October 2015

DynaPhoPy

How to use

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 unit cell data

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Prepare Molecular Dynamics calculation

- Using VASP

Obtain **XDATCAR** file with Molecular Dynamics information

Refer to VASP manual for further information

- Using Lammps

Obtain **lammpstrj** file with Molecular Dynamics information

Refer to LAMMPS manual for further information

*The input file used for 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 is 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 inside input file are optional, if not specified default parameters are taken.
You can specify only the necessary ones for the requested calculation.
See input examples for several compounds in DYNAPHOPY folder

Execute DYNAPHOPY

Command line execution:

./dynaphopy **input_file** **XDATCAR/lampstrj** [-options]

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

Interactive execution:

./dynaphopy -i **input_file** **XDATCAR/lampstrj** [-options]

time.

Options

-n N
Use only the lasts N steps of the trajectory file

-q N1 N2 N3
Wave vector in with the projection will be done

-r INI END
Frequency range used in the calculation of the power spectra

-pd
Plot the full power spectrum

-sd FILENAME
Save the full power spectrum to file

-pw
Plot wave vector projected power spectrum

-sw FILENAME
Save wave vector projected power spectrum to file

-pp
Plot phonon mode projected power spectrum

-sp FILENAME
Save phonon mode projected power spectrum

-psm N
Change power spectrum algorithm (1:Maximum entropy method, 2: FFT method)

-cf N
Number of coefficients used in Maximum entropy method

-pa
Peak analysis.Fit phonon projected power spectrum to Lorentzian and get properties

-pad X Y Z
Plot the atomic displacements of each atom in direction X Y Z

-sad X Y Z FILENAME
Save the atomic displacements of each atom in direction X Y Z to file

-sfc FILENAME
Save renormalized force constants to file

--silent
Text only results (No plots are displayed)

Final notes

For more information check DynaPhoPy web page
http://abelcarreras.github.io/DynaPhoPy/

You can follow DynaPhoPy development on GitHub
https://github.com/abelcarreras/DynaPhoPy