

A Step-by-Step Guide for *ab initio*
Calculation of the Hole Mobility of Si
using Quantum ESPRESSO and
aMoBT on nanoHub.org

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Remarks

- Hole mobility of Si is just one example that was chosen for availability and simplicity of Quantum ESPRESSO (QE) calculation of this material on nanoHub
- Similar steps can be taken for calculating electronic properties of other semiconductors
- Both VASP and QE are compatible with aMoBT: ab initio model for calculating the mobility in Boltzmann Transport framework
- Steps:
 1. ab initio calculations
 2. aMoBT calculations

***Ab initio* electronic transport model with explicit solution to the linearized Boltzmann transport equation**

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Accurate models of carrier transport are essential for describing the electronic properties of semiconductor materials. To the best of our knowledge, the current models following the framework of the Boltzmann transport equation (BTE) either rely heavily on experimental data (i.e., semiempirical), or utilize simplifying assumptions, such as the constant relaxation time approximation (BTE-cRTA). While these models offer valuable physical insights and accurate calculations of transport properties in some cases, they often lack sufficient accuracy—particularly in capturing the correct trends with temperature and carrier concentration. We present here a transport model for calculating low-field electrical drift mobility and Seebeck coefficient of *n*-type semiconductors, by explicitly considering relevant physical phenomena (i.e., elastic and inelastic scattering mechanisms). We first rewrite expressions for the rates of elastic scattering mechanisms, in terms of *ab initio* properties, such as the band structure, density of states, and polar optical phonon frequency. We then solve the linear BTE to obtain the perturbation to the electron distribution—resulting from the dominant scattering mechanisms—and use this to calculate the overall mobility and Seebeck coefficient. Therefore, we have developed an *ab initio* model for calculating mobility and Seebeck coefficient using the Boltzmann transport (aMoBT) equation. Using aMoBT, we accurately calculate electrical transport properties of the compound *n*-type semiconductors, GaAs and InN, over various ranges of temperature and carrier concentration. aMoBT is fully predictive and provides high accuracy when compared to experimental measurements on both GaAs and InN, and vastly outperforms both semiempirical models and the BTE-cRTA. Therefore, we assert that this approach represents a first step towards a fully *ab initio* carrier transport model that is valid in all compound semiconductors.

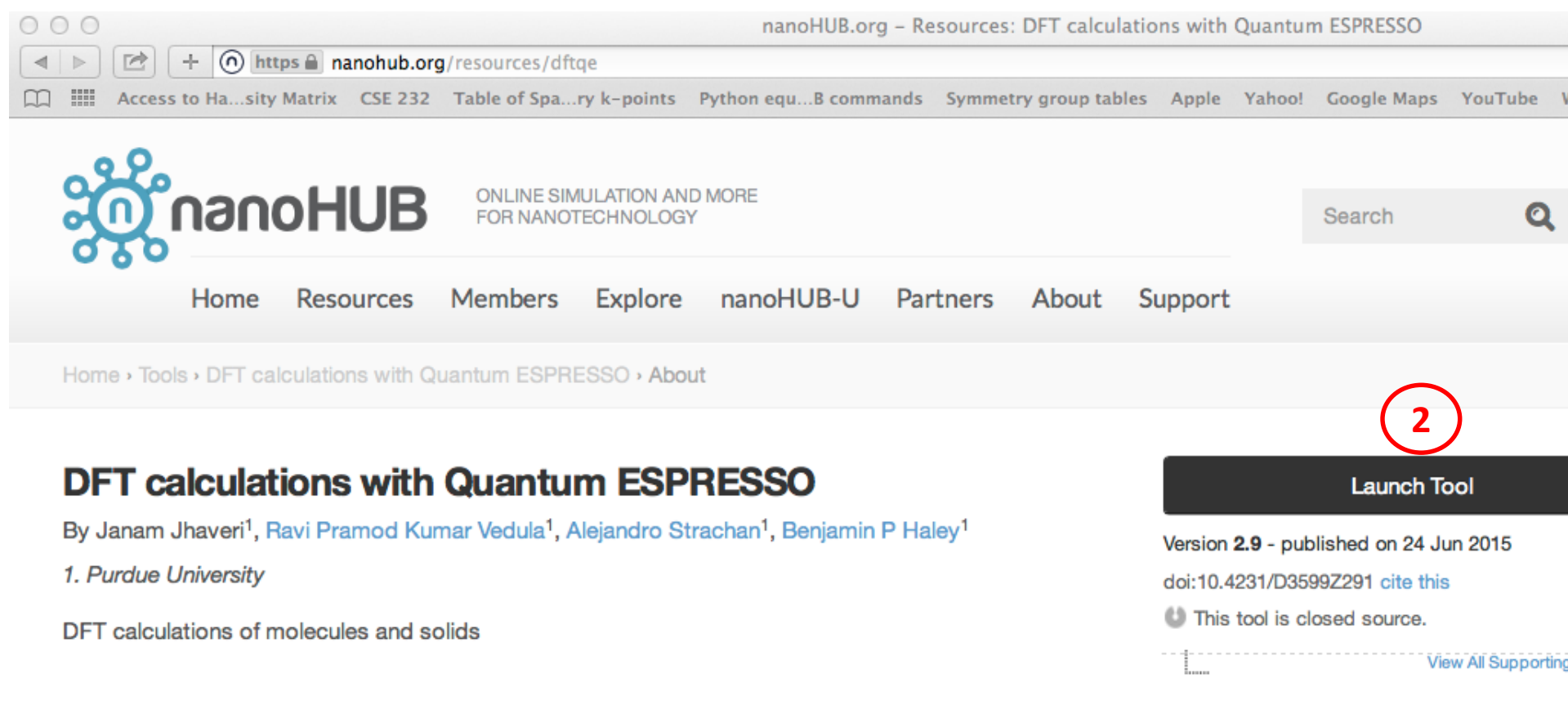
Section 1: Generating the Quantum ESPRESSO output on nanoHub.org

You can skip to Section 2 if you use VASP or if you use Quantum ESPRESSO in Unix.

* If you use QE in Unix, start from slide 12.

1) ab initio calc.: QE on nanoHub for simplicity


1. Open <https://nanohub.org/resources/dftqe>
2. Select Launch Tool




The screenshot shows a web browser window with the URL <https://nanohub.org/resources/dftqe>. The page title is "nanoHUB.org - Resources: DFT calculations with Quantum ESPRESSO". The nanoHUB logo is visible, along with the tagline "ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY". A search bar is present in the top right. The navigation menu includes "Home", "Resources", "Members", "Explore", "nanoHUB-U", "Partners", "About", and "Support". The breadcrumb trail is "Home > Tools > DFT calculations with Quantum ESPRESSO > About". The main heading is "DFT calculations with Quantum ESPRESSO", followed by the authors: "By Janam Jhaveri¹, Ravi Pramod Kumar Vedula¹, Alejandro Strachan¹, Benjamin P Haley¹". The affiliation is "1. Purdue University". The description is "DFT calculations of molecules and solids". On the right side, there is a "Launch Tool" button circled in red, with the number "2" inside the circle. Below the button, it says "Version 2.9 - published on 24 Jun 2015", "doi:10.4231/D3599Z291 cite this", and "This tool is closed source." A link for "View All Supporting" is partially visible at the bottom right.


- You need to sign-in using one of the following methods or simply signup in the website free of charge.


Login




Choose your sign in method:

 With an affiliated institution: ▾

 Sign in with Facebook >

 Sign in with Google >

 Sign in with LinkedIn >

— or —

Sign in with your nanoHUB.org account

- Leave the first tab as default. It should look like the one below

DFT calculations with Quantum ESPRESSO

⚙️ Terminate ▶️ Keep for later

1 Input → 2 Simulate [? About this tool Questions?](#)

Input Geometry | Energy Expression | Phonons | Band Structure/DOS | Advanced Options

Create the model

Premade atomistic structure: Si diamond

Atomic Coordinates: Fractional

Structure type: cubic F (fcc)

Title of Run: Silicon band structure

Atomic Structure:
2
Silicon diamond structure
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25

Cell Vectors (A):
-2.715 2.715 0.000
-2.715 0.000 2.715
0.000 2.715 2.715

Lattice Parameter "a" (A): 5.43

Ratio Lattice Parameters "b/a": 1

Ratio Lattice Parameters "c/a": 1

1. Change the number of kpoints to 20 in each direction (see below)

- Input Geometry
- Energy Expression
- Phonons
- Band Structure/DOS
- Advanced Options

Exchange and Correlation functional: LDA
Relax: No

K-grid spacing (Reciprocal-space)

X direction: 20
Y direction: 20 **1**
Z direction: 20

Number of bands: 8
Wavefunction Kinetic Energy cutoff (Ry): 16.0
Charge Density Kinetic Energy cutoff (Ry): 96.0
SCF Convergence Criterion (Ry): 1E-6
SCF maximum steps: 100 [+ -]
Enable occupation options: yes

Occupations Options

Occupation: tetrahedra
Smearing: Gaussian
Gaussian Spreading (Ry): 0

1. Choose not to calculate the band structure or density of states (DOS)
2. Simulate

The screenshot shows the Quantum ESPRESSO web interface. At the top, the title is "DFT calculations with Quantum ESPRESSO". There are three buttons: a gear icon, "Terminate", and "Keep for later". Below the title bar, there are two steps: "1 Input" and "2 Simulate". A green question mark icon is labeled "About this tool Questions?". The main content area has five tabs: "Input Geometry", "Energy Expression", "Phonons", "Band Structure/DOS", and "Advanced Options". Under the "Band Structure/DOS" tab, there are two rows of controls:

- "Band Structure Calculations: ● no" (The is circled in red with the number 1.)
- "Density of States Calculations: ● no" (The is circled in red with the number 1.)


At the bottom right, there is a "Simulate >" button, which is circled in red with the number 2.

1. Select the download button to download the output

DFT calculations with Quantum ESPRESSO

⚙️ Terminate ▶▶ Keep for later

1 Input → 2 Simulate 🗨️ About this tool Questions?

Result: SCF Output Log 

```
Program PWSCF      v.4.1.1  starts ...
  Today is  2Nov2015 at 12:14:21

  Parallel version (MPI)

  Number of processors in use:      1



  For Norm-Conserving or ultrasoft (Vanderbilt) Pseudopotentials or PAW

  Current dimensions of program pwscf are:
  Max number of different atomic species (ntypx) = 10
  Max number of k-points (npk) = 40000
  Max angular momentum in pseudopotentials (lmaxx) = 3
  Waiting for input...

  Subspace diagonalization in iterative solution of the eigenvalue problem:
  Too few procs for parallel algorithm
  we need at least 4 procs per pool
  a serial algorithm will be used

  Planes per process (thick) : nr3 = 24 npp = 24 ncplane = 576
  Planes per process (smooth): nr3s= 20 npps= 20 ncplanes= 400

  Proc/  planes cols      G      planes cols      G      columns      G
  Pool   (dense grid)    (smooth grid)    (wavefct grid)
  1      24      349      4285    20      235      2277      85      531
```

Find:   Select All

1. In the popped-up window, you may need to scroll down to see the “Save As ...” button.
2. Click on the “Save As ...” button and choose where you want to download the output file.

The screenshot displays the nanoHUB.org interface for DFT calculations with Quantum ESPRESSO. The main window shows a terminal output for the 'SCF Output Log'. The output text includes:

```
Program PWSCF v.4.1.1 starts ...
Today is 2Nov2015 at 12:14:21

Parallel version (MPI)

Number of processors in use: 1

For Norm-Conserving or ultrasoft (Vanderbilt) pseudopotentials:
Current dimensions of program pwscf are:
Max number of different atomic species (nat) = 100
Max number of k-points (npk) = 40000
Max angular momentum in pseudopotentials (lmax) = 10
Waiting for input...

Subspace diagonalization in iterative solution of the eigenvalue problem:
Too few procs for parallel algorithm
we need at least 4 procs per pool
a serial algorithm will be used

Planes per process (thick) : nr3 = 24 npp = 24 ncplane = 576
Planes per process (smooth): nr3s= 20 npps= 20 ncplanes= 400

Proc/ planes cols 6 planes cols 6 columns 6
Pool (dense grid) (smooth grid) (wavefct grid)
1 24 349 4285 20 235 2277 85 531
```

Overlaid on the terminal is a 'nanoHUB.org' banner with the text 'ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY' and 'an ncn project'. Below the banner are two buttons: 'Save As...' and 'Print...'. The 'Save As...' button is circled in red with the number '2'. The 'Print...' button is circled in red with the number '1'. A red 'X' icon is visible in the top right corner of the banner area.

1. Download “QE-to-VASP.py” python code from here:
<https://nanohub.org/resources/amobt/supportingdocs>
2. Once “QE-to-VASP.py” and your QE output file (which we call “SCFOutputLog.txt” here) in the same folder run the python code as follows:

```
python QE-to-VASP.py -f SCFOutputLog.txt
```

or basically:

```
python QE-to-VASP.py -f your_QE_output_file
```

This should generate the EIGENVAL and OUTCAR files which contain information regarding the lattice dimensions and its volume. These two files are minimum requirements for aMoBT for calculating the mobility and Seebeck coefficient (next section).

3. If you don't have python, you can download the resulting EIGENVAL and OUTCAR from the following links to continue this example:

<https://www.dropbox.com/s/8v0l4a3xecmhb1b/EIGENVAL?dl=0>

<https://www.dropbox.com/s/ka025rbtf1r3uvj/OUTCAR?dl=0>

Section 2: Calculating the mobility and Seebeck coefficient using aMoBT

It is assumed in this section that you have the EIGENVAL and OUTCAR files ready for upload.

2) aMoBT calculations

1. Open <https://nanohub.org/tools/amobt>
2. Select Launch Tool

ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation

By [Alireza Faghaninia](#)¹, [Joel Ager](#) (editor)², [Cynthia S Lo](#) (editor)¹

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ab initio electronic transport model to calculate low-field electrical mobility and Seebeck coefficient of semiconductors in Boltzmann transport framework.

2

Launch Tool

Version 2.1.0 - published on 29 Oct 2015

doi:10.4231/D38C9R524 [cite this](#)

 This tool is closed source.

[View All Supporting Documents](#)

About

Usage

Citations

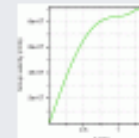
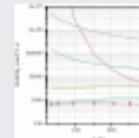
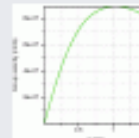
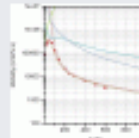
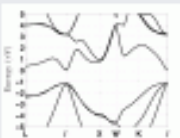
Questions

Reviews

Wishlist


Versions

Supporting Docs





1. You need to sign-in using one of the following methods or simply signup in the website free of charge.


Login




Choose your sign in method:

 With an affiliated institution: ▾

 Sign in with Facebook >

 Sign in with Google >

 Sign in with LinkedIn >

— or —

Sign in with your nanoHUB.org account

1. From the “Material” drop-down menu, select “New”

The screenshot shows the 'ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation' interface. At the top right, there are icons for settings, 'Terminate', and 'Keep for later'. Below the title bar, the 'Material:' dropdown menu is open, showing 'GaAs_example.xml' as the current selection. The dropdown list includes 'New 1' (circled in red), 'Upload...', 'Download', '---', 'n-GaAs example', 'n-InN example', and 'n-ZnS example'. To the right of the dropdown is a yellow bar with a 'Simulate' button, 'new input parameters' text, and a 'Questions?' link. Below this is the 'aMoBT' description and a 'Simulate' button. The main form contains various input fields: 'Compare to experiment?' (radio buttons for 'no'), 'Maximum number of iterations to obtain g:' (input field with '6' and +/- buttons), 'Free electron DOS?' (radio buttons for 'no'), 'k-point of CBM/VBM for n-/p-type conductivity:' (input field with '0.0 0.0 0.0'), 'Polar optical phonon frequency, w_{po} (THz):' (input field with '8.16'), 'Static dielectric:' (input field with '12.18'), 'High-frequency dielectric:' (input field with '10.32'), 'Deformation potential, E_d (eV):' (input field with '6.04eV'), 'Piezoelectric coefficient, P:' (input field with '0.081'), 'Dislocation density, N_{dis} (1/cm²):' (input field with '0.1'), 'Carrier concentration, n (1/cm³):' (input field with '3e+13'), and 'Experimental data for mobility:' (input field with '4.5 92557;'). At the bottom, there is a 'Storage (manage)' bar showing '35% of 10GB' and system icons for power, refresh, and zoom (824 x 479).



ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation

Material: Uploaded data

- New
- Upload... **1**
- Download
-
- n-GaAs example
- n-InN example
- n-ZnS example

Simulate

aMoBT

ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation. This model that uses Boltzmann Transport Equation (BTE) to obtain the electron distribution function. Current transport as well as charge carrier scattering are included in the model. For more information, see the paper by Ager, and C. S. G. 235123, Jun 2008.

Compare to experiment?: no

Iterations to obtain g: + -

Free electron DOS?: yes

n/p-type conductivity:

Frequency, w_po (THz):

Static dielectric:

High-frequency dielectric:

Deformation potential, Ed (eV):

Piezoelectric coefficient, P:

Dislocation density, Ndis (1/cm2):

Carrier concentration, n (1/cm3):

Experimental data for mobility:

Exp. data for Seebeck coeff.:

EIGENVAL:

PROCAR:

OUTCAR:

DOSCAR:

1. Select "Upload ..." from the "Material" drop-down
2. Choose EIGENVAL file
3. Choose OUTCAR file
4. Upload

Material: Upload...

ab initio band structure and density of states: Upload...

! Upload starting... A web browser page should pop up from this site to handle the upload operation. If the upload form doesn't pop ups from this site, you may have trouble with the version of the browser. Support area for details.

Maximum number of files: 10

k-point of CBM/VBM for n-/p-type conductivity: 0.0

Polar optical phonon frequency, w_po (THz): 10

Static dielectric: 10

High-frequency dielectric: 5

Deformation potential, Ed (eV): 5eV

Piezoelectric coefficient, P: 0.15

Dislocation density, Ndis (1/cm2): 0.1

Carrier concentration, n (1/cm3): 1e+16

Experimental data for mobility: 300 100

Exp. data for Seebeck coeff.: 1e16 -100

EIGENVAL:

PROCAR:

OUTCAR:

DOSCAR:

nanoHUB.org ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

Upload

Use this form to upload data for ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation. If you don't specify a file for a particular input, that input won't be modified by the Upload operation.

EIGENVAL:

Upload a file Copy/paste text

2 Choose File

PROCAR:

Upload a file Copy/paste text

Choose File

OUTCAR:

Upload a file Copy/paste text

3 Choose File

DOSCAR:

Upload a file Copy/paste text

Choose File

4 Upload

1. Select “Type of the conductivity” to be :
“p-type”
2. Optical phonon frequency at Γ : 15.23 THz
 - Calculated via DFPT(VASP)+Phonopy
3. Static dielectric: 12.02
 - Calculated via DFPT(VASP)
4. High frequency dielectric: 11.66 (=12.02x(15/15.23)^2)
 - Calculated via Lyddane–Sachs–Teller relation: $(\omega_{LO}/\omega_{TO})^2 = \epsilon_s/\epsilon_\infty$
5. Carrier Concentration: 1e14
6. Leave the rest to default
7. Simulate

Material:

ab initio band structure and density of states:

Type of the conductivity: 1

Type of formulation:

Temperature, T (K):

Compare to experiment?: no

Maximum number of iterations to obtain g: + -

Free electron DOS?: yes

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

Polar optical phonon frequency, w_po (THz): 2

Static dielectric: 3

High-frequency dielectric: 4

Deformation potential, Ed (eV):

Piezoelectric coefficient, P:

Dislocation density, Ndis (1/cm2):

Carrier concentration, n (1/cm3): 5

Experimental data for mobility:

Exp. data for Seebeck coeff.:

EIGENVAL:

2	2	1	1
0.2376594E+02	0.40		
65993E-09	0.4065993E		

PROCAR:

OUTCAR:

DOSCAR:

Simulate

7

aMoBT

ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport equation (3:5). This model solves the Boltzmann Transport Equation (BTE) to obtain the carrier distribution as a function of energy and momentum. It takes into account the piezoelectric effect and the polar optical phonon scattering. For more information, see the paper by C. S. Lo, Phys. Rev. B, 2014.

- The calculation should finish in about 53 seconds
 - The hole mobility of Si is 450 cm²/V.s at 300K
1. Use the drop-down menu to see other outputs (e.g. group velocity)

ab initio Model for Mobility and Seebeck coefficient using Boltzmann Transport (aMoBT) equation

Material: Uploaded data

Use this to load examples.

ab initio band structure and density of states: Uploaded data

Type of the conductivity: p-type

Type of formulation: automatic

Temperature, T (K): 300K

Compare to experiment?: no

Maximum number of iterations to obtain g: 6

Free electron DOS?: yes

k-point of CBM/VBM for n-/p-type conductivity: 0.0 0.0 0.0

Polar optical phonon frequency, w_po (THz): 15.23

Static dielectric: 12.02

High-frequency dielectric: 11.66

Deformation potential, Ed (eV): 5eV

Piezoelectric coefficient, P: 0.15

Dislocation density, Ndis (1/cm2): 0.1

Carrier concentration, n (1/cm3): 1e+14

Experimental data for mobility: 300 100

1e+16 100

Simulate

About this tool Questions?

Result: Mobility (cm2/V.S) **1**

Mobility (cm2/V.S)

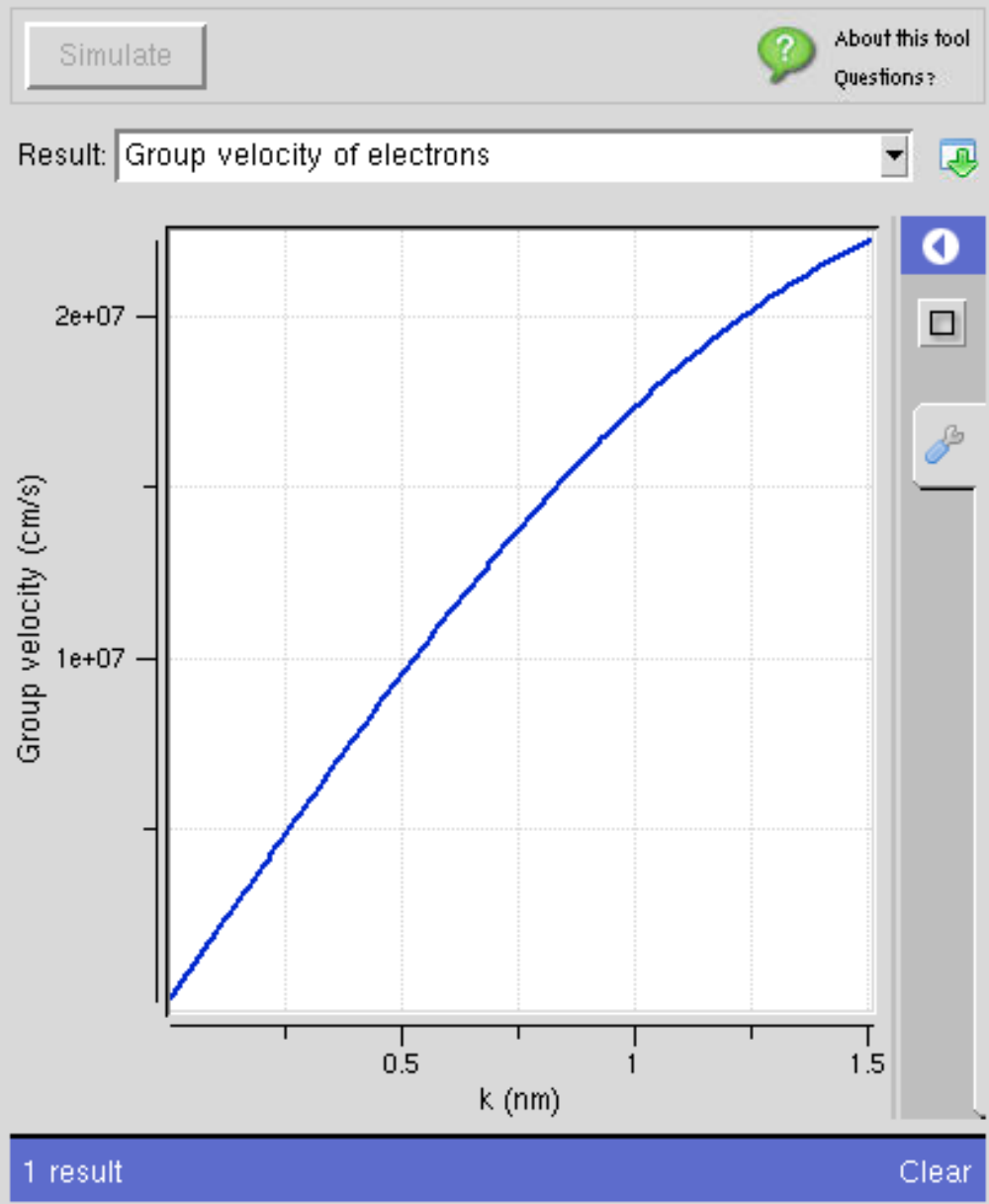
#2 Simulation

1 result Clear

Storage (manage) 46% of 10GB

986 x 507

- You can use a similar procedure to calculate the mobility and Seebeck coefficient of other semiconductors.
- The output depends on the accuracy of the calculated band structure and other properties such as phonon frequencies and dielectric constants.
- Questions? please see the manual <https://nanohub.org/resources/amobt/supportingdocs> or contact alireza@wustl.edu



Simulate ? About this tool Questions?

Result: Output ↓

```

Iteration 4 in BTE: at T = 300.00 K. Average change in g_2 = 2.993
Iteration 5 in BTE: at T = 300.00 K. Average change in g = 3.14975
Iteration 5 in BTE: at T = 300.00 K. Average change in g_2 = 9.923
Iteration 6 in BTE: at T = 300.00 K. Average change in g = 1.62411
Iteration 6 in BTE: at T = 300.00 K. Average change in g_2 = 2.800
mobility = 519.694845224375
sigma = 0.00832642904568270

Hole concentration = 1.00e+14 in cm^-3
N_dis = 0.10000000000000000
mobility = 519.694845224375
thermopower = 1137.68849777640

Total Simulation Time: 53 seconds
  
```

Find: ↓ ↑ Select All

1 result Clear