

lmf, lmfa, lmchk

We need ctrl file ctrl.foobar for inputs.

lmfa: spherical atom calculations

Example:

```
lmfa si
```

It finishes instantaneously.

```
lmfa si |grep conf
```

shows electronic configurations. It gives electron densities of spherical atoms contained in the primitive cell specified by .

With the superposition of the densities From which, we construct initial electronic density for lmf.

In addition, **lmfa** generates

lmf: solving the Kohn-Sham equation

- **Usage:** `mpirun lmf TARGET [options] > llmf`

Example:

```
mpirun -np 4 lmf si [options] > llmf
```

PROF

This is a case we have ctrl.si.

options

- quit option at some point. `--quit=band`, `--quit=ldau`... We need to do 'grep cmdopt SRC//.f90|grep quit' to know details.
- `--tdos`
total dos calculation.
- `-vfoobar=xxx` : This override const foobar=yyy defined in ctrl, and used as {foobar} in ctrl file.
This is shown in save file explained below.

We have some kinds of options for electron density plot, boltztrap and so on.
(not yet described).

Input files

- `syml.target`
symmetry line for band plot (usually `job_band` calls `lmf` internally)
- `sigm.target`
a part of QSGW calculation
- Usually (when `READP=T` in `ctrl`), we need `atmpnu*` generated by `lmfa`.

Output files

- `rst.target`
restart file : it mainly contains electron density.
- `save.target`
This contains very minimum history for you to execute `lmf`, `lmf`, `lmchk`, and total energies for each iteration step of `lmf`.
- `mix.target`
mixing file for electron density. When you stop iteration at the middle, you may need to delete this.

** Main Source** : `SRC/main/lmf.f90`

lmchk: Check crystal symmetry.

`lmchk` gives useful information of space group symmetry recognized by `lmf`. In addition, it determines MT radius.