October 2014

DynaPhoPy

How to use (quick guide)

Prepare PHONOPY harmonic lattice dynamics calculation

Obtain **FORCE_SETS** file from PHONOPY:

phonopy -f vasprun{000..}.xml

Refer to PHONOPY manual for further information

Keep original **POSCAR** file used in the calculation containing unaltered structural data (VASP 5.x style required)

Prepare VASP Molecular Dynamics calculation

Obtain **OUTCAR** file with Molecular Dynamics information

Refer to VASP manual for further information

*The input file used for VASP MD calculation must be a super cell of the structure in POSCAR file used in PHONOPY calculation. SPOSCAR file generated by PHONOPY may be used.

Prepare input file for DYNAPHOPY

Create an **input file** that contains information referred to:

Files location (**FORCE_SETS** and **POSCAR**).

If not specified, POSCAR file and FORCE_SETS are read (in the same directory)

Primitive matrix

Matrix that defines the primitive cell. If not specified identity matrix is used.

PHONOPY calculation super cell matrix

Matrix that defines the supercell used in PHONOPY calculation.

Bands definition

Defines the phonon dispersion bands that will be plotted in “obtain dispersion spectra” option. If not defined direction (0,0,0) -> (0,0,0.5) is used.

Each parameter is preceded by a label which indicates parameter type in input file (see examples).
All the parameters are optional, except PHONOPY calculation super cell matrix.
See input examples for several compounds in DYNAPHOPY folder

Execute DYNAPHOPY

Command line execution:

./dynaphopy **input_file** **OUTCAR** [-options]

*Execute “./dynaphopy -h “ for options information

Interactive execution:

./dynaphopy -i **input_file** **OUTCAR** [-options]

Final notes

-n flag in DYNAPHOPY execution takes the last specified steps from MD OUTCAR file to perform the calculations. By default it takes only 2000 which is good as a first approximation, but for line widths calculation is recommended to take at least 20000.

-i interactive flag is compatible with the other options (like -n, -q, -r) but is not recommended to request calculations through flags and using interactive mode at the same time.