User's Guide

May 30, 2014

VASPKIT

Postprocessing tool for the VASP code

* Bug report: please send a copy of both input and output files to

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1. Features

VASPKIT version: 0.3 (14 Apr. 2014)

Choose the problem to solve:
========== Structural Options ==========
4: Building Supercell *(New added)*
5: EOS Fitting
========== Electronic Options ==========
11/12: Total/Projected DOS
13: l-m Decomposed DOS
21/22: Total/Projected Band Structure
========== Charge Density & Potential Options ==========
31/32: Charge/Spin Density
33: Spin-Up & -Down Density *(New added)*
34/35: Charge/Spin Density Difference *(New added)*
41/42: Planar Average Charge/Potential *(New added)*
========== Optical options ==========
51: Linear Optics

0: Quit ————>>

2. Installation

For the VASPKIT installation, basic UNIX/LINUX environment and *fortran compiler* are required. Also, you can install VASPKIT on WINDOWS system using MinGW program.

Compiling the program is very simple, please use the following commands.
$ tar -zvxf vaspkit.*.tar.gz
$ cd vaspkit.*/src
$ modify the *Makefile* file based on your machine environment;
$ make
** Note that the formats of POSCAR, CONCAR and CHGCAR files in VASP.5.x are slightly different from those in VASP.4.x. Please set the vasp5=.false. in the src/module.f90 file if you use VASP.4.x;*

3. Usage

Table 1: Current available option, function and the corresponding input (output) files.

Option	Function	Read file	Output file
4	Building Supercell	POSCAR/CONTCAR	SC***.VASP[1]
5	EOS Fitting	EOS.IN	*.DAT[2]
11	Total DOS	DOSCAR	TDOS.DAT, ITDOS.DAT
12	Projected DOS	DOSCAR	PDOS.No.*.DAT, IPDOS.No.*.DAT
13	l-m Decomposed DOS	DOSCAR	LMDOS.No.*.DAT, ILMDOS.No.*.DAT
21	Band Structure	PROCAR, KPOINTS	BAND.DAT, KPATH.DAT
22	Projected Band Structure	PROCAR, KPOINTS	PBAND.DAT, KPATH.DAT
31	Charge Density	CHG	CHARGE.VASP
32	Spin Density	CHG	SPIN.VASP
33	Spin-Up & -Down Density	CHG	SPIN.UP.VASP, SPIN.DOWN.VASP
34	Charge Density Difference	CHG1*, CHG2*[3]	CHGDIFF.VASP
35	Spin Density Difference	CHG1*, CHG2*	SPINDIFF.VASP
41	Planar Average Charge	CHG	PAVG.DAT
42	Planar Average Potential	LOCPOT	PAVG.DAT
51	Linear Optics	REAL.IN and IMAG.IN	*.DAT

[1] Open *.VASP files with VESTA code (http://jp-minerals.org/vesta/en/).

[2] Open *.DAT files with scientific 2D plotting program, such as Origin, Gnuplot, Grace and so on.

[3] The file names of CHG1* and CHG2* can only consist of letter and number.

3.1 EOS fitting

The equation of state (EOS) sub-program for fitting energy-volume data was implemented from elk code (http://elk.sourceforge.net/). You need to prepare the ***EOS.IN*** file before performing EOS fitting. The following variables are set in the file EOS.IN:

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cname : name of crystal up to 256 characters

natoms : number of atoms in unit cell

etype : equation of state type (see below)

vplt1, vplt2, nvplt : volume interval over which to plot energy, pressure etc. as well as the number of points in the plot

nevpt : number of energy-volume points to be inputted vpt(i)

ept(i) : energy-volume points (VASP default units, *i.e.,* $\AA^3$ *and* eV)

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* *Note that the input units are VASP default values, i.e., Å^3 and eV. See an example in vaspkit.*/examples/eos/*

The equations of state currently implemented are:

1. Universal EOS (Vinet P et al., J. Phys.: Condens. Matter 1, 1941 (1989))
2. Murnaghan EOS (Murnaghan F D, Am. J. Math. 49, 235 (1937))
3. Birch-Murnaghan 3rd-order EOS (Birch F, Phys. Rev. 71, 809 (1947))
4. Birch-Murnaghan 4th-order EOS
5. Natural strain 3rd-order EOS (Poirier J-P and Tarantola A, Phys. Earth Planet Int. 109, 1 (1998))
6. Natural strain 4th-order EOS
7. Cubic polynomial in (V-V_0)

3.2 Linear optics

The absorption coefficient, refractive coefficient, reflectivity coefficient, extinction coefficient and energy-loss function as a function of photon energy can be calculated. You need to prepare the ***REAL.IN*** and ***IMAG.IN*** files which include the real and imaginary parts of frequency-dependent complex dielectric function. The REAL.IN and IMAG.IN consist of the following data:

energy	*xx*	*yy*	*zz*	*xy*	*yz*	*zx*
..	..	..	..	..	..	..
..	..	..	..	..	..	..

energy is the photon energy (in eV). *xx*, *yy*, *zz*, *xy*, *yz* and *zx* are the calculated values of frequency dependent dielectric tensor writted in vasprun.xml. There is a bash script ***optics.sh*** as a reference in the vaspkit.*/examples/optic/ could help you to prepare the real.in and imag.in files.

3.3 Misc

Under construction .....