Longxun inc., Beijing

User guide

use pwmat to calculate phonons

PWmat2Phonopy 0.2.1

Author:
Peng Chen

email:
peng.chen.iphy@gmail.com

November 15, 2017

Abstract

PWmat2Phonopy provides an interface to phonopy, which can help PWmat user perform phonon calculations. You might find it most useful for tasks you already have a relaxed atom.config. The best thing of PWmat2Phonopy is that, with almost only one click, the phonon spectrum will be calculated for you.

1 Install

Firstly, download PWmat2Phonopy-x.x.x.tar.gz from github (https://github.com/PaulChern/PWn
    Secondly, unzip the PWmat2Phonopy-x.x.x wherever you prefer.
    Thirdly, include /where/you/put/PWmat2Phonopy-x.x.x in you PYTHON-PATH and /where/you/put/PWmat2Phonopy/bin in your PATH.
    Finally, all things are settled.

2 Usage

2.1 quick start

Just type in PWmatRunPhonopy.py in the directory where atom.config, etot.input, and PP are strored.

2.2 for experienced users

The PWmatRunPhonopy.py will call PWmat2Phonopy, a PWmat version of phonopy with an interface to PWmat format and all the functions in phonopy. Other than using the PWmatRunPhonopy.py directly, you can acturally use PWmat2Phonopy too. The use of the PWmat2phonopy is exactly the same as phonopy, except that you should include –pwmat in the args when you are using a PWmat calculator. If you use –vasp, –wien2k, –abinit, and et. al., PWmat2Phonopy will work exactly the same as the phonopy does. So, if you want to learn all the functions and how to use, you can consult phonopy website or user guide.