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<td>September 3, 2020</td>
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<td>0.2.2 (2020-08-18)</td>
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High throughput
Building structure (lattice, atomic, supercell etc.) and calculating properties automatically
Submit multi-structures only one command line

Expert settings
Settings without additional convergence tests

Robust
Checking symmetry including strain, energy and bond distance

Finite temperature
Free energy including electron and phonon contribution

Shoulders of giants
pymatgen: materials analysis and I/O
Custodian: calculation error recovery
FireWorks: workflow packages
atomic: materials calculate environment
The goal of DFTTK is to make high-throughput first-principles calculations as simple as possible. The density functional theory (DFT) based software VASP is employed to perform first-principles calculations. In addition thermodynamic properties via the quasiharmonic approach, we proposed that any property, as long as it is dependent on the volume or strain, can be predicted using a quasi-static approach implemented by our group according to (i) the predicted property-volume/strain relationship from first-principles calculations directly and (ii) the volume/strain-temperature relationship of materials from the quasiharmonic approach.

For a given structure and elements, calculate all kinds of thermodynamic properties at finite temperature and pressure by first-principles approach based on density functional theory, including lattice vibration, thermal electron excitation, Seebeck coefficient, Lorenz number, effective charge carrier concentration etc.
By its definition, the term of “first-principles” represents a philosophy that the prediction is to be based on a basic, fundamental proposition or assumption that cannot be deduced from any other proposition or assumption. This implies that the computational formulations are based on the most fundamental theory of quantum mechanics - Schrödinger equation or density functional theory (DFT) and the inputs to the calculations must be based on well-defined physical constants – the nuclear and electronic charges. In another word, once the atomic species of an assigned material are known, the theory should predict the energy of all possible crystalline structures, without invoking any phenomenological fitting parameters.

However, to perform DFT calculations in reality, it still needs the user to have extensive experiences on a variety of parameter choices and a lot of human handling on numerical or system exceptions. In the last decade, we have been working on solving the problem by integrating our experiences accumulated on high-throughout DFT calculations into a software package named as DFTTK (DFT based toolkits) and opened to the community (https://www.dfttk.org).
CHAPTER THREE

THE MAIN FUNCTIONS OF DFTTK

• Structure maker by prototype and elemental substitution;
• Robust 0 K equilibrium volume optimization;
• Robust 0 K energy-volume curve optimization;
• Quasiharmonic phonon calculation;
• Born effective charge calculation;
• Elastic constant calculations.
• MongoDB database management
• Thermodynamic calculations and figure plots
To perform DFT calculation using DFTTK, the user only needs to name the structure file called POSCAR by VASP, either prepared by user or produced by DFTTK by elemental substitution on given prototype. DFTTK is developed on atomate from the Materials Project which is built on three open-source Python libraries. The main benefits of atomate are its flexibility and data management platform, in particular the numerical convergence control and computational exception handling. DFTTK is able to predict properties at finite temperatures by phonon or Debye model for both stoichiometric and solution phases, featured by:

- High-throughput DFT calculation and postprocess;
- Postprocess plenty of data stored in MongoDB with one simple command;
- Compatible with Yphon package and phonopy;
- Can recover data from certain fizzled calculations;
- Can account thermal electron contribution to thermodynamic properties;
- Can calculate thermodynamic properties at 0 K and a few tenth K;
- Can perform doping calculations for semiconductors or thermoelectric materials under rigid band approximation;
- Can account the effect of thermal expansion/temperature on Seebeck coefficient, Lorenz number, thermal carrier concentrations;
- Automatic plot figures for more than 20 thermodynamic properties in the publishable resolution, including atomic volume, free energy, entropy, enthalpy, linear thermal expansion coefficient, isobartic specific heat, constant volume specific heat, lattice only specific heat, bulk modulus, Debye temperature, Seebeck coefficient, Lorenz number, absolute thermal electric force, etc.
CHAPTER FIVE

THE OUTLINE OF FLOW CHART OF DFTTK

Provide robust density functional theory workflows for calculating thermodynamic properties in temperature and composition space. The work flow control of DFTTK is given by the following blueprint.
DFTTK makes it automatic to going through these ISIF options by the workflow shown in the figure in the right.

The purpose of DFTTK robust relaxation is to find the lowest energy structure within a given threshold of a given symmetry. This information is especially useful in the case, for example

1. Random solution phase;
2. High temperature phase which is unstable in low temperature;
3. The calculation of energetics for endnumber for CALPHAD modeling.

The solution is to make the best use of ISIF control parameter in VASP, which controls:

<table>
<thead>
<tr>
<th>ISIF</th>
<th>calc. force</th>
<th>relax stress tensor</th>
<th>relax ions</th>
<th>change cell shape</th>
<th>change cell volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>1</td>
<td>yes</td>
<td>trace only</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>2</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>3</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>4</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>5</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
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</tr>
<tr>
<td>6</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
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</tr>
<tr>
<td>7</td>
<td>yes</td>
<td>yes</td>
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</tr>
</tbody>
</table>
6.1 License

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The MIT License (MIT)

6.2 Installation

It is recommended to install DFTTK under the anaconda environment. Under the linux command prompt (or anaconda powershell prompt for Windows), one can create a preferred directory and then run

- Release version

```
pip install dfttk
```

- Development version

```
git clone https://github.com/PhasesResearchLab/dfttk.git
cd dfttk
pip install -e .
```

- Alpha interanal daily test version

```
git clone https://github.com/yiwang62/dfttk.git
cd dfttk
pip install -e .
```

to get the laste updates for the Alpha version based on one’s current version, run

```
git fetch origin
git checkout 20210405 #20210405 is a branch name which may be change in a time maner
```

mkdir a folder named config whereever you want to followed by copy the file db.json, my_launchpad.yaml from your MongoDB manager into config/. See the section Config MongoDB

```
dfttk config -all --nodes 1 --ppn 16 --pmem 32gb -aci -M yourcomputer -qt yourbatch -mpi PMG_MAPI_KEY
```

where
vasp_psp is a place holding your vasp pseudopotentials
yourcomputer is your computer name, such as aci-rour, cori-knl, cori-ksw, bridges2, stampede2
yourbactch can be pbs, slurm
PMG_MAPI_KEY can be obtained by: Go to the materials project website, https://materialsproject.org/, under the API section, you will easily find you API Keys number.
finally, you need to change the account number and queue/partition number in the config/my_qadapter.yaml file

6.2.1 Config MongoDB

DFTTK needs MongoDB to manage DFT calculations and outputs. The users of DFTTK can either buy the commercial MongoDB database service or set up their own MongoDB server.

Ask the MongoDB system manager for two json files: one named db.json and another named my_launchpad.yaml and save them in a config folder wherever you choose.

db.json used by FireWorks through MongoDB to access the DFTTK output results, templated as follows.

```json
{
    "database": "userid-results",
    "collection": "tasks",
    "admin_user": "userid",
    "admin_password": "pass1",
    "readonly_user": "userid-ro",
    "readonly_password": "pass2",
    "host": "146.186.149.69",
    "port": 27018,
    "aliases": {}
}
```

my_launchpad.yaml used by FireWorks through MongoDB for DFT job managements, templated as follows.

```yaml
host: 146.186.149.69
name: userid-fws
password: pass3
port: 27018
ssl_ca_file: null
strm_lvl: INFO
user_indices: []
username: userid
wf_user_indices: []
```

6.2.2 Access MongoDB database from desktop

One can install robo3T from https://robomongo.org/. One needs to use the information from the db.json file to setup robo3T connection as indicated below
#note

1. PSU-VM is a label of your choice to remark the MongoDB connection;
2. 146.186.149.69 is the ip address of the MongoDB server;
3. One needs to replace userid with the one (i.e. the value field of admin_user) from the db.json file together with the the value field of admin_password

6.2.3 YPHON

To postprocess the finite properties, the Yphon package is required. Yphon can be installed by run

```
cd ~
git clone https://github.com/yiwang62/YphonPackage
#Note: Usually the precompiled binaries should be executable in the common Linux/Unix environment. If not, do the following:

cd YphonPackage/YPHON/YPHON
make
#Note: If errors reported in the compiling stage, insert one line #define R_OK 1 after
...

```

For csh user: the command search path should be changed by inserting line below into the .cshrc (.tcshrc) file

```
set path = (. ~/YphonPackage/YPHON/YPHON $BIN_PATH $path)
```

For bsh user: the command search path should be changed by inserting the lines below into the .bash_profile (.bashrc) file

```
PATH=.:~/YphonPackage/YPHON/YPHON:$BIN_PATH:$PATH
export PATH
```
6.3 Examples

The Examples folder is designed to keep the data for user to test the DFTTK package. The two subfolder are:

- dir `Al` - contains all data for test run for Al
- dir `ZrSiO4` - contains all data for test run for ZrSiO4
- dir `ExptData` - contains a json file `ExptData.json` which saves the experimental thermodynamic data for a collection of materials.

Within the Al or the ZrSiO4 subfolder, one see two subfolders

- dir input - contain input setup files using Al as the example on E-V, phonon, and thermodynamic property calculations
- Al_Fm-3m_225PBE - contain outputs by postprocessing data that saved in MongoDB by the above Al example.

For the data within Al_Fm-3m_225PBE/

- dir Yphon - all data input/output for Yphon, e.x., hessian matrix (superfij.out), calculated phonon dos
- dir figures - plots in png format for most of the thermodynamic properities
- file readme - extensive summary of the calculated results in json format
- file fvib_ele - tablated data containing the calculated thermodynamic properties
- file fvib_eij - tablated data containing the calculated thermal expansion coefficient tensor
- file record.json - SGTE fitting record for heat capacity, Gibbs energy, enthalpy, and entropy at given temperature range

To run the Example for the VASP calculation, say Al, run

```
cd Al/input
dfttk run -wf robust -f POSCAR.Al -l -m 1
```

To postprocess calculations after the VASP calculation done, run

```
cd Al
dfttk thfind -py -td -50 -plot find_or_DFT -eq 4 -smooth -el 1 -renew -get -metatag
   0c1887fa-0cb4-4ce2-9559-7f90ffaf1a -expt ../ExptData/ExptData.json
   #note that the key "0c1887fa-0cb4-4ce2-9559-7f90ffaf1a" is obtained from the file
   "input/METADATAS.yaml" automatically produced by the VASP calculation step.
```

The above will produce more than 20 figures stored in the folder “Al_Fm-3m_225PBE/figures/” and they can be view them using the linux command `display` to show the figure, for example

```
display Al_Fm-3m_225PBE/figures/LTC.png #to see the linear thermal expansion coefficient
```
display Al_Fm-3m_225PBE/figures/Heat_capacities.png  #to see the heat capacitity, and so on
### 6.4 Quick guide to run DFTTK

#### 6.4.1 Submit dfttk DFT batch job

The DFT calculations are managed by the run modules by the command `dfttk run`

- Submit a single calculation

Go to any folder under ytests folder say `cd dfttk/ytests/ex55`, then run

```bash
   dfttk run -f POSCAR.Al -l -m 1
```

![Graph of Heat capacities vs. Temperature](image-url)
6.4.2 Postprocess DFTTK results

To postprocess the DFTTK results and get thermodynamic properties.

- Single postprocess

```
dfttk thelec -renew -plot find_or_DFT -metatag metatag.
```

where metatag is the metadata tag automatically produced after one submits the dfttk job, the argument -renew instruct thelec to redo the calculations even already done previously, and the arguments -plot find_or_DFT instruct thelec to find the label for theoretical curve from the MongoDB database (in the above case, it found PBE) and use DFT if not found. In the above example, one can find out metatag in the value field of tag by cat dfttk/ytests/ex55/METADATA.yaml

The run of the above command will cost a couple of minutes. After the command done, one will see a folder with name like compound_xxx-xxx (in the above example, the folder name will be Al_Fm-3m_225PBE within which the fcontents are:

- folder figures - plots in png format for most of the thermodynamic properties;
- file readme - contain key information in json format;
- file fvib_ele - text table contains the thermodynamic properties
- file record.json - json file contains Shomate Equation (SGTE) fitting of Cp, G-H298.15, H-H298.15, and S; and
- folder Yphon - extracted data to run Yphon for further analysis

The figures stored in the figures folder can viewed by the command display, e.x, to see the evolution of Helmholtz energy as functions of volume and temperature

```
display Al_Fm-3m_225PBE/figures/Helmholtz_energy.png
```
6.5 Configuration of DFTTK

6.5.1 Content

- On batch job
- Preparation
- Configure all with one command
- Configure separately
  - Configuration for atomate
  - Configuration for pymatgen
- Example
- Validation for configuration
6.5.2 On batch job

- SLURM sbatch instruction
- SLURM sbatch example

6.5.3 Preparation

For configure dfttk, the following file you need to prepare.

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>current_folder</td>
<td>-psp [specified by -psp]</td>
</tr>
<tr>
<td>pseudopotential_content</td>
<td>[required if you didnot configurate pymatgen]</td>
</tr>
<tr>
<td>config</td>
<td>[specified by -c parameter]</td>
</tr>
<tr>
<td>db.json</td>
<td>[required]</td>
</tr>
<tr>
<td>my_launchpad.yaml</td>
<td>[required]</td>
</tr>
<tr>
<td>FW_config.yaml</td>
<td>[optional]</td>
</tr>
<tr>
<td>my_fworker.yaml</td>
<td>[optional]</td>
</tr>
<tr>
<td>my_qadapter.yaml</td>
<td>[optional]</td>
</tr>
<tr>
<td>vaspjob.pbs</td>
<td>[optional, specified by -q parameter]</td>
</tr>
</tbody>
</table>

After prepared the above **required** file, simply run `dfttk config -all` to finish the configuration. If such command successes, you can skip all of the reset part of this documents. If not, please reading the following parts.

- **pseudopotential_content**: The vasp pseudopotential.
  - **PRL Group Notes**: For PRL group, if you use ACI at PSU, you can skip this part, using `-aci` parameter
  - It can be compressed file (*.tar.gz) or uncompressed folder. The name is handled as follows:
**PSP Name**

**Note:** 1. The split can recognize \(.,-,+,=,^*\) and space.

**2.** After split, the name will be a list. The condition e.g. `contain 52` is the elements' level. It means `52` should be a elements of the list. But `US` is string level, which means `US` only need be a sub-string of the elements of the list.

**3.** For compressed file, it support `*.tar.gz` and `*.tar`

e.g. `potpaw_PBE`, `PBE.tar.gz` and `potpaw_PBE_5254` will be recognized as `PBE`.

`potpaw_PBE.52` and `potpaw_PBE_52` will be recognized as `PBE_52`

`potUSPP_LDA` and `POT_LDA_US` will be recognized as `LDA_US`

After prepare, the file structure should look like as follows:
The original pseudopotential file, please ask those who are in charge of vasp in your group.

- **MAPI_KEY**: The API key of Materials Project, ref. API KEY

- **vaspjob.pbs**: The submitting script of your queue system. **Currently, only pbs system is supported**

- **other config files**: At least, you need prepare two files, db.json and my_launchpad.yaml. The template is shown in the config folder.
  - For more details, please ref. Configure database connections and computing center parameters

- **PRL GROUP NOTES**:
  - For db.json and my_launchpad.yaml file, please ask Brandon for help.
  - vaspjob.pbs for ACI can be download from github
  - For pseudopotential, two choices: 1. using the pseudopotentials in ACI account (Using -aci parameter). 2. Download the pseudopotential from group’s box (Group Documents/VASP_potential note: only PBE_54 and LDA_54).

### 6.5.4 Configure all with one command

- dfttk config -all

- For ACI at PSU user, please use dfttk config -all -aci

```
usage: dfttk config [-h] [-all] [-p PATH_TO_STORE_CONFIG] [-a]
                 [-c CONFIG_FOLDER] [-q QUEUE_SCRIPT] [-qt QUEUE_TYPE]
                 [-v VASP_CMD_FLAG] [-mp] [-aci] [-psp VASP_PSP_DIR]
                 [-mapi MAPI_KEY] [-df DEFAULT_FUNCTIONAL]
```

The meaning of the parameters, please ref Help for dfttk config command or just run dfttk config -h

### 6.5.5 Configure separately

**Configuration for atomate**

- Config manual, ref Configure database connections and computing center parameters

- dfttk config -a

```
usage: dfttk config -a [-p PATH_TO_STORE_CONFIG] [-c CONFIG_FOLDER] [-q QUEUE_SCRIPT]
                    [-qt QUEUE_TYPE] [-v VASP_CMD_FLAG]
```

The meaning of the parameters, please ref Help for dfttk config command or just run dfttk config -h
Configuration for pymatgen

- Config manual, ref POTCAR setup in pymatgen
- `dfttk config -mp`

```bash
```

The meaning of the parameters, please ref Help for dfttk config command or just run dfttk config -h

---

**6.5.6 Example**

```bash
dfttk config -all -p test_config -mapi test_api
```

In `test_config` folder

```
test_config
config
db.json
FW_config.yaml
my_fworker.yaml
my_launchpad.yaml
my_qadapter.yaml
logs
vasp_psp
    POT_GGA_PAW_PBE_54
    Ac
    ...
    POT_LDA_PAW_54
    Ac
    ...
```

In `~/.bashrc`

```bash
export FW_CONFIG_FILE=/gpfs/scratch/mjl6505/test/dfttk/tutorial/config/test_config/config/FW_config.yaml
```

in `~/.pmgrc.yaml`

```yaml
PMG_DEFAULT_FUNCTIONAL: PBE
PMG_MAPI_KEY: test_api
PMG_VASP_PSP_DIR: /gpfs/scratch/mjl6505/test/dfttk/tutorial/config/test_config/vasp_psp
```

---

6.5. Configuration of DFTTK
6.5.7 Validation for configuration

- `dfttk config -t`

  This command will validate the configuration, and give some error or tips for the incorrect configuration

  ```
dfttk config -t [{all,pymatgen,atomate,none}]
  ```

  - Currently only support validation for the configuration of pymatgen

6.5.8 Help for `dfttk config` command

`dfttk config -h`

DFTTK version: 0.1.121.g8fddda3.dirty
Copyright Phases Research Lab (https://www.phaseslab.com/)

Usage: dfttk config [-h] [-all] [-p PATH_TO_STORE_CONFIG] [-a]
       [-c CONFIG_FOLDER] [-q QUEUE_SCRIPT] [-qt QUEUE_TYPE]
       [-v VASP_CMD_FLAG] [-mp] [-aci] [-psp VASP_PSP_DIR]
       [-mapi MAPI_KEY]
       [-df {LDA,LDA_52,LDA_54,LDA_US,PBE,PBE_52,PBE_54,PW91,PW91_US,Perdew-
Zunger81}]
       [-t [{all,pymatgen,atomate}]]

Optional arguments:
  -h, --help           show this help message and exit
  -all, --all           Configure atomate and pymatgen.
  -p PATH_TO_STORE_CONFIG, --prefix PATH_TO_STORE_CONFIG
                       The folder to store the config files. Default: .
                       (current folder)
  -a, --atomate         Configure atomate.
  -c CONFIG_FOLDER, --config_folder CONFIG_FOLDER
                       The folder containing config files, at least contain db.json
                       and my_launchpad.yaml. Default: './'
  -q QUEUE_SCRIPT, --queue_script QUEUE_SCRIPT
                       The filename of the script for submitting vasp job. It
                       will search in current folder and sub-folders.
                       Default: vaspjob.pbs
  -qt QUEUE_TYPE, --queue_type QUEUE_TYPE
                       The type of queue system. Note, only pbs is supported
                       now. Default: pbs
  -v VASP_CMD_FLAG, --vasp_cmd_flg VASP_CMD_FLAG
                       The flag to distinguish vasp_cmd to other commands in
                       queue_script. Default: vasp_std
  -mp, --pymatgen       Configure pymatgen.
  -aci, --aci           Using the pseudopotential on the ACI cluster at PSU.
  -psp VASP_PSP_DIR, --vasp_psp_dir VASP_PSP_DIR
                       The path of pseudopotentials. Default: psp

(continues on next page)
-mapi MAPI_KEY, --mapi_key MAPI_KEY
  The API key of Materials Projects
-df \{LDA,LDA_52,LDA_54,LDA_US,PBE,PBE_52,PBE_54,PW91,PW91_US,Perdew-Zunger81\}, --
default_functional \{LDA,LDA_52,LDA_54,LDA_US,PBE,PBE_52,PBE_54,PW91,PW91_US,Perdew-
Zunger81\}
  The default functional. Default: PBE
-t \[{all,pymatgen,atomate}\], --test_config \[{all,pymatgen,atomate}\]
  Test for configurations. Note: currently only support for pymatgen.

6.6 Settings file

The user can change the settings for dfttk calculations by providing a settings file.

6.6.1 File name instruction

Global settings

By default, the global settings file is named as SETTINGS.yaml or SETTINGS.json.
The user can change the name by -s parameter in dfttk run. e.g. if the user run dfttk by dfttk run -s SET, then the files named with SET.yaml or SET.json is the global settings file.

Individual settings

The user can provide individual settings for some structures whose settings is different with others.
The individual settings file should be named with SETTINGS-Filename_With_Ext.yaml(json) or Filename_With_Ext-SETTINGS.yaml(json)

Note:

- Filename_With_Ext is the file name of structure with extension.
- SETTINGS is case insensitive, both settings and SETTINGS are OK.

E.g. In the working folder, there are some structure files as follows:

<table>
<thead>
<tr>
<th>Fe3Ni.cif</th>
</tr>
</thead>
<tbody>
<tr>
<td>POSCAR</td>
</tr>
<tr>
<td>POSCAR-2</td>
</tr>
</tbody>
</table>

Then the following files will be recognized as settings files.

<table>
<thead>
<tr>
<th>SETTINGS-Fe3Ni.cif.yaml</th>
</tr>
</thead>
<tbody>
<tr>
<td>POSCAR-SETTINGS.yaml</td>
</tr>
<tr>
<td>settings-POSCAR-2.yaml</td>
</tr>
</tbody>
</table>
6.6.2 Keywords in the file

Default settings

The settings file is optional, if the user does not provide the settings file, the default value will be used.

- Common settings
<table>
<thead>
<tr>
<th>Keywords</th>
<th>Default Value</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>magmom</td>
<td>No</td>
<td>The MAGMOM for each atom, e.g. [4, 4, -4, 4]. <em>Note</em>, the length must agree with the number of atoms</td>
</tr>
<tr>
<td>metadata</td>
<td>No</td>
<td>The metadata of the calculation. If the user provides it, DFTTK will find the existing calculations in the database. If not, it will generate by uuid4.</td>
</tr>
<tr>
<td>isif4</td>
<td>False</td>
<td>If run ISIF=4 following ISIF=7 in RobustOptimizeFW</td>
</tr>
<tr>
<td>level</td>
<td>1</td>
<td>Optimize level. If run ISIF=2 after last ISIF=4 in RobustOptimizeFW 1 for run and 2 for not</td>
</tr>
<tr>
<td>override_symmetry_tolerances</td>
<td>None</td>
<td>Override the default symmetry tolerance, if None, {'tol_strain':0.05, 'tol_energy':0.025, 'tol_bond':0.10}</td>
</tr>
<tr>
<td>override_default_vasp_params</td>
<td>{}</td>
<td>Override the default vasp settings. The optional keys is 'user_incar_settings', 'user_kpoints_settings', 'user_potcar_functional'. For more details, ref. <a href="https://pymatgen.org/pymatgen.io.vasp.sets.html">https://pymatgen.org/pymatgen.io.vasp.sets.html</a></td>
</tr>
<tr>
<td>modify_incar_params</td>
<td>{}</td>
<td>Modify the incar settings in the fireworks level. e.g. modify_incar_params = {'Full relax': {'incar_update': {'LCHARG':False}}, 'static': {'incar_update': 'LAECHG':True}}</td>
</tr>
<tr>
<td>modify_kpoints_params</td>
<td>{}</td>
<td>Modify the kpoints settings in the fireworks level.</td>
</tr>
<tr>
<td>store_volumetric_data</td>
<td>False</td>
<td>Store the volumetric data (True) or not (False)</td>
</tr>
<tr>
<td>verbose</td>
<td>False</td>
<td>print(True) or not(False) some informations, for debug</td>
</tr>
<tr>
<td>passinitrun</td>
<td>False</td>
<td>Pass init vasp result. <strong>It will be dropped in the future</strong></td>
</tr>
<tr>
<td>run_isif2</td>
<td>False</td>
<td>If run ISIF=2 before ISIF=4 (True) or not (False). <strong>It will be dropped in the future</strong></td>
</tr>
<tr>
<td>pass_isif4</td>
<td>False</td>
<td>Whether pass isif=4 calculation. <strong>It will be dropped in the future</strong></td>
</tr>
<tr>
<td>symmetry_tolerance</td>
<td>0.05</td>
<td>The tolerance for symmetry. <strong>It will be dropped in the future</strong></td>
</tr>
<tr>
<td>relax_path</td>
<td>''</td>
<td>The path of relaxation. <strong>It will be dropped in the future</strong></td>
</tr>
</tbody>
</table>

- Phonon settings
### Keywords

<table>
<thead>
<tr>
<th>Keywords</th>
<th>Default Value</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>phonon</td>
<td>False</td>
<td>Run phonon (True) or not (False, Debye model)</td>
</tr>
<tr>
<td>phonon_supercell_matrix</td>
<td>Matrix, e.g.</td>
<td>The supercell matrix for phonon calculations. It can take the following</td>
</tr>
<tr>
<td></td>
<td></td>
<td>values: Matrix, e.g. [[2, 0, 0], [0, 2, 0], [0, 0, 2]] String: atom/lattice/volume (the first letter works) Determining the supercell matrix automatically by atoms/lattice/volume ranges</td>
</tr>
<tr>
<td>phonon_supercell_matrix_min</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>phonon_supercell_matrix_max</td>
<td>130</td>
<td></td>
</tr>
<tr>
<td>force_phonon</td>
<td>False</td>
<td>Force run phonon (True) or not (False), No matter ISIF=4/stable_tor pass or not</td>
</tr>
<tr>
<td>stable_tor</td>
<td>0.01</td>
<td>Sample tolerance (The percentage of negative dos), If the negative part of DOS is larger than this value, DFTTK won’t run phonon for this structure.</td>
</tr>
</tbody>
</table>

- **QHA settings**

<table>
<thead>
<tr>
<th>Keywords</th>
<th>Default Value</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_deformations</td>
<td>7</td>
<td>The number of deformations/structures</td>
</tr>
<tr>
<td>deformation_fraction</td>
<td>[-0.1, 0.1]</td>
<td>The range of deformation, 0.1 means 10%</td>
</tr>
<tr>
<td>eos_tolerance</td>
<td>0.01</td>
<td>The tolerance for eos fitting. If larger than this value, DFTTK will append volumes automatically</td>
</tr>
<tr>
<td>t_min</td>
<td>5</td>
<td>The minimum of temperature in QHA process</td>
</tr>
<tr>
<td>t_max</td>
<td>2000</td>
<td>The maximum of temperature in QHA process</td>
</tr>
<tr>
<td>t_step</td>
<td>5</td>
<td>The step of temperature in QHA process</td>
</tr>
<tr>
<td>volume_spacing_min</td>
<td>0.03</td>
<td>Minimum ratio of Volumes spacing. This keyword will be dropped in the future</td>
</tr>
</tbody>
</table>

- **Elastic settings**

<table>
<thead>
<tr>
<th>Keywords</th>
<th>Default Value</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>strain_states</td>
<td>None</td>
<td>Strain modes, if it is None, it will generated by atomate</td>
</tr>
<tr>
<td>stencils</td>
<td>None</td>
<td>The amplitude of the strain modes/states</td>
</tr>
<tr>
<td>analysis</td>
<td>True</td>
<td>Analysis (True) or not (False)</td>
</tr>
<tr>
<td>sym_reduce</td>
<td>False</td>
<td>Reduce the strain according to the symmetry or not</td>
</tr>
<tr>
<td>order</td>
<td>2</td>
<td>The order of the elastic constants</td>
</tr>
<tr>
<td>conventional</td>
<td>False</td>
<td>Convert the structure into conventional format or not</td>
</tr>
</tbody>
</table>

### 6.7 Get Started

#### 6.7.1 Content

- **Run dfttk with dfttk run command**
  - Run dfttk for a single structure or a single folder
  - Write out the workflow
  - Run dfttk for a folder and its sub-folder
  - Run dfttk with individual settings
  - Submit job to launchpad and queue system
6.7.2 Run dfttk with dfttk run command


The help of dfttk run command, please ref. Help for dfttk run command or simply run dfttk run -h

All the examples is run under current folder (get_started)

get_started
NaCl.cif
NotSupportFile
POSCAR

test_folder
Fe3Ni.cif
Fe3Ni-settings.yaml
POSCAR
POSCAR-2
SETTINGS-POSCAR.yaml
SETTINGS.yaml
sub_folder
POSCAR

Run dfttk for a single structure or a single folder

-f parameter, specify the structure or folder containing structure

dfttk run -f STRUCTURE/STRUCTURE_FOLDER

- When the parameter value of -f is a file it run this file; if it is a folder, it will search all supported files in the specified folder.
- It support POSCAR, CONTCAR, CHGCAR, LOCPOT, cif, vasprun.xml, pymatgens structures, mcsqs's structure, more details, ref pymatgen.core.structure.IStructure.from_file
  - For POSCAR or CONTCAR, the name should be *POSCAR* or *CONTCAR* or *.vasp
  - For CHGCAR or LOCPOT, the name should be *CHGCAR* or *LOCPOT*
  - For cif, the name should be *.cif* or *.mcif*
  - For vasprun.xml, the name should be vasprun*.xml*
  - For pymatgen's structure, the name should be *.json or *.yaml
  - For atat's structure, the name should be *rndstr.in* or *lat.in* or *bestsq*

TO TOP
Write out the workflow

-o parameter, write out work flow

• When add -o parameter, the work flow for every structure will be write out

• The file name of the work flow is `dfttk_wf- + filename of the structure + .yaml` (e.g. `dfttk_wf-POSCAR.yaml`)

```
dfttk run -f POSCAR -o
```

It will write out the work flow in current folder as `dfttk_wf-POSCAR.yaml`

• The file will write out in the same folder with corresponding structure.

```
dfttk run -f ./test_folder/POSCAR -o
```

It will write out the work flow as `./test_folder/dfttk_wf-POSCAR.yaml`

Run dfttk for a folder and its sub-folder

-r parameter, recursive the folder

-mh parameter, specify the match pattern

• Add -r parameter, it will searching the folder (specified by -f parameter) and its sub-folder

```
dfttk run -f . -r
```

It will run the following structure

```
get_started/NaCl.cif
get_started/POSCAR
get_started/test_folder/Fe3Ni.cif
get_started/test_folder/POSCAR
get_started/test_folder/POSCAR-2
get_started/test_folder/sub_folder/POSCAR
```

• Add -mh parameter, it will filter the filename by the value of -mh, the pattern should be placed in quotes (" or ")

```
dfttk run -r -mh "*.cif"
```

It will run the following structure

```
get_started/NaCl.cif
get_started/test_folder/Fe3Ni.cif
```

TO TOP
Run dfttk with individual settings

-s parameter, specify the name for settings, default: SETTINGS

- SETTINGS.yaml or SETTINGS.json: The global settings for current folder
- SETTINGS-*_.yaml(json) or -*SETTINGS.yaml(json): The individual settings, * is the name of the structure (without ext)
- Case insensitive. (both SETTINGS and settings are OK)
- The value of -s parameter will replace SETTINGS.
- Examples:

  dfttk run -f test_folder -s set

  It will take ./test_folder/Fe3Ni-SET.yaml as setting file, and ./test_folder/Fe3Ni-settings.yaml will not taken as setting file.

Submit job to launchpad and queue system

-l parameter, launch to launchpad

-m parameter, launch to queue system and determine the number of jobs
- Add -1 parameter, it will submit the job to launchpad
- Add -m N parameter, it will submit the job to queue system. N specifies the number of jobs run at the same time. (Note: This only work when -l parameter is added.)

  dfttk run -l
  dfttk run -l -m 1
  dfttk run -l -m 2

  - When -m 1, it will run qlaunch singleshot (fireworks command)
  - When -m N (N>1), it will run qlaunch rapidfire -m N (fireworks command)
  - For more details, please ref. Fireworks: Launch Rockets through a queue

6.7.3 Run dfttk with python script
### 6.7.4 Help for dfttk run command

**dfttk run -h**

```
DFTTK version: 0.1+98.ge7aa39c.dirty
Copyright  Phases Research Lab (https://www.phaseslab.com/)

usage: dfttk run [-h] [-f STRUCTURE_FOLDER] [-mh MATCH_PATTERN] [-s SETTINGS]
               [-r] [-wf WORKFLOW] [-l] [-m [MAX_JOB]] [-o]

optional arguments:
  -h, --help    show this help message and exit
  -f STRUCTURE_FOLDER, --structure_folder STRUCTURE_FOLDER
                The folder/file containing the structure, Default: '.'
  -mh MATCH_PATTERN, --match_pattern MATCH_PATTERN
                The match pattern for structure file, e.g. *POSCAR*,
                Default: * -- everything except SETTING files, ref. -s
  -s SETTINGS, --setting SETTINGS
                Specify the name of SETTINGS files (yaml or json file)
                Default: SETTINGS (case insensitive and without ext)
                The following filename will be treat as SETTINGS file
                SETTINGS (global settings in the folder) Start with
                SETTINGS- (individual settings for struct) End with
                -SETTINGS (individual settings)
  -r, --recursive
                Recursive the path.
  -wf WORKFLOW, --workflow WORKFLOW
                Specify the workflow to run. Default: get_wf_gibbs
                (NOTE: currently, only get_wf_gibbs is supported.)
  -l, --launch
                Launch the wf to launchpad
  -m [MAX_JOB], --max_job [MAX_JOB]
                Run the job, only works when -l is specified. Default:
                0 (Not submit to queue) 1: qlaunch singleshot (single
                job) N(N>1): qlaunch rapidfire -m N
  -o, --write_out_wf
                Write out the workflow
```

---

### 6.8 Dfttk postprocessing mechanism

#### 6.8.1 Flow controls

Depending on the given condition, postprocessing can take data from

- The qha-phonon collection
- The qha collection (Debye model)
- The phonon collection (in case of qha-phonon calculations failed)

Then, invoke Yphon to recalculate the phonon properties based on the force constants obtained from the database
6.8.2 Scheme to find equilibrium volume

If the data quality is excellent, use central symmetric 7-point difference
If the data quality is very good, fit the free energies use 4-parameter Birch-Murnaghan
If the data quality is good (may use as default), fit the 0-K total energies using 4-parameter Birch-Murnaghan
Fit the finite T part of the free energies by UnivariateSpline

6.8.3 Scheme to calculate derivative

1. 7-point symmetrical central difference

\[
\text{Deriv} = \frac{1}{3} \sum_{i=1}^{3} \frac{f(X_{N+i}) - f(X_{N-i})}{X_{N+i} - X_{N-i}}
\]

2. Birch-Mannhan Euqations of state fitting

\[
\text{Deriv} = -\frac{2}{3} bx^{\frac{2}{3}} - \frac{4}{3} cx^{\frac{4}{3}} - \frac{6}{3} dx^{\frac{6}{3}}
\]

6.8.4 Scheme for LTC

1. By entropy derivative

\[
\alpha = \frac{1}{B_T} \frac{\partial S}{\partial V}
\]

where \(B_T\) is isothermal bulk modulus

2. By internal energy derivative via Birch-Mannhan fitting

\[
\alpha = \frac{1}{B_T T} \left( \frac{\partial U}{\partial V} + P \right)
\]

where \(P\) is pressure

3. When the data quality is fair (~20% cases)

Fit the 0-K total energies using 4-parameter Birch-Murnaghan; and
fit the finite T part of the free energies by linear function \(f=a+b*V\)
6.9 More about run DFTTK

To run DFTTK, the user should use the following Linux command style:

```
dfttk 'module' [option]
```

where the available module can be:

<table>
<thead>
<tr>
<th>module</th>
<th>function</th>
</tr>
</thead>
<tbody>
<tr>
<td>run</td>
<td>DFT job submission. Call VASP to perform 0 K E-V, phonon, elastic moduli, Born effective charge (dielectric tensor), etc</td>
</tr>
<tr>
<td>config</td>
<td>Set basic dfttk run environment, such as path to pseudopotential, batch job prototype</td>
</tr>
<tr>
<td>db_remove</td>
<td>Remove certain data in MongoDB to save storage cost</td>
</tr>
<tr>
<td>thelec</td>
<td>Download data from MongoDB database &amp; postprocess them to get thermodynamic properties, elastic constant, etc</td>
</tr>
<tr>
<td>thfind</td>
<td>Check the MongoDB database for DFT results followed by calling the thelec module to get thermodynamic properties when the option -get is given.</td>
</tr>
<tr>
<td>EVfind</td>
<td>Find the metadata tags that have 0 K static calculation finished.</td>
</tr>
</tbody>
</table>

6.9.1 Examples

- Check run results

To get a brief summary for data in the database, use

```
dfttk thfind -v 1
```

this will report the metadata, number of finished phonon calculations, number of finished static calculations, supercell size used for the phonon calculations, brief phase name; and the following command reports the location where the DFT calculations were submitted

```
dfttk thfind -v 1 -jobpath parentfolder
```

where parentfolder is the parent folder whose subfolders hold the individual DFT calculation job submission data.

- Batch postprocessing results

```
dfttk thfind -get -py -td -50 -plot find_or_DFT -eq 4 -renew -ss 30 -w Pb-Ti-O
```

where -get instruct thfind to call thelec module to postprocess the data, -py to use Yphon to recalculate the phonon density of states based on the force constants saved in the phonon collection, -td -50 to use the self-adapted temperature mesh, -eq 4 to use Birch-Murnaghan fitting to get equilibrium volume, -ss 30 means only handle results with supercell size larger than 30, -w elist means only extract for compounds with all elements in the list of elist. Other enhanced screening conditions can be combinations of the follows

- all elist # compounds must contain all elements in the list of elist;
- any elist # compounds contain any elements in the list of elist;
- xall elist # compounds must not contain all elements in the list of elist;
- xany elist # compounds must not contain any elements in the list of elist.
6.9.2 Batch run dfttk

Depend on the cases, dfttk postprocess may take longer time to finish. If it is the case, it is recommended to submit batch job. When submit batch, make sure compatibilities of non-ascii character by including the following in the job script:

```
export LC_ALL='en_US.utf8' # for bsh;
setenv LC_ALL en_US.utf8 # for csh
```

6.9.3 Usage of run module

- dfttk run: call VASP to perform 0 K E-V, phonon, elastic moduli, Born effective charge (dielectric tensor), etc

```
usage: dfttk run [-h] [-f STRUCTURE_FOLDER] [-mh MATCH_PATTERN] [-s SETTINGS] 
[-o]
```

optional arguments:

- `-h`, `--help` show this help message and exit
- `-f STRUCTURE_FOLDER`, `--structure_folder STRUCTURE_FOLDER` The folder/file containing the structure, Default: '
- `-mh MATCH_PATTERN`, `--match_pattern MATCH_PATTERN` The match pattern for structure file, and it should be place in quotes. e.g. '*POSCAR*'. Default: * --
- `-s SETTINGS`, `--setting SETTINGS` Specify the name of SETTINGS files (yaml or json file) Default: SETTINGS (case insensitive and without ext) The following filename will be treat as SETTINGS file SETTINGS (global settings in the folder) Start with SETTINGS- (individual settings for struct) End with -SETTINGS (individual settings)
- `-r`, `--recursive` Recursive the path.
- `-wf WORKFLOW`, `--workflow WORKFLOW` Specify the workflow to run. Default: robust (run get_wf_gibbs_robust workflow) (NOTE: currently, only robust and born are supported.)
- `-ph`, `--phonon` Run phonon. This is equivalent with set phonon=True in SETTINGS file
- `-tag TAG`, `--tag TAG` Specify the tag for continue mode
- `-a`, `--append` Append calculation according to metadata, e.g. appending volumes or phonon
- `-l`, `--launch` Launch the wf to launchpad
- `-m [MAX_JOB]`, `--max_job [MAX_JOB]` Run the job, only works when -l is specified. Default: 0 (Not submit to queue) 1: qlaunch singleshot (single job) N(N>1): qlaunch rapidfire -m N
- `-o`, `--write_out_wf` Write out the workflow
6.9.4 Usage of thelec module

- **thelec** [Download data from MongoDB database & postprocess them to get] thermodynamic properties, elastic constant, etc
- **try dfttk thelec -h** for command available line options

```
dfttk thelec [-h] [-py] [-T0 [T0]] [-T1 [T1]] [-dT [TD]] [-xdn [XDN]]
               [-xup [XUP]] [-dope [DOPE]] [-ne [NDOSMX]]
               [-natom [NATOM]] [-e [EVERYTY]] [-gauss [GAUSSIAN]]
               [-i [DOSCAR]] [-o [OUTF]] [-noel] [-metatag [METATAG]]
               [-qhamode [QHAMODE]] [-pn [PHASENAME]] [-eq [EQMODE]]
               [-el [ELMODE]] [-s] [-plot] [-g] [-expt [EXPT]]
               [-xlim [XLIM]]
```

optional arguments:

```
-h, --help                              show this help message and exit
-py, --pyphon                             use Yphon to recalculate vibrational properties.
                                           Default: False
-T0 [T0], --t0 [T0]                      Low temperature limit. Default: 0
-T1 [T1], --t1 [T1]                      High temperature limit. Default: 1300
-dT [TD], --td [TD]                      Temperature increment. Default: 10
-xdn [XDN], --xdn [XDN]                  Low band energy limit. Default: -100 (eV)
-xup [XUP], --xup [XUP]                  High band energy limit. Default: 100
-dope [DOPE], --dope [DOPE]              dope level (electrons). Default: -1.e-8 for numerical
                                           stability
-ne [NDOSMX], --ndosmx [NDOSMX]          new DOS mesh. Default: 10001
-natom [NATOM], --natom [NATOM]          number of atoms in the DOSCAR. Default: 1
-e [EVERTY], --everyT [EVERTY]           number of temperature points skipped from QHA
                                           analysis. Default: 1
-gauss [GAUSSIAN], --gauss [GAUSSIAN]    densing number near the Fermi energy. Default: 1000
-i [DOSCAR], --doscar [DOSCAR]           DOSCAR filename. Default: DOSCAR
-o [OUTF], --outf [OUTF]                 output filename for calculated thermoelectric
                                           properties. Default: fvib_ele
-noel, --noel                             do not consider the thermal electron contribution.
                                           Default: False
-metatag [METATAG], --metatag [METATAG]  metatag: MongoDB metadata tag field. Default: None
-qhamode [QHAMODE], --qhamode [QHAMODE]  quasiharmonic mode: debye, phonon, or yphon. Default: debye
-pn [PHASENAME], --phasename [PHASENAME] assign phase name. Default: None
-eq [EQMODE], --eqmode [EQMODE]          (continues on next page)
6.9.5 Usage of thfind module

- `thfind`: Check the MongoDB database for DFT results followed by calling the 'thelec' module to get thermodynamic properties when the option '-get' is given.
- `try dfttk thfind -h` for command available line options

```
dfttk thfind [-h] [-q [QHAMODE]] [-w [WITHIN]] [-all [CONTAINALL]]
    [-any [CONTAINANY]] [-v [NV]] [-ss [SUPERCELLN]] [-get]
    [-py] [-T0 [T0]] [-T1 [T1]] [-dT [TD]] [-xdn [XDN]]
    [-xup [XUP]] [-dope [DOPE]] [-ne [NDOSMX]]
    [-natom [NATOM]] [-e [EVERYT]] [-gauss [GAUSSIAN]]
    [-i [DOSCAR]] [-o [OUTF]] [-noel] [-metatag [METATAG]]
    [-qhamode [QHAMODE]] [-eq [EQMODE]] [-el [ELMODE]] [-s]
    [-plot] [-g] [-expt [EXPT]] [-xlim [XLIM]]
```

optional arguments:

```
-h, --help
    show this help message and exit
-q [QHAMODE], --qhamode [QHAMODE]
    Collection. 'phonon', 'qha'. Default: 'phonon'
-w [WITHIN], --within [WITHIN]
    find calculations within element list Default: None
-all [CONTAINALL], --containall [CONTAINALL]
    find calculations must contain all elements in the list Default: None
-any [CONTAINANY], --containany [CONTAINANY]
    find calculations contain any elements in the list Default: None
-v [NV], --nv [NV]
    Return phonon calculations finished for number of volumes larger or equals to. Default: 6
-ss [SUPERCELLN], --supercellsize [SUPERCELLN]
    only return phonon calculation with supercell size larger than. Default: 0
-get, --get
    get the thermodynamic data for all found entries.
```
-py, --pyphon
  use Yphon to recalculate vibrational properties.
  Default: False
-T0 [T0], -t0 [T0]
  Low temperature limit. Default: 0
-T1 [T1], -t1 [T1]
  High temperature limit. Default: 1300
-dT [TD], -td [TD]
  Temperature increment. Default: 10
-xdn [XDN], --xdn [XDN]
  Low band energy limit. Default: -100 (eV)
-xup [XUP], --xup [XUP]
  High band energy limit. Default: 100
-dope [DOPE], --dope [DOPE]
  dope level (electrons). Default: -1.e-8 for numerical stability
-ne [NDOSMX], --ndosmx [NDOSMX]
  new DOS mesh. Default: 10001
-natom [NATOM], --natom [NATOM]
  number of atoms in the DOSCAR. Default: 1
-e [EVERYT], --everyT [EVERYT]
  number of temperature points skipped from QHA analysis. Default: 1
-gauss [GAUSSIAN], --gauss [GAUSSIAN]
  densing number near the Fermi energy. Default: 1000
-i [DOSCAR], --doscar [DOSCAR]
  DOSCAR filename. Default: DOSCAR
-o [OUTF], -outf [OUTF]
  output filename for calculated thermoelectric properties. Default: fvib_ele
-noel, --noel
  do not consider the thermal electron contribution. Default: False
-metatag [METATAG], --metatag [METATAG]
  metatag: MongoDB metadata tag field. Default: None
-qhamode [QHAMODE], --qhamode [QHAMODE]
  quasiharmonic mode: debye, phonon, or yphon. Default: debye
-eq [EQMODE], --eqmode [EQMODE]
  Mode to calculate LTC. 0: Symmetrical Central differential; 4: 4-parameter BM fitting. 5:
  5-parameter BM fitting. Default: 0
-el [ELMODE], --elmode [ELMODE]
  Mode to interpolate thermal electronic contribution:
  0: interp1d; 1: UnivariateSpline. Default: 0
-s, --smooth
  smooth the LTC. Default: False
-plot, --plot
  plot the figure. Default: False
-g, --debug
  turn on debug mode by reducing the mesh. Default: False
-expt [EXPT], --expt [EXPT]
  json file path for experimental thermodynamic properties for plot. Default: None
-xlim [XLIM], --xlim [XLIM]
6.10 Job monitoring

The following briefly some common automate commands for DFT jobs submitted by dfttk run.

- Monitor workflows

To check running status of all submitted dfttk jobs, use

```
lpad get_wflows
```

To find the running calculations

```
lpad get_fws -s RUNNING
```

To find the jobdir for a job with specific fw_id (The number portion of job id reported by lpad get_wflows), use

```
lpad get_launchdir fw_id
```

- FIZZLED jobs

FIZZLED means failed. The following command can summarize all FIZZLED jobs:

```
lpad get_fws -s FIZZLED; or
lpad get_wflows -s FIZZLED
```

One can rerun FIZZLED by

```
lpad rerun_fws -s FIZZLED
```

For more details, see ref. FIZZLED.

To get help for the subcommands, try lpad get_fws -h or lpad get_wflows -s FIZZLED -h

6.11 Useful help from FireWork

Controlling the Worker that executes a Firework
Querying FireWorks and Workflows/Generating Reports
Dealing with Failures and Crashes
Writing Queue Adapters

6.12 Troubleshooting

This document covers how to handle jobs that have fizzled. There are three main sections: common troubleshooting, general troubleshooting workflow to find the root cause of issue and specific issues and their fixes.
6.12.1 Common troubleshooting

1. In the config stages, one may need properly set up VASP environments, such as

   module load intel impi vasp

2. Make the latest automate installed;

3. In .bashrc or .cshrc, make sure not messed up with your other automate FW config;

4. Make sure the setup in the .bashrc file

   export FW_CONFIG_FILE=~/dfttk/config/FW_config.yaml

   or equivalently in the .cshrc file

   setenv FW_CONFIG_FILE /storage/work/y/yuw3/dfttk/config/FW_config.yaml

5. git push issue for contributors, see https://docs.github.com/en/github/authenticating-to-github/adding-a-new-ssh-key-to-your-github-account

6. for batch run of the postprocessing modules, make sure compatibilities of non-ascii character by:

   export LC_ALL='en_US.utf8' #for bsh;
   setenv LC_ALL en_US.utf8 #for csh

7. For phonon calculations, due to certain reasons (such as temperature range too high), one may not see results in the qha_phonon or qha MongoDB collections. In this case, the subcommand dfttk thfind will try to find results from the phonon collection and process the data by calling Yphon

8. When you are interesting in revising the code, if have job running in the system before your changes, the codes in the batch system might not be updated and the results might be not as you assumed. It takes me two days to figure out this problem. The solution is to kill all the dfttk running job and resubmit them. Following are the steps of adding API key number on DFTTK.

9. How to solve the install warning of ‘PMG_MAPI_KEY’ is empty.

   1. Go to the materials project website, https://materialsproject.org/, under the API section, you will easily find you API Keys number.

   2. Go to the .pmgrc.yaml file

   vi ~/.pmgrc.yaml

   3. Add your API key number into your .pmgrc.yaml file. For example

   PMG_MAPI_KEY: ######(your API key number)

10. How to find the reason for FIZZLED job.

11. VasprunXMLValidator found from the command “lpad get_fws -i fw_id -d more”

   If you get an error from the VasprunXMLValidator, that means that the vasprun.xml failed to be parsed and/or validated. Usually that means the VASP job did not run or failed for a reason that was not caught and handled by Custodian. Check the output files in the launch directory and see if there are any errors in the VASP output or stdout/stderr.
6.12.2 pymatgen 2021 issue

You may meet numpy version issues using pymatgen, reporting:

```python
pymatgen 2021.2.16 requires numpy>=1.20.1, but you'll have numpy 1.19.2 which is incompatible.
```

In such case, please upgrade numpy by:

```
pip install numpy --upgrade
```

6.12.3 conda issues

In some cases, such as in the Windows environment, one may meet the error:

```
ModuleNotFoundError: No module named 'ruamel' #106
```

This is due to conda bug on namespace of ruamel.yaml vs ruamel.yaml. One can resolve this by open the Anaconda Powershell Prompt as administrator and reinstall ruamel.yaml by:

```
conda install ruamel.yaml
```

6.12.4 Troubleshooting Workflow

My job has fizzled! The following steps can help you get information about how your job. You can imagine it as a decision tree. Check one thing before moving on to the next one.

1. Check that the job ran and has raised an exception with a traceback.
   
   Run `lpad get_fws -i <ID> -d more`, replacing `<ID>` with the integer id of the Firework. Search the output for `_exception`. What you see is the Python exception that was raised when running the Firework.
   
   **TIP:** Searching works well when you pipe the output to `less` with `lpad get_fws -i <ID> -d more | less` and search using `/
   
   **todo:** If you don’t see a traceback, that means... (this is the first step, but does this actually happen?)

2. Check the traceback is not a common error.

   See the Common Errors section

6.12.5 Common Errors

**Custodian VasprunXMLValidator failed**

In this error, you get a traceback that looks something like:

```python
Traceback (most recent call last):
  File "/storage/home/bjb54/.conda/envs/wfs/lib/python3.7/site-packages/custodian/...custodian.py", line 320, in run
    self._run_job(job_n, job)
  File "/storage/home/bjb54/.conda/envs/wfs/lib/python3.7/site-packages/custodian/...custodian.py", line 428, in _run_job
...
```

(continues on next page)
raise CustodianError(s, True, v)
custodian.custodian.CustodianError: (CustodianError(...), 'Validation failed: <custodian.
  vasp.validators.VasprunXMLValidator object at 0x2af45b1d3908>')

During handling of the above exception, another exception occurred:

Traceback (most recent call last):
  File "/storage/home/bjb54/.conda/envs/wfs/lib/python3.7/site-packages/fireworks/core/
    rocket.py", line 262, in run
    m_action = t.run_task(my_spec)
  File "/storage/home/bjb54/.conda/envs/wfs/lib/python3.7/site-packages/atomate/vasp/
    firetasks/run_calc.py", line 204, in run_task
    c.run()
  File "/storage/home/bjb54/.conda/envs/wfs/lib/python3.7/site-packages/custodian/
    custodian.py", line 330, in run
    .format(self.total_errors, ex))
RuntimeError: 0 errors reached: (CustodianError(...), 'Validation failed: <custodian.
  vasp.validators.VasprunXMLValidator object at 0x2af45b1d3908>). Exited...

With the key being that Custodian fails to validate the vasprun.xml. After running VASP, Custodian will try to parse the vasprun.xml file using pymatgen.

There are usually two possible triggers for this failure:

1. VASP failed to run at all (more common) or quit in a way that custodian did not detect (less common)
2. The vasprun.xml file could not be parsed by pymatgen.

To investigate this, first check that VASP ran (e.g. the OUTCAR shows that the run completed successfully). If VASP did not run, find out why and fix that issue. If VASP did run successfully, it was probably an issue parsing the vasprun.xml file. Try parsing the vasprun.xml file using the pymatgen.io.vasp.outputs.Vasprun class. If it throws an error when you try to parse, that’s what made Custodian fail and you should fix that.

### 6.13 MongoDB VM hosting

This section is for the dfttk users who want to host their MongoDB by themselves.

MongoDB is one of the most popular document-oriented databases under the banner of NoSQL database. The schema-free implementation of MongoDB eliminates the prerequisites of defining a fixed structure required by the SQL database.

In computing, a virtual machine (VM) is an emulation of a computer system. Virtual machines are based on computer architectures and provide functionality of a physical computer. Their implementations may involve specialized hardware, software, or a combination. See [https://en.wikipedia.org/wiki/Virtual_machine](https://en.wikipedia.org/wiki/Virtual_machine)

Our MongoDB databases are currently hosted by Penn State's VM hosting service that provides cost-effective, reliable VM for departments, colleges, and research units at Penn State University.

In our case, we have changed the default tcp port from 27017 into 27018 due to historical reason.
6.13.1 VM operation

Connect your VM by ssh (ssh youruserid@146.186.149.69 in our case). One should use VPN if you have firewall for your system

- To add user to your VM linux system

Run the following command under Linux

```
sudo adduser newuser
usermod -aG sudo newuser # add admin user to your VM
```

Note on adding other users to access the VM. In order to add other users to access the VM from the Morpheus portal you would need to add them to the VM. For the VM itself you would need to add their user ID to the /etc/security/access.conf file and if they need sudo access you would need to add their ID to the /etc/sudoers.d/sudo-users file as well.

6.13.2 MongoDB installation/configuration

These are the one time setup steps for MongoDB:

Assuming you are on Ubuntu and using the apt package manager:

```
apt update
apt install mongodb
```

This may be an outdated MongoDB. To follow the best security practices and get the latest features, you should install something more recent. More information about installing and configuring MongoDB 3.6 is available here: https://docs.mongodb.com/manual/tutorial/install-mongodb-on-ubuntu/

Additional configuration info for MongoDB 4.4 can be found here: https://www.digitalocean.com/community/tutorials/how-to-install-mongodb-on-ubuntu-18-04-source

More broadly, the MongoDB security checklist should be followed. Critically, you should enable access control and set up an authentication database and credentials for at least one administrator.

Some key things to configure in /etc/mongodb.conf:

- Set the path of the database to the correct location. You may need to sudo chown mongodb /path/to/database for permissions to work
- Add the public IP of the server to bind_ip setting so it reads like 127.0.0.1,XXX.XXX.XXX.XX for your server’s IP XXX.XXX.XXX.XX.
- Set a non-standard port if you want one
- Enable authentication (assuming you enabled authentication and set up an administrator database and user)

6.13.3 MongoDB operation

Managing the MongoDB service

This section assumes that you already have your VM set up and you are managing it under linux environment.

The MongoDB server is managed by a systemd service that is managed through systemctl. Common commands are:

- Check status of mongodb service:

```
sudo systemctl status mongodb
```
- Start mongodb service:
  
  ```
  sudo systemctl start mongodb
  ```

- Shut down mongodb service:

  ```
  sudo systemctl stop mongodb
  ```

- Restart mongodb service (if it's already running):

  ```
  sudo systemctl restart mongodb
  ```

### Connecting to the MongoDB server console

This section deals with your MongoDB database management to locally or remotely operate on it. This is to say you are going to manage your database from your local computer by `mongo` or `mongosh`.

Note: `mongosh` by MongoDB Shell is the quickest way to connect, configure, query, and work with your MongoDB database.

- Create admin user for mongodb

These are the one time setup steps for MongoDB:

With access control enabled, ensure you have a user with userAdmin or userAdminAnyDatabase role in the admin database. This user can administrate user and roles such as: create users, grant or revoke roles from users, and create or modify customs roles.

For more details on MongoDB user management, see [https://docs.mongodb.com/manual/tutorial/enable-authentication/](https://docs.mongodb.com/manual/tutorial/enable-authentication/)

1. Connect to the instance by open another terminal in your VM and connect a mongo shell to the instance:

   ```
   mongod --port 27018
   ```

   after the prompt “>” input:

   ```
   use admin
db.createUser(
    {
      user: "admin",
pwd: "xxxxxxxxxx", // xxxxxxxxxx is the admin password of your choice
      roles: [ { role: "userAdminAnyDatabase", db: "admin" }, "readWriteAnyDatabase" ]
    })
   ```

2. Re-start the MongoDB instance with access control
   a. Shut down the mongod instance
   b. Exit the mongo shell by run the command `exit` or give an EOF (Ctrl+D)
   c. Start the mongod with access control enabled by
      - adding the security.authorization configuration file setting

    ```
    security:
    authorization: enabled
    ```
• or If you start the mongod from the command line

```
mongod --auth --port 27018
```

• Create general user

Assuming the service is running and configured with authentication (see above), Connect to your mongoDB as admin user locally by:

```
mongo --port 27018 --authenticationDatabase "admin" -u "admin" -p
```
or remotelly by:

```
mongo 146.186.149.69:27018 --authenticationDatabase admin -u <admin username> -p <admin password>
```
or remotelly use mongosh by:

```
mongosh --username <admin username> --password --authenticationDatabase admin --host 146.186.149.69 --port 27018
```

followed by inputting the following lines after the prompt “>”:

```
use userid-fws
db.createUser({user: "userid", pwd: "B5nRcUvoCZ92", roles: [{role: "dbOwner", db: "userid-fws"}]})

use userid-results
db.createUser({user: "userid", pwd: "BeFihJ2mrKGm", roles: [{role: "dbOwner", db: "userid-results"}]})
db.createUser({user: "userid-ro", pwd: "QIvaUT9ca6H8", roles: [{role: "read", db: "userid-results"}]})
```

These lines can be produced by dfttk by run a python code named `mongodb_user.py` which can be downloaded from [https://github.com/PhasesResearchLab/dfttk/tree/master/dfttk/scripts](https://github.com/PhasesResearchLab/dfttk/tree/master/dfttk/scripts) After download the code, one can run it by:

```
python mongodb_user.py
```

The run will prompt the MongoDB system manager to input an userid for the user. After you input userid and hit enter, one gets the above outputs in the screen.

Meanwhile, a file named `db.json` in the JSON format containing something similiar to the following lines which should be sent to the MongoDB user:

```json
{
    "database": "userid-results",
    "collection": "tasks",
    "admin_user": "userid",
    "admin_password": "BeFihJ2mrKGm",
    "readonly_user": "userid-ro",
    "readonly_password": "QIvaUT9ca6H8",
    "host": "146.186.149.69",
    "port": 27018,
    "aliases": {} }
```

The MongoDB user should save this data in a json file named `db.json` under the path `dfttk/config` that created by `dfttk config -mp -aci` command.

6.13. MongoDB VM hosting
6.14 Changelog

6.14.1 0.3.1 (2021-02-03)

(Contributor: @YiWang, @mxf469, @bocklund)

• Change List:
  • Made a significant online documentation using readthedocs
  • Documentation open online by www.dfttk.org

6.14.2 0.3.0 (2020-12-10)

(Contributor: @YiWang, @mxf469, @bocklund)

• Change List:
  • formally release dfttk version 0.3.0
  • Revised dfttk/script/run_dfttk.py
  • made workflow get_wf_gibbs run on robust with get_wf_gibbs_robust
  • changed test module from get_wf_gibbs into get_wf_gibbs_robust
  • Add elasticity calculation model
  • Add Born effective charge calculations

6.14.3 September 17, 2020

• Bug fixes:
  • Replaced curve-fit by ployfit for BM fitting
  • Fixed bugs on result checks
  • Summarizing installation/run documents for DFTTK (This documents)

6.14.4 September 3, 2020

• Added a module EVfind per discussion with Shunli and enhanced calculation summary
  • E-V, P-V, Stress-V, Strain-V
  • Implemented 4 numerical schemes for evaluating LTC
  • Enhanced plots
  • LO-TO splitting were marked
  • Gamma point phonon frequencies
  • Prepared ~50 testing structures/compounds
• Made LDA pseudopotential as an option
• Speed up calculation
• Turned on LREAL=Auto from default
• Change into ISPIN=1 for nonmagnetic system from default
• For better relaxation
• Turned on EDIFF=1.e-8 (why it showed 2e-7 in the OUTCAR?)
• Turned on EdiffG=-1.e-3 (testing, could be the reason for poor phonon data quality)
• Data report
• Phonon quality
• LTC quality
• Found phonopy was unable handle Cv below 1 K
• Added experimental data for plotting results
• Working on
• Calculate Born effective charge/dielectric tensors for insulators
• Launch by module EVfind when band gaps found and if not calculated

6.14.5 0.2.2 (2020-08-18)

(Contributor: @YiWang, @mxf469)

• Change List:
  • added codes in the dfttk/scripts directory:
    • run_dfttk_ext.py
    • handle the argumentns for the thelec and thfind modules
  • added python code in the dfttk directory:
    • pyfind.py
    • database search engine
    • pythelec.py
    • for compatibiliy with Yphon
    • generating the majority of thermodynamic properties, such as thermal expansion coeffi-
      cient, Seebech coefficients, Lorenz number etc
    • pyphon.py for
    • calculate the phonon contributions to the various thermodynamic properties
  • added python code in the dfttk/analysis directory:
    • database
    • for plot phonon dispersions for all crystalline systems
    • ywutils.py
    • general utils code
• ywplot.py
  • for plots of ~20 different phonon and thermodynamic properties in the png format
• made Yphon compatible with phonopy
  • added codes in the CRO-soc directory:
    – phonopy2yphon, phonopy2yphon.py
    – convert the phonopy force constant matrix in hdf5 format into superfij.out format used by Yphon
• changed codes:
  • in the dfttk/scripts directory:
    • run_dfttk.py
      • added the following lines aimed to handle the arguments for the thelec and thfind modules
        # extension by Yi Wang, finalized on August 4, 2020 #
        from dfttk.scripts.run_dfttk_ext import run_ext_thelec
        run_ext_thelec.run_ext_thelec(subparsers)
  • in the dfttk/analysis directory:
    • debye.py is renamed as debye_ext.py
    • to include the vibrational entropy ($S_{vib}$) and heat capacity ($C_{vib}$) into the “qha”
      MongoDB collection
    • quasiharmonic.py:
      • copy the $S_{vib}$ and $C_{vib}$ from the “phonon” collection into the “qha_phonon”
        MongoDB collection

6.14.6 0.2 (2020-03-30)

New features
(Contributor: @bocklund, @Peng_Gao, @hitliaomq)
• The relax scheme is optimized. (from ISIF=3 to ISIF=2 followed by ISIF=4) (@Peng_Gao)
• Change the static workflow to dynamic workflow. (EVcheck_QHA.py increase the data points atomately if the
  fitting of initial points is incorrect) (@Peng_Gao)
• Support run dfttk by command. (Add dfttk run [options]) (@hitliaomq)
• Support configrate dfttk automately. (Add dfttk config [options]) (@hitliaomq)
• Documents’ enhance. (@hitliaomq)
• Bug fix. (Including #8) (@bocklund, @Peng_Gao, @hitliaomq)
6.14.7 0.1 (2018-08-28)

Initial release. Includes

(Contributor: @bocklund, @mxf469)

- Gibbs workflow for stable structures
- Analysis code and libraries for calculation quasiharmonic Gibbs energies with 0K, vibrational and thermal electronic contributions
- Useful utilities for interfacing with structure, calculations and the Materials Project

6.15 Contribution Guide

6.15.1 Style Guidelines

In general, code style should follow PEP8 and PEP20. Specifics are summarized below:

- Code should be indented using spaces, not tabs. One indentation = 4 spaces
- Lines longer than 100 should be manually wrapped, but prefer readability
- Minimize blank lines: 2 around top level classes/functions, 1 in nested functions
- Workflows, Fireworks, and Firetasks should follow the same naming scheme as in atomate
- Include docstrings for classes and functions (see code), add comments where needed
- Function and variable names should be descriptive (not ‘x’ or ‘xx’) and all lowercase_with_underscores
- Class names should be descriptive CapitalWords

6.15.2 How to Contribute

It is recommended to first install anaconda if one does not have it installed yet.

1. Register an account in www.github.com or www.gitlab.com, depending on where the package that you want to contribute to is resided.
2. Sign into your web account
3. find the the package that you want to contribute to
4. make a fork by click the Fork sign on top-right corner of the repository (for instance, see the web site of DFTTK)
5. go back to your web account, you will see the forked repository shown in your account
6. login in your local machine
7. clone the repository to your local machine and go to/create a folder that you want to reside your contribution, then install the development version by

```bash
git clone https://github.com/PhasesResearchLab/dfttk.git
cd dfttk
pip install -e .
dfttk config -mp -aci #a folder named "config" will be created where running
←environmental info saved
```
8. Create a new branch for your addition or changes (`git checkout -b mybranchname`), something like

```
git checkout -b yourname  # "yourname" is a name that you preferred to use
```

9. Write codes or make changes and commit them to your branch. (#Note from me, try your best not changing the original codes, only focusing expanding codes will save a lot of troubles when merging your changes to the package)

```
git commit -am "your notation for the changes"
```

10. Push your branch to the repository

```
git push #push your changes to github/gitlab
```

11. *When and only when your are sure that your changes are completely correct*, submit a pull request by going to your web account and click the sign of 🚀 Pull requests on the top-left side of your repository

After you submit a merge request, other members of the group are able to review your changes and give feedback. Someone with a rank of Master or higher in the project can merge your commits into the master branch.

### 6.16 Releasing DFTTK

When releasing a new version of DFTTK

1. `git pull` to make sure you haven’t missed any last-minute commits. After this point, nothing else is making it into this version.

2. Ensure that all tests pass locally on develop.

3. `git push` and verify all tests pass on all CI services.

4. Generate a list of commits since the last version with `git --no-pager log --oneline --no-decorate 0.1^..origin/master` Replace 0.1 with the tag of the last public version.

5. Condense the change list into something user-readable. Update and commit CHANGES.rst with the release date:

```
git tag 0.2 master -m "0.2" Replace 0.2 with the new version. git show 0.2 to ensure the correct commit was tagged git push origin master --tags
```

7. The new version is tagged in the repository. Now the public package must be built and distributed.

### 6.16.1 Uploading to PyPI

1. `rm -R dist/*` on Linux/OSX or `del dist/*` on Windows

2. With the commit checked out which was tagged with the new version: `python setup.py sdist` Make sure that the script correctly detected the new version exactly and not a dirty / revised state of the repo.

   Assuming a correctly configured .pypirc:

   `twine upload -u bocklund dist/*`
6.16.2 Some useful commands are following

```bash
git checkout master
#
git pull
git pull upstream master
git --version
git remote set-url --all upstream git@github.com:PhasesResearchLab/dfttk.git
git remote set-url --add upstream git@github.com:PhasesResearchLab/dfttk.git
git remote set-url --delete upstream git@github.com:PhasesResearchLab/dfttk.git
git remote remove upstream
git remote rm upstream
git remote -v
git remote add upstream git@github.com:PhasesResearchLab/dfttk.git
#
git tag -d 0.3.0
git push --delete upstream 0.3.0
git tag 0.3.0 master -m "0.3.0"
git push upstream master --tags
rmdir/*
python setup.py sdist
twine upload -u yiwang62 dist/*
```

6.17 Recipes

6.17.1 Construct a series of Debye workflows by substituting into a template structure

```python
DRY_RUN = True  # Don't submit the workflows
VERBOSE = True  # Turn on printing of substitutions

# Filename of the template structure to use, usually a dilute or SQS structure
TEMPLATE_STRUCTURE_FILENAME = 'structures/FCC_A1.sqs.12Ni-4Fe.POSCAR'

# sublattice configuration of the template structure.
# This will be substituted exactly, this does not need to be sorted,
# however the individual configurations to build should be sorted.
TEMPLATE_SUBLATTICE_CONFIGURATION = [['Fe', 'Ni']]
TEMPLATE_SUBLATTICE_OCCUPANCIES = [[0.25, 0.75]]
SUBLATTICE_SITE_RATIOS = [1.0]

PHASE_NAME = 'FCC_A1'

configurations_to_build = [  # list of sublattice configurations in DFTTK
    [['Cr', 'Ni']],
    [['Fe', 'Ni']],
    # [['V', 'Ni']],  # should not use this because it's out of order, make a second script with the templates flipped
```
Dictionary of densities for each pure element.
Not necessary, using the periodic_table in pymatgen instead

```python
DENSITY_DICT = {
    'V': 6.313,  # bcc
    'Cr': 7.463,  # bcc
    'Ni': 9.03,  # fcc
    'Ti': 4.58,  # hcp
    'Fe': 8.028  # bcc
}
```

# SCRIPT #

Should not need to edit below this line.

```python
from pymatgen import Structure
from fireworks import LaunchPad
from dfttk import get_wf_gibbs
from dfttk.structure_builders.substitutions import substitute_configuration_with_metadata

workflows = []

temp_struct = Structure.from_file(TEMPLATE_STRUCTURE_FILENAME)

for config in configurations_to_build:
    struct, meta = substitute_configuration_with_metadata(temp_struct, TEMPLATE_SUBLATTICE_CONFIGURATION, config, TEMPLATE_SUBLATTICE_OCCUPANCIES, PHASE_NAME, TEMPLATE_SUBLATTICE_SITE_RATIOS)
    if VERBOSE:
        print("PHASE: {}  CONFIGURATION: {}  OCCUPANCIES: {}  STRUCTURE: {}".
              format(PHASE_NAME, config, TEMPLATE_SUBLATTICE_OCCUPANCIES, struct.composition.hill_formula))
    workflows.append(get_wf_gibbs(struct, deformation_fraction=(-0.05, 0.10), phonon=False, num_deformations=11, t_max=2000, metadata=meta))

# Load everything in the LaunchPad

if VERBOSE:
    print("{} workflows.".format(len(workflows)))

if DRY_RUN:
    exit()

if VERBOSE:
    print("Adding workflows to LaunchPad")

lpad = LaunchPad.auto_load()

(continues on next page)
for workflow in workflows:
    lpad.add_wf(workflow)

### ESPEI datasets from a QHA database

The following code snippet will take ESPEI datasets from a QHA database, optionally writing the (nicely named) files to dict. The QHA database requires the following metadata schema:

```python
{
    'metadata': {
        'phase_name': 'FCC_A1',
        'tag': 'ed447049-ad67-4090-ba99-378188d3416b',
        'sublattice': {
            'configuration': [['Cr', 'Ni']],
            'occupancies': [[0.03125, 0.96875]]
        }
    }
}
```

```
# EDIT #
#
#
phase_name = 'BCC_A2'
configuration_to_find = [['Ni', 'V']]
sublattice_site_ratios = [1.0]
```

```
db_username = 'BrandonResultsRO'
db_password = 'piqhg38hap3'
db_uri = 'mongodb://206.189.190.225:27018'
WRITE_FILES = True

```

```
temperature_index = 59  # index of 300 K temperature (close to 298 K), found by hand
```

```
refstate_tags = {
    'Fe': '4ac77fce-0e43-4c07-8418-4843a2cd5723',
    'Ni': '0059ee69-4a8f-4e86-9895-9b40cf67dd96',
    'Cr': '8ccceb186-2796-4488-ba8c-2380c5278f62',
    'V': 'fba46b6b-1699-419f-b5e1-da9533530701',
}
```

```
# SCRIPT
```

```
from dfttk.analysis.formation_energies import get_formation_energy, get_thermal_props
from dfttk.espei_compat import make_dataset, dfttk_config_to_espei, dfttk_occupancies_to_espei
from pymatgen import Structure
import numpy as np
```

(continues on next page)
from dfttk.utils import recursive_flatten
import json
from pymongo import MongoClient

# create the MongoClient
cli = MongoClient(db_uri)
db = cli.results
db.authenticate(name=db_username, password=db_password)
coll = db.qha

# construct the energies, assumption of same temperature grid
# energies are J/mol-atom
refstate_energies = {}
for el, tag in refstate_tags.items():
    qha_result = coll.find_one({
        'metadata.tag': tag
    })
    refstate_energies[el] = get_thermal_props(qha_result)

# calculate all the dataset values
configs = []
occupancies = []
hm_values = []
sm_values = []
cpm_values = []

# we'll change the T to the right temperatures later
fixed_conds = {'P': 101325, 'T': 0}
temp_conds = {'P': 101325, 'T': 0}

for qha_res in coll.find({
    'metadata.sublattice.configuration': configuration_to_find,
    'metadata.sublattice.phase_name': phase_name
}):  
    configs.append(qha_res["metadata"]['sublattice']["configuration"])
    occupancies.append(qha_res["metadata"]['sublattice']["occupancies"])

    tprops = get_thermal_props(qha_res)
    struct = Structure.from_dict(qha_res['structure'])
    hm_form = get_formation_energy(tprops, struct, refstate_energies, 'HM',
    -idx=temperature_index)
    sm_form = get_formation_energy(tprops, struct, refstate_energies, 'SM',
    -idx=temperature_index)
    cpm_form = get_formation_energy(tprops, struct, refstate_energies, 'CPM', thin=10)[:2]
    fixed_temp = tprops['T'][temperature_index]
    cpm_temps = tprops['T'][::10][-2]

    fixed_values.append(hm_form)
    sm_values.append(sm_form)
    cpm_values.append(cpm_form)

fixed_conds['T'] = fixed_temp.tolist()
temp_conds['T'] = cpm_temps.tolist()
# make the HM, SM, CPM values arrays of the proper shape
hm_values = np.array([hm_values])
sm_values = np.array([sm_values])
cpm_values = np.array(cpm_values).T[np.newaxis, ...]

if WRITE_FILES:
    # write JSON files
    comps = [c.upper() for c in sorted(recursive_flatten(configuration_to_find))]
    for prop, vals, conds in [('HM_FORM', hm_values, fixed_conds), ('SM_FORM', sm_values, fixed_conds), ('CPM_FORM', cpm_values, temp_conds):
        ds = make_dataset(phase_name, prop, sublattice_site_ratios, configs, conds, vals, occupancies=occupancies, tag=tag)
        with open('{}-{}-DFTTK.json'.format('-'.join(comps), phase_name, prop), 'w') as fp:
            json.dump(ds, fp)

6.18 FAQ

6.18.1 What do the references to DFTTK-style or ESPEI-style configurations or occupancies mean?

ESPEI is separate software for fitting thermodynamic databases within the CALPHAD method. The CALPHAD method requires descriptions of the formation and mixing energies of phases described by sublattices, as in the compound energy formalism.

DFTTK is an excellent tool for calculating the temperature and composition dependent thermodynamic properties of sublattice configurations within the compound energy formalism.

In both ESPEI and DFTTK, there are three key aspects to describing a phase in the CEF: sublattice site ratios, sublattice configurations, and sublattice occupancies. Sublattice site ratios are a list of integer or fraction ratios of the sublattice. There are no constraints on the order or values. Some valid ones would be:

- 1 sublattice
- 3.0, 2.0 # 2 sublattices with 3 occurrences of species in sublattice 1 and 2 in sublattice 2
- 1, 0.5 # 2 sublattices with 1 occurrence of species in sublattice 1 and 1/2 in sublattice 2
- 16, 11 # 2 sublattices with 16 occurrences of species in sublattice 1 and 11 in sublattice 2

DFTTK describes a sublattice configuration as a list of sublattices, where each sublattice is also a list of the components occupying that sublattice. Some examples are:

- [[Fe, Ni]] # 1 sublattice with mixing of Fe and Ni
- [[Mg], [Cu]] # 2 sublattices with no mixing in each sublattice.
- [[Cr, Fe], [Cr], [Cr, Fe]] # 3 sublattices with mixing in the first and last sublattice

The ordering of sublattices themselves have no distinct meaning. As a convention, DFTTK sorts the components in each sublattice by component name, e.g., Cr (starts with C) always comes before Fe (starts with F)). ESPEI requires each sublattice to be ordered in this way.
Sublattice occupancies or occupations describe how a sublattice is filled with each particular element. The shape of these corresponds exactly to the configuration that the occupancy list describes. The sorting of the occupancies therefore is also in the same order of the configuration.

DFTTK includes several tools to help build ESPEI-compatible sublattice descriptions. The only difference between DFTTK and ESPEI configurations and occupancies is that a singly occupied sublattice, e.g. \([\text{[Fe]}]\) in DFTTK, is not wrapped in the sublattice parenthesis for both the configuration and occupancies. Some examples of ESPEI configuration and occupancy lists are given below:

\[
\begin{align*}
\text{[[Fe, Ni]}], \text{[[0.5, 0.5]]} & \quad \# \text{this is the same as DFTTK, there are no single occupations} \\
\text{[Mg, Cu], [1.0, 1.0]} & \quad \# \text{each sublattice is singly-occupied and is not wrapped in the \(\_\_\_\text{parenthesis}\)} \\
\text{[[Cr, Fe]}, \text{Cr}, [\text{[Cr, Fe]}], \text{[[0.5, 0.5], 1, [0.3, 0.7]]} & \quad \# \text{the second sublattice is singly-occupied and is not wrapped}
\end{align*}
\]

As a final note, ESPEI format typically uses all uppercase, consistent with the CALPHAD community, while DFTTK usually uses standard element capitalization. The conversion tools take this into account.

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6.20 Indices and tables

- genindex
- modindex
- search