## 0.1 Input parameters

The code is written in python language and the input parameters are read from the ”inpner.in” file. Please mind that the transport distribution functions (prefix_tdf1.dat and prefix_tdf2.dat ) are always required.

`real :: smrT`

The smearing temperature in the units of K.

`character :: ratecode`

The code used for the scattering rate calculation. Available options, not case sensitive, are AMSET, PERTURBO, ELECTRA, CUSTOM, and CRTA (constant relaxation time approximation).

`real :: Evwan`

The top of the valence band of the wannierized band structure in the units of eV.

`character :: prefix`

prefix of the DFT calculation. It has to be consistent in all steps: DFT, wannierization, and scattering rates.

`real :: Eg`

The experimental band gap in the units of eV.

`real :: Ev`

The top of the valence band from the nscf calculation for the scattering rate calculation in the units of eV.

`real :: mubn`

The chemical potential span in conduction and valence bands in the units of eV.

`real :: mustep`

The chemical potential step size in the units of eV.

`integer :: ner_bext`

The magnitude of the external magnetic field applied to calculate the transport distribution function in the Wannier90 package, the same as ner_bext in the $prefix$.win file.

`real :: Bex`

The external magnetic field along z-axis that is applied for the thermomagnetic properties calculation. It does not have to be the same as nerbext. According to the Jones-Zener expansion, the transport distribution function is a linear function of the magnetic field, therefore, the thermomagnetic properties can be computed at any arbitrary magnetic field which is determined by Bex. Bex is in the units of T.

`integer :: amesh`

The mesh grid printed in the output of scattering rate calculation by AMSET.

`real :: eps0`

The tolerance value for the derivative of the Fermi–Dirac distribution function.

`integer :: calcdos`

Whether density of states is calculated (1) or not (0). If set to 1, the density of states from band "bni" to band "bnf" will be calculated on the interpolated bands. **Only implemented with AMSET.**

`integer :: bni`

The initial band index for the calculation of the density of states. **Keep in mind that these band indices are the interpolated bands which might differ from the original DFT band indices.**

`integer :: bnf`

The final band index for the calculation of the density of states. **Keep in mind that these band indices are the interpolated bands which might differ from the original DFT band indices.**

`character :: elctcharge`

Charge carrier type used in ElecTra, h for holes and e for electrons.

`real :: Tmin`

The minimum temperature in the units of K **only for CRTA**.

`real :: Tmax`

The maximum temperature in the units of K **only for CRTA**.

`real :: Tstep`

The temperature step size in the units of K **only for CRTA**.

`integer :: calcseeb`

Whether the Seebeck effect related properties are calculated (1) or not (0).

`integer :: savematrix`

Whether the the response functions of the Seebeck and Nernst effects are saved (1) or not (0). For further information Ref should be consulted.

## 0.2 Output files

Assume we have scattering rates at the temperature of $t$ in Kelvin and the doping concentration (chemical potential) of $dop$ in $cm^{-3}$ (eV) and a magnetic field of Bex is applied for the thermomagnetic properties, multiple files will be generated.

`T$t$dop$p$rate.txt`

Scattering rates at the temperature of $t$ and doping concentration/chemical potential of $p$ due to various scattering mechanisms. The first column is energy the rest columns are scattering rates in then units of second as many columns as the scattering mechanisms.

`T$t$dop$p$Sig.txt`

The electrical conductivity tensor for the Seebeck effect in the units of $1/\Omega.m$ at the temperature of $t$ and doping concentration/chemical potential of $p$ . The first column is the chemical potential in the units of eV and 9 columns of the electrical conductivity in possible directions.

`T$t$dop$p$S.txt`

The Seebeck coefficient tensor in the units of $V/K$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical potential in the units of eV and 9 columns of the Seebeck coefficient in possible directions.

`T$t$dop$p$Kap.txt`

The electronic thermal conductivity tensor in the units of $W/m.K$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical potential in the units of eV and 9 columns of the electronic thermal conductivity in possible directions.

`T$t$dop$p$Bmat.txt`

The B-matrix response function for the Seebeck effect in the units of $V/K.m.\Omega$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical potential in the units of eV and 9 columns of the B-matrix response function in possible directions.

`T$t$dop$p$K.txt`

The K-matrix response function for the Seebeck effect in the units of $W/m.K$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical potential in the units of eV and 9 columns of the K-matrix response function in possible directions.

`T$t$dop$p$TDF1.txt`

The transport distribution function of the Seebeck effect in the units of $C^2S/kg.m^3$ at the temperature of $t$ and doping concentration of $p$. The first column is the energy in the units of eV and 9 columns of the transport distribution function in possible directions.

`T$t$dop$p$RB$Bex$.txt`

The Hall coefficient in the units of $\Omega.m/T$ at the temperature of $t$ and doping concentration/chemical potential of $p$ . The first column is the chemical potential in the units of eV and the second column is the Hall coefficient.

`T$t$dop$p$NB$Bex$.txt`

The Nernst coefficient in the units of $V/K.T$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical potential in the units of eV and the second column is the Nernst coefficient.

`T$t$dop$p$EB$Bex$.txt`

The Ettingshausen coefficient in the units of $K.m/A.T$ at the temperature of $t$ and doping concentration/chemical potential of $p$ . The first column is the chemical potential in the units of eV and the second column is the Ettingshausen coefficient.

`T$t$dop$p$SigB$Bex$.txt`

The electrical conductivity tensor for the Nernst effect in the units of $1/\Omega.m$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the chemical

potential in the units of eV and 9 columns of the electrical conductivity for the Nernst effect in possible directions. For further information Ref should be consulted.

`T$t$dop$p$BmatB$Bex$.txt`

The B-matrix response function for the Nernst effect in the units of $V/K.\Omega.m$ at the temperature of $t$ and doping concentration/chemical potential of $p$ . The first column is the chemical potential in the units of eV and 9 columns of the B-matrix response function for the Nernst effect in possible directions. For further information Ref should be consulted.

`T$t$dop$p$KB$Bex$.txt`

The K-matrix response function for the Nernst effect in the units of $W/m.K$ at the temperature of $t$ and doping concentration/chemical potential of $p$ . The first column is the chemical potential in the units of eV and 9 columns of the K-matrix response function for the Nernst effect in possible directions. For further information Ref should be consulted.

`T$t$dop$p$TDF2B$Bex$.txt`

The transport distribution function of the Nernst effect in the units of $C^2.S/m^3.kg$ at the temperature of $t$ and doping concentration/chemical potential of $p$. The first column is the energy in the units of eV and 9 columns of the transport distribution function for the Nernst effect in possible directions. For further information Ref should be consulted.

## 0.3 AMSET

The output of the AMSET code, mesh_a×a×a.h5, needs to be in the working directory. The parameter a is the interpolation grid and specified by "amesh" in the input file.

## 0.4 Perturbo

The electron-phonon self energy (prefix.imsigma) and the temperature array (prefix.temper) have to be provided.

## 0.5 ElecTra

After successfully running ElecTra, scattering rates are stored in a binary MATLAB file named 'TE_prefix_kScan_electrons.mat'. You need to run "alltau.m" file in the MATLAB workspace to save the total scattering rates in the format required by **NERTAW.py**. Ad-

ditionally, from the MATLAB workspace, save the variables "EF_matrix" and "T_array.in" into files "elcmu.in" and "elcT.in", respectively. The charge carrier, e or h, has to be selected by "elctcharge" flag in the inpner.in file.

## 0.6 Custom

Temperature in the units of Kelvin (Tarray.in), chemical potential/doping in the units of eV (muarray.in), and scattering rates (rarray.in) in the units of 1/s are required. The "rarray.in" file has to follow a specific format, a space separated file in which the first column is energy (eigenvalues) followed by the scattering at each temperature over all doping (chemical potential). e.g. if we have T=300,400 and n=$10^{15}$, $10^{16}$, $10^{17}$ then the scattering rate file needs to have 7 columns. The 2nd,3rd, and 4th columns are the rates at T=300 and n=$10^{15}$, $10^{16}$, $10^{17}$ respectively. The 5th,6th, and 7th columns correspond to T=400 and n=$10^{15}$, $10^{16}$, $10^{17}$ respectively.

## 0.7 CRTA

For the case of the constant relaxation time approximation (CRTA), the constant value for the relaxation time is supplied by "ctau" in the input file.