**Usage of diffusion coefficient calculation tool code**

1. This code currently supports 5(fcc) and 8(hcp) frequency models.
2. The code currently will work in the same directory with other MAST generated folders (neb\_vac\*, phonon\_vac\*, etc.)
3. Type “diff.py –i <input>” to run. (<input> is the same as the MAST input file)
4. The input file has a new session in a $freq - $end pair, where the directories of energy and attempting rates are specified with respect to different frequencies.
   1. The order of different lines does not matter.
   2. There can be as many ‘\n’ between lines or as many spaces between words, and they will not affect the code.
   3. The keyword at the beginning of each line matters:
      1. ‘type’ means which frequency model to choose. Either ‘5’ or ‘fcc’ tells the code 5-freq is applied, while either ‘8’ or ‘hcp’ the 8-freq.
      2. ‘E\*’ and ‘v\*’ means energy and attempting rate, respectively. (Currently doesn’t support other characters such as ‘w’).
      3. For 5-freq, ‘E0’~’E4’ should be used to specify their relations with certain directories; for 8-freq, ‘Ea’,’Eb’,’Ec’,’EX’,’Eap’(‘p’ means ‘prime’),’Ebp’,’Ecp’ and ‘EXp’ should be used. Note they are all ***case sensitive*** and should be exactly the same as
      4. Generally speaking, each keyword (‘E\*’ or ‘v\*’) is followed by two words. The first indicates the configuration of the starting/end point of NEB and the second represents the saddle point. This order should not be changed.
      5. The user can also type only ***one single float*** behind the keyword, and the code will then not refer to the directory for the related energy or attempting rate, but simply use the data given.
      6. ‘HVf’ means the formation energy of vacancy and ‘HB’ means binding energy (4 configurations will be used for ‘HB’, so 4 words or 1 float are expected after ‘HB’).
      7. Current code will not likely to work if these keywords are spelt incorrectly.

Below are two examples of the $freq part in the input file:

**Ex1:**

$freq

type 5

v1 vac1 vac10-vac1

v2 2

v3 vac3 vac4-vac3

v4 5

v0 vac0 vac00-vac0

E1 vac1 vac10-vac1

E2 vac2 vac20-vac2

E3 0.5

E4 vac4 vac4-vac3

E0 vac0 vac00-vac0

HVf 0.5

HB perfect sub vac-sub vac

$end

**Ex2:**

$freq

type hcp

HVf 0.44

HB -0.1

Ea 0.5

Eb 0.5

Ec 0.5

EX 0.5

Eap 0.5

Ebp 0.5

Ecp 0.5

EXp 0.5

va 5

vb 5

vc 5

vX 3

vap 5

vbp 5

vcp 3

vXp 4

$end

Issues:

1. The code currently does not do quite well in the calculation of attempting rate according to the file FREQ\* in phonon\_vac\*\_parse generated by ‘phon\_henry’. In my test, the 2x2x2 cell case gives proper results, but 3x3x3 gives much more frequencies than I expected – not only the frequency of He, but also of Mg and O are calculated by ‘phon\_henry’, and it certainly confuses the code: Should all the frequencies be used? If not, which ones should be used? So I wonder if there is a way to wisely select the phonon frequencies so as to improve the code.
2. Should some information of the system such as lattice parameters *a*, *c* and the number of atoms in the perfect cell (needed when calculating the formation energy of vacancy) also added to the $freq session? Current code requires the user copy the POSCAR of the supercell as well as the primitive cell to the working directory in order to obtain those data.