **LMX** increased for Sr
- **LMXA** increased for Ti
  ($l$ cut-off for augmentation)
- difference in empty states due to large
  $r_{mt} = 3.6$bohr on Sr
  (**blm --wsrmax=3.0** fixes this)
- **blm** probably better than my guesses!

# Advice

- ctrl file:
  - use the **blm** to setup $r_{mt}$; use `--gw` for $GW$ setup
  - check the `--help` and `--input` to see if what you want is there
- LDA setup
  - use a large basis (eg, `AUTOBAS_LMTO=5`)
  - the default basis setup (`EH,RSMH`) should be satisfactory "out of the box"
  - (also **`lmf --optbas`**, ..!)
  - semicore local orbitals should be included when present
  - use **lmfa** recommendation for `GMAX`, but test for convergence
  - consider plane waves for tricky open structures (`PWEMAX=2Ryd` goes a long way)
- in general
  - *many* tools and utilities to setup different systems, obtain properties and analyse data
  - just ask us! ☺
  - Se relaxation: https://www.questaal.org/tutorial/lmf/molstat/