syml.foobar

Symmetry line for the band plot.
We can generate `syml.foobar` by `getsyml`.

Get symmetry lines for band plot and Brillouwin zone plot.

`syml.*` is generated from `ctrl.*`. `syml.*` is needed for band plot.
After generated, you can easily edit `syml.*` for `job_band`.

At ecalj/GetSyml, we have getsyml.py, which is based on the
seekpath at https://github.com/giovannipizzi/seekpath/
and spglib at https://anaconda.org/conda-forge/spglib

Usage:

We make softlink getsyml to ecalj/SRC/GetSyml/getsyml.py during the install by InstallAll.py.
Run

```
getsyml nio
(or)
getsyml ctrls.nio
```

. This show 3D Brillouin zone together with symmetry lines for band plot.
See BZsamples here.
The symmetry lines are written into the `syml.*` file for ecalj.
The number of divisions for `syml` is give by a crude algorism, so edit it if necessary.

Needed citations for getsyml

PROF

In addition to usual ecalj acknowledgement, following citations are required when you make a publication.

1.Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, I. Tanaka,
Band structure diagram paths based on crystallography,
Comp. Mat. Sci. 128, 140 (2017)

2.You should also cite spglib that is an essential library used in the implementation.
https://github.com/atztogo/spglib.git

- See Lincence.txt for spglib and seekpath.

(memo for developer)

a.Modify lmchk to write required information to supply reasonable.
For example, ndiv (mesh size along lines).

b.Numerical accuracy of calculations.
np.set_printoptions(precision=16) is not meaningful since we read output of lmchk

symmetry-line file : input for plotting energy bands along selected symmetry lines or for generating constant-energy contours such as a Fermi surface. This file (whose name is specified as a modifier with the command-line argument --band, described in the "Command-line switches" section) can take on of several forms.

format of syml

```
generate bands along specific symmetry lines.
The following sample input illustrates input for lines
X->Gamma and Gamma->M for the simple cubic lattice.
   21  .5 0  0    0  0  0         X     Gamma
   21  0  0  0    .5 .5 0         Gamma  M
   0   0  0  0    0  0  0
The first number designates how many points along each line.
The next six label the starting and ending q-points,
respectively.  Note that the last line must contain zeros.
```