

aMoBT User's Manual

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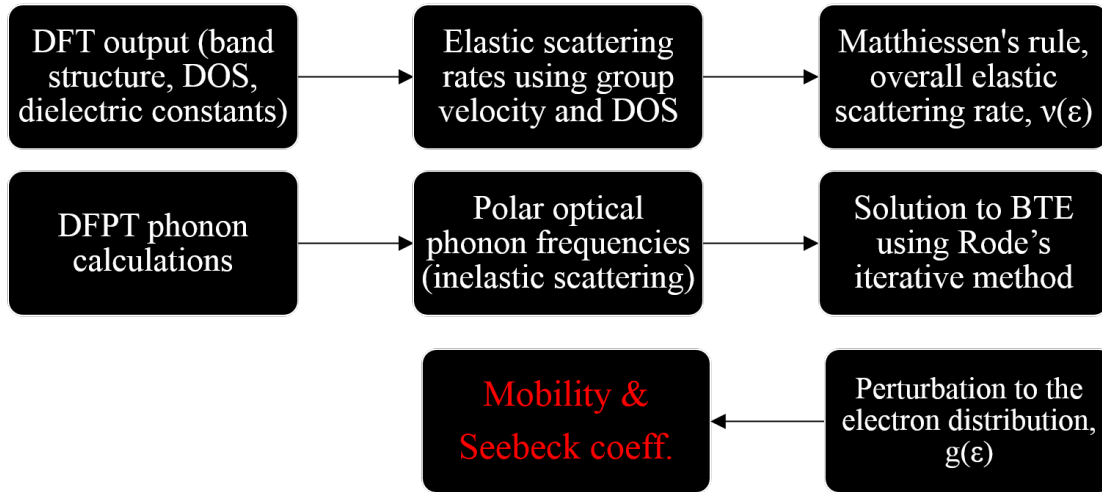


Figure 1: Flowchart of aMoBT, from *ab initio* calculations to the calculated mobility and Seebeck coefficient. For more detailed information regarding aMoBT, see [1].

Disclaimer: This document is meant to be a guide for the users of aMoBT to facilitate a complete employment of the available features. The content is NOT guaranteed to be scientifically accurate and certified/peer-reviewed and the researchers should use the suggestions at their own responsibility.

1 Introduction

ab initio Model for Mobility calculation using Boltzmann Transport equation (aMoBT) is a model that uses the *ab initio* band structure (preferably using GW) and explicitly solves BTE to obtain the small perturbation to the electron distribution assuming low-field transport.

Currently ionized impurity scattering as well as charged dislocation and piezoelectric and deformation potential scatterings are taken into account as elastic scattering mechanisms and polar optical phonon as an inelastic scattering mechanism. You can go through the examples and change parameters to see the effect on transport properties or you can upload your own band structure and density of states files generated with VASP (Vienna *ab initio* Simulation Package) for transport calculations. Figure 1 provides an overview of aMoBT from *ab initio* calculations to the calculated mobility and Seebeck coefficient. For more detailed information, see [1].

If you want to upload your VASP files for your system, you need to choose the "New" option from the top left drop-down menu in aMoBT and then upload the EIGENVAL file from a non-self consistent calculations in a dense k-point mesh around your CBM/VBM (for an n-type/p-type semiconductor) as well as PROCAR (generated with LORBIT = 11 flag in INCAR). Also, you need to upload DOSCAR and OUTCAR from the self-consistent calculations. It is preferable that the DOSCAR is generated with NEDOS more than 3000 and less than 10,000 (if it is 10000 or more, this number is not readable from DOSCAR). If you had any questions, feel free to send an email to alireza@wustl.edu

2 Logistics

The graphical user interface (GUI) for aMoBT has been prepared using Rappture which is available on nanoHub.org. We present, in the following, some features of this GUI from which 3 and 4 are only relevant to some users.

1. You can run several simulations with different values for temperature, dielectric constants, etc. You can access those simulation through the blue bar on the lower right side of the window. To save the output of different simulations, you can access and download the Output for each simulation.
2. To calculate mobility at different temperatures, rather than running separate simulations at those temperatures, you can run one simulation at different temperatures which is much faster since band structure fitting is done only once. To do that, you can simply enter your data points in Experimental data for mobility field like the following example and then switch Compare to experiment? to "yes". In the following, the first column is temperature and the second is the mobility. The column for mobility should not be left empty. If you have experimental data at those temperatures, of course they can be entered instead of repeated "1000":

```
50 1000;
100 1000;
200 1000;
300 1000;
400 1000;
500 1000;
600 1000
```

3. If you are running aMoBT on Internet Explorer, the screen might go dark. Refresh will fix it. For more information, please contact nanoHub.org.
4. If you are running aMoBT on windows 8 touch screen laptop, if you use Google Chrome, you might not be able to use the mouse. If only the touch screen is working, an alternative solution is to use a different browser. Generally, the users might have some difficulty using the tool with Google Chrome. For more information, please contact nanoHub.org

In the following all the inputs and outputs of aMoBT are briefly described:

3 Inputs

3.1 Material

Material: Here you can choose your material of interest, currently there are 3 examples available together with corresponding mobility and Seebeck coefficient experimental data. The followings are the options for this input:

- Option* 1. n-GaAs example (default): this example is for a pure GaAs sample with a very low electron concentration of $n = 3.0 \times 10^{13}$. Other parameters are obtained *ab initio*[1]. In order to make this example faster to run, the band structure and the density of states are already carefully fitted to polynomials in a dense mesh containing 8531 k-points.
- Option* 2. n-InN example: the purpose of this example is to illustrate the effect of charge dislocation scattering on limiting the mobility of InN. Here again, all the default parameters are obtained *ab initio*. Furthermore, to make this example faster to run, the band structure and the density of states are already carefully fitted to polynomials in a dense mesh containing 8531 k-points.
- Option* 3. n-ZnS example: this is an example of uploaded data with all four files, EIGENVAL, PROCAR, OUTCAR and DOSCAR (output files of VASP[2-5]) already uploaded. The main purpose of this example is for user to see how the next option, "New", should look like.
- Option* 4. New: this option can be used for uploading the files for a new system. Note that choosing this option will generate new set of default values for parameters that are not for any specific material.

The user is responsible for choosing the appropriate values for each parameter. However, the deformation potential, E_d , and piezoelectric constant, P , might not be important particularly at higher temperatures ($>200\text{K}$). It is a good idea to run the simulation with correct polar optical frequency and dielectric constants, etc. and change E_d and P only if they are limiting the mobility at the selected temperature(s).

Option 5. Upload: this option is used to upload all necessary VASP files together. You can select this after choosing "New" to upload all the files. Otherwise, by right clicking on the white field in front of each file, and choosing "Upload...", that specific file can be uploaded.

Option 6. Download: you can use this option to download the files for ZnS example as sample files for a working example.

3.2 *ab initio* band structure and density of states

This field is just an indicator for the program to use either the pre-fitted band structures for faster calculations in the examples, or to use the uploaded band structure (If Material is set to "New"). After the user chooses any option for Material, this field will automatically set to the proper option and it should not be changed after that.

3.3 Type of the conductivity

This field decides whether electron (n-type) or hole (p-type) mobility is calculated. If "n-type" is chosen, aMoBT will calculate the transport properties based on the conduction band edge, at and around the "reference k-point". If "p-type" is chose, aMoBT will calculate the transport properties based on the valence band edge, at and around the k-point determined as the reference k-point . It should be noted that changing the type does not affect the results of the two examples: "n-GaAs" and "n-InN" as their conduction bands are pre-set to fitted polynomials to provide a faster demonstration.

3.4 Type of formulation

This field determines whether aMoBT uses single-band model or coupled band. Coupled band model is relevant in degenerate CBM or VBM where interband scattering exist. For more information on this formulation see [6] This option should be left to the default: "automatic" in which case appropriate formulation will be used depending on the type of the input band structure: coupled-band formulation will be used only if degenerate band exists which is the case for most p-type semiconductors; otherwise, a single band formulation will be used. One may manually choose "single band" or "coupled band" options to compare the two formulation but of course only one of them is relevant and correct for each input. It is recommended to leave this field unchanged from "automatic".

3.5 "Tempearture, T(K)" and "Compare to experiment?"

This is the temperature at which the properties are calculated if the field "Compare to experiment?" is set to "no". Otherwise, if the data is compared to experiment, the mobility and Seebeck coefficient are evaluated at the experimental data entry points that are specified in Experimental data for mobility. It should be noted that the Seebeck coefficient in this case is only at the specified Carrier concentration. Unfortunately, currently, if the user wants to calculate the Seebeck coefficient at different T's and n's, they have to switch "Compare to experiment?" to "no" and then calculate each point separately as opposed to a single simulation run.

3.6 Maximum number of iterations to obtain g

This is the maximum number of iterations set when solving the Boltzmann transport equation using Rode's[7] iteration method to obtain the perturbation to the electron distribution, g. Usually the average

difference in two consecutive g's (Printed in Output) drop by one or two orders of magnitude within 5 iterations.

3.7 Free electron DOS?

If this is set to "no" then the uploaded *ab initio* density of states (DOS) will be used in transport calculations and everything will be integrated in energy space. Otherwise, if "yes", the free-electron DOS will be used which works better at high carrier concentrations and high temperatures. Everything will be integrated in k-space in this case. See [1] for more details.

3.8 k-point of CBM/VBM for n-/p-type conductivity

Here you can set the fractional coordinate of the k-point at which the conduction band minimum (CBM) or the valence band maximum (VBM) is located in either the n- or p-type semiconductor. Here we call this the "reference k-point". It should be noted that for accurate calculation of the transport properties, one should use the k-point mesh that is suggested (or a denser one) in "Supporting Docs". However, if the CBM/VBM does not occur at the Γ -point with the coordinate "0.0 0.0 0.0", one should generate a new k-point mesh using the `KPOINTS_generator_for_aMoBT.m` available under the tab "Supporting Docs" using the new reference k-point and calculate the EIGENVAL based on that.

3.9 Polar optical phonon frequency, ω_{po} (THz)

To calculate this parameter *ab initio*, one needs to calculate the phonon band structure and density of states. One method is to use Phonopy [8] code, after the force constants are obtained using DFPT, to get these frequencies in THz. For the available examples of aMoBT calculations: GaAs, InN and ZnS, the optical phonon frequency at Γ point, ω_{po} , that we are looking for, is in very good agreement with experimental measurements. There is an approximation in choosing the optical phonon frequency from the last phonon DOS peak. Users are responsible for the accuracy of the values they set for all input parameters of aMoBT particularly ω_{po} , ϵ_0 and ϵ_∞ (see the next section) on which the results are sensitive.

3.10 Dielectric constants: ϵ_0 and ϵ_∞

Dielectric constants can be calculated *ab initio*. You can refer to VASP manual. However, the calculated values are not always accurate. The calculated properties are sensitive to the values of dielectric constants [1]. It is relatively simple to calculate the high frequency dielectric constant, ϵ_∞ , based on the calculated static dielectric constant, ϵ_0 , from DFPT which is generally reliable. Once the phonon density of states (DOS) is calculated which is required for ω_{po} anyway, ϵ_∞ can be calculated via Lyddane-Sachs-Teller relation (equation 1):

$$\epsilon_\infty = \epsilon_0 \times \left(\frac{\omega_{TO}}{\omega_{LO}} \right)^2 \quad (1)$$

where ω_{TO} and ω_{LO} are transverse and longitudinal optical phonon frequencies respectively.

3.11 Deformation Potential

Deformation potential is "how much the energy level of CBM/VBM changes per unit change in the volume" times "the equilibrium volume". In order to obtain this value *ab initio* please see [1]. Also, experimental values for deformation potential for some III-V semiconductors are available in [7].

3.12 Piezoelectric coefficient, P

The piezoelectric coefficient is a unitless parameter which is a function of piezoelectric and elastic constants of the material all of which can be calculated *ab initio*. The user can run the simulation with default

values first to check if the mobility is limited by piezoelectric scattering at the corresponding temperature(s). The experimental values for this input parameter for some III-V semiconductors can be found in the literature [7]. Piezoelectric coefficient, P, can be calculated using equation 2 for sphalerite crystal structure :

$$P^2 = h_{14}^2 \epsilon_0 [(12/c_l) + (16/c_t)] / 35 \quad (2)$$

$$c_l = (3c_{11} + 2c_{12} + 4c_{44}) / 5 \quad (3)$$

$$c_t = (c_{11} - c_{12} + 3c_{44}) / 5 \quad (4)$$

Also, for wurtzite crystal structure, P can be calculated using equation 5[7]:

$$P_{\perp}^2 = 4\epsilon_0 \left(21h_{15}^2 + 6h_{15}h_x + h_x^2 \right) / 105c_t + \epsilon_0 \left(21h_{33}^2 - 24h_{33}h_x + 8h_x^2 \right) / 105c_l \quad (5)$$

$$P_{\parallel} = 2\epsilon_0 \left(21h_{15}^2 + 18h_{15}h_x + 5h_x^2 \right) / 105c_t + \epsilon_0 \left(63h_{33}^2 - 36h_{33}h_x + 8h_x^2 \right) / 105c_l \quad (6)$$

$$h_x = h_{33} - h_{31} - 2h_{15} \quad (7)$$

$$c_l = (8c_{11} + 4c_{13} + 3c_{33} + 8c_{44}) / 15 \quad (8)$$

$$c_t = (2c_{11} - 4c_{13} + 2c_{33} + 7c_{44}) / 15 \quad (9)$$

where h_{ij} and c_{ij} are independent elements of piezoelectric and elastic tensors respectively. Also, c_l and c_t are longitudinal and transverse spherically averaged elastic constants. For more information, see [7].

3.13 Dislocation density, N_{dis} ($1/cm^2$)

In some materials, such as InN, charged linear dislocations cause electron scattering and limit the electron mobility. See [9] for more information. The density of these linear dislocations are measured and reported in $1/cm^2$; however, for electron scattering the overall density is required. We assume that these dislocations are homogeneously distributed along the c-axis. Therefore, the value entered for "Dislocation density, N_{dis} ($1/cm^2$)" will be divided by 0.565 nm which is the equilibrium lattice constant of InN. The user must recalibrate "Dislocation density, N_{dis} ($1/cm^2$)" based on this number and the actual lattice constant of their material.

3.14 Carrier concentration, n ($1/cm^3$)

The carrier concentration can be explicitly entered here. It should be noted that this carrier concentration is assumed to be constant at all temperatures ($>20K$). The Fermi level is calculated based on this value. See [1] for more information.

The experimental values for input parameters described in sections 3.9-3.14 for some III-V semiconductors can be found in the literature [7].

3.15 Experimental data for mobility

This field is for the mobility vs. temperature data to compare with the calculated mobility. Once Compare to experiment? is set to "yes", the transport properties will be calculated at each temperature that is specified in this field. For example, if the input is the following (note the correct format):

```
300 1000;
400 500
```

then the transport properties will be calculated at 300K and 400K to be compared with $1000 \text{ cm}^2/V \cdot s$ and $500 \text{ cm}^2/V \cdot s$ respectively.

3.16 Exp. data for Seebeck coeff.

This field has to be filled out similar to Experimental data for mobility but for Seebeck coefficient, S, vs. carrier concentration, n, data. Unfortunately, S vs. T plot is not currently available. The users can run single-point calculations at different temperatures for S vs. T comparisons.

3.17 Input files: EIGENVAL, PROCAR, OUTCAR, DOSCAR

If "New" is selected for Material, then, 4 input files can be uploaded two of which are required: EIGENVAL and OUTCAR. As described in Introduction, the EIGENVAL file should be from a non-self consistent calculations in a dense k-point mesh around your CBM/VBM (for an n-type/p-type semiconductor) as well as PROCAR (generated with LORBIT = 11 flag in INCAR). The number of k-points must be less than 10,000 points. Also, you need to upload DOSCAR and OUTCAR from the **self-consistent** calculations. It is preferable that the DOSCAR is generated with NEDOS more than 3000 and less than 10,000 (if it is 10000 or more, this number is not readable from DOSCAR). EIGENVAL is required for the band structure and group velocity calculations. OUTCAR is required for extracting lattice matrix and volume. PROCAR is optional for more accuracy in calculation of s-p hybridization in the conduction band; if PROCAR is not available the conduction(valence) band wave function is assumed to be completely s-like(p-like). DOSCAR is optional for extracting the total density of states to be used when Free electron DOS? is set to "no"; if DOSCAR is not available, the free electron DOS is used.

4 Outputs

4.1 Mobility ($\text{cm}^2/\text{V}\cdot\text{s}$)

This simply plots the calculated mobility at the specified temperature. In case that "Compare to experiment?" is set to "yes", this will be the calculated mobility at the **last** temperature point that is specified in Experimental data for mobility as input.

4.2 Seebeck coefficient ($\mu\text{V}/\text{K}$)

This simply plots the calculated Seebeck coefficient at specified carrier concentration. Unlike the previous plot, even if "Compare to experiment?" is set to "yes", this will be the calculated Seebeck coefficient at the **specified** carrier concentration that is specified in Carrier concentration, n ($1/\text{cm}^3$) as input.

4.3 Effective mass (average)

The calculated average effective mass based on the uploaded band structure. For more details on how the effective mass is calculated, see [1].

4.4 Group velocity of electrons

The plot of the calculated electron group velocity vs. k, based on the uploaded band structure. For more details on how the group velocity is calculated from the polynomials that are fitted to the conduction band, see [1].

4.5 Mobility vs. T

The calculated and experimental mobility vs. temperature all in one plot. If Compare to experiment? is set to "yes" the calculated mobilities will be plotted at all the temperatures that were specified by the user at Experimental data for mobility as input. Each line represent the mobility if it was only limited by a specific scattering mechanism. Furthermore, the overall mobility is also plotted to be compared to the experimental values entered before. It should be noted that if Compare to experiment? is set to "no" only the experimental data (if any) will be plotted.

4.6 Seebeck coefficient vs. n

The calculated and experimental Seebeck coefficient vs. carrier concentration. Unlike the previous plot, even if Compare to experiment? is set to "yes" the calculated Seebeck coefficients will be plotted at only

the specified Carrier concentration, n ($1/\text{cm}^3$). It should be noted that if Compare to experiment? is set to "no" only the experimental data (if any) will be plotted.

4.7 Output

This is the printed output with some useful information such as the accuracy of the fit to the band structure, DOS, etc. as well as the calculated effective mass, mobilities, Seebeck coefficient. This file also contain some warnings in case, for example, more data points are required for fitting polynomials, etc.

5 Version notes

5.1 Version 2.1.1

The PROCAR and DOSCAR files are no longer required. Only EIGENVAL file and OUTCAR file are required. If DOSCAR is not uploaded a free electron density of state is assumed and if PROCAR is not uploaded the conduction(valence) band is assumed to be fully s-like(p-like).

For Quantum ESPRESSO (QE) users: the Python code named "QE-to-VASP.py" is now available under the supporting documents. This code generates the EIGENVAL and OUTCAR files from a QE self consistent or non-self consistent calculation (line-mode band structure is not supported). Usage: python QE-to-VASP.py -f YOUR-QE-OUTPUT-FILE

5.2 Version 2.0.1

Substantial changes were made compared to the previous versions. A coupled band formulation is added to the program to take into account the inter-band scattering in semiconductors with degenerate bands. aMoBT now automatically decides which formulation to be used based on the uploaded EIGENVAL file. This version has been tested with p-type GaAs with a degenerate valence band. DFT band structure with spin orbit coupling taken into account was used as the input band structure. Very good agreement with experimental data was obtained.

5.3 Version 1.1.1

Based on the uploaded OUTCAR, aMoBT now automatically calculates the predicted density of the material. Furthermore, based on the value of LSORBIT printed in the OUTCAR file that is uploaded by the user, aMoBT determines whether the *ab initio* calculations have been done with spin-orbit coupling. Subsequent treatment of EIGENVAL and PROCAR will be determined based on this. This is particularly important in semiconductors with a degenerate band.

5.4 Version 1.1.0

The k-point at which the conduction band minimum (CBM) or the valence band maximum (VBM) is located in the semiconductor can now be entered as an input. See reference k-point for more information.

The type of the semiconductor (n-type/p-type) can be determined for calculating the electron/hole mobility, conductivity, etc.

5.5 Version 1.0.2

The low-field mobility and Seebeck coefficient can be calculated in a semiconductor with a single conduction band governing the transport properties with the CBM at Γ -point. If the conduction band has a single dominant band (an example is shown in the snapshots of aMoBT) but not at Γ point, the transport properties can still be easily calculated but not with this version on nanoHub.

Please contact alireza@wustl.edu if you had any question. Comments and feedbacks are most certainly always welcome.

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