

Transport Properties of Graphene on Hexagonal Boron Nitride

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MSE 690

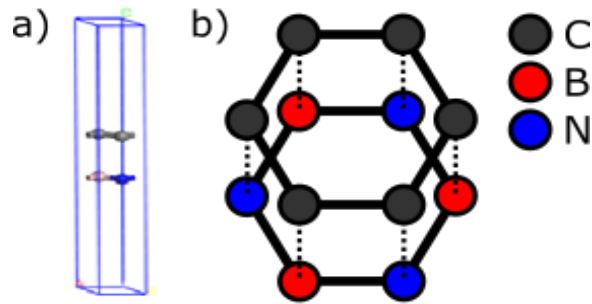
PROF. ALE STRAHAN

Work Flow

Step 1

Input Structure

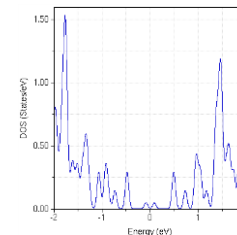
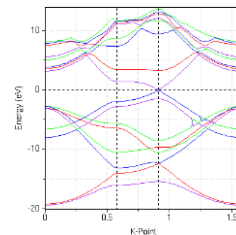
- Atomic Structure (Fractional or Cartesian)
- Cell Vectors (\AA)



Step 2

DFT Calculations (DFT MatProp)

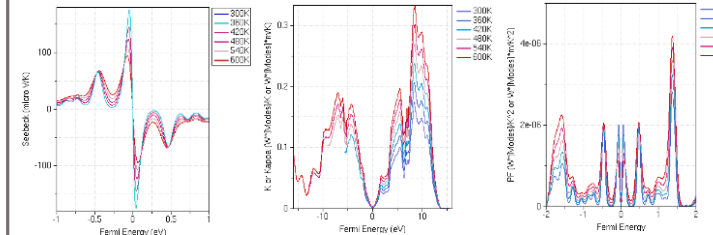
- Band Diagrams
- Density of States
- Input Data for LanTraP



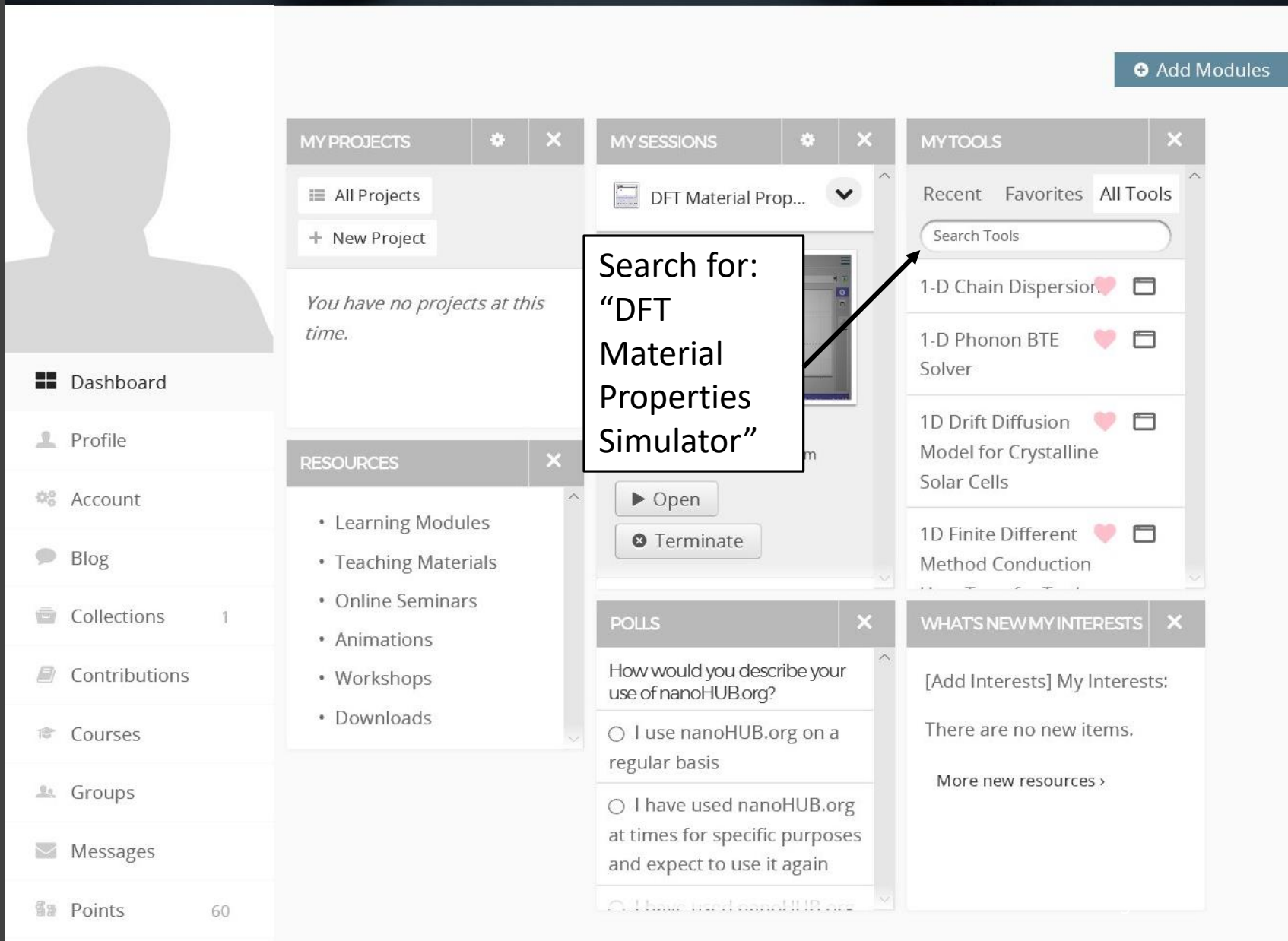
Step 3

Landauer Transport (LanTraP)

- Seebeck Coefficient (S)
- Conductivity (σ)
- Power Factor (PF)



First Part: DFT



The screenshot displays the nanoHUB user interface with several panels:

- MY PROJECTS:** Contains 'All Projects' and 'New Project' buttons. A message states: "You have no projects at this time."
- MY SESSIONS:** Shows an active session titled "DFT Material Prop..." with "Open" and "Terminate" buttons.
- MY TOOLS:** A search results panel with a search bar and a list of tools:
 - 1-D Chain Dispersion
 - 1-D Phonon BTE Solver
 - 1D Drift Diffusion Model for Crystalline Solar Cells
 - 1D Finite Different Method Conduction
- RESOURCES:** A list of resource categories including Learning Modules, Teaching Materials, Online Seminars, Animations, Workshops, and Downloads.
- POLLS:** A poll titled "How would you describe your use of nanoHUB.org?" with options for regular use, occasional use, and no use.
- WHAT'S NEW MY INTERESTS:** A section for tracking new items, currently showing "There are no new items."

A callout box with the text "Search for: 'DFT Material Properties Simulator'" has an arrow pointing to the search bar in the MY TOOLS panel.

1 Input → 2 Simulate

Basic Input | Geometric Input | Energy Expression | Band Structure/DOS | Dielectric

Task: Thermoelectric Calculations

Material Type: Semiconductor

Semiconductors: Graphite

Advanced Options: yes

1-Click DFT

Simu

Select:
"Thermoelectric
Calculations"

Enable Advanced
Options

Select the following:
Material Type: Semiconductor
Semiconductors: Graphite

Define Basic Inputs

1 Input → 2 Simulate

Basic Input | **Geometric Input** | Energy Expression | Band Structure/DOS | Dielectric

Atomic Structure:

C	0.333330044	0.666670085	0.580000019
C	0.666670034	0.333330023	0.580000019
N	0.333330044	0.666670085	0.419999981
B	0.666670034	0.333330023	0.419999981

Cell Vectors (A):

2.4684000015	0.0000000000	0.0000000000
-1.2342000008	2.1376971080	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Equation of State Calculations: no

Advanced Options: yes

Fill with data shown here

No need to enable

Define Geometric Input

1 Input → 2 Simulate

Basic Input | Geometric Input | Energy Expression | Band Structure/DOS | Dielectric

Exchange and Correlation functional: LDA
Relax: No

Number of K-Points
X direction: 30
Y direction: 30
Z direction: 1

Number of K-Points (for Non-Self Consistent Field Calculation)
X direction: 30
Y direction: 30
Z direction: 1

Wavefunction Kinetic Energy cutoff (Ry): 40.0
Charge Density Kinetic Energy cutoff (Ry): 160.0
SCF Convergence Criterion (Ry): 1E-6
SCF maximum steps: 100
Enable occupation options: yes

Occupations Options
Occupation: smearing
Smearing: Gaussian
Gaussian Spreading (Ry): .0038

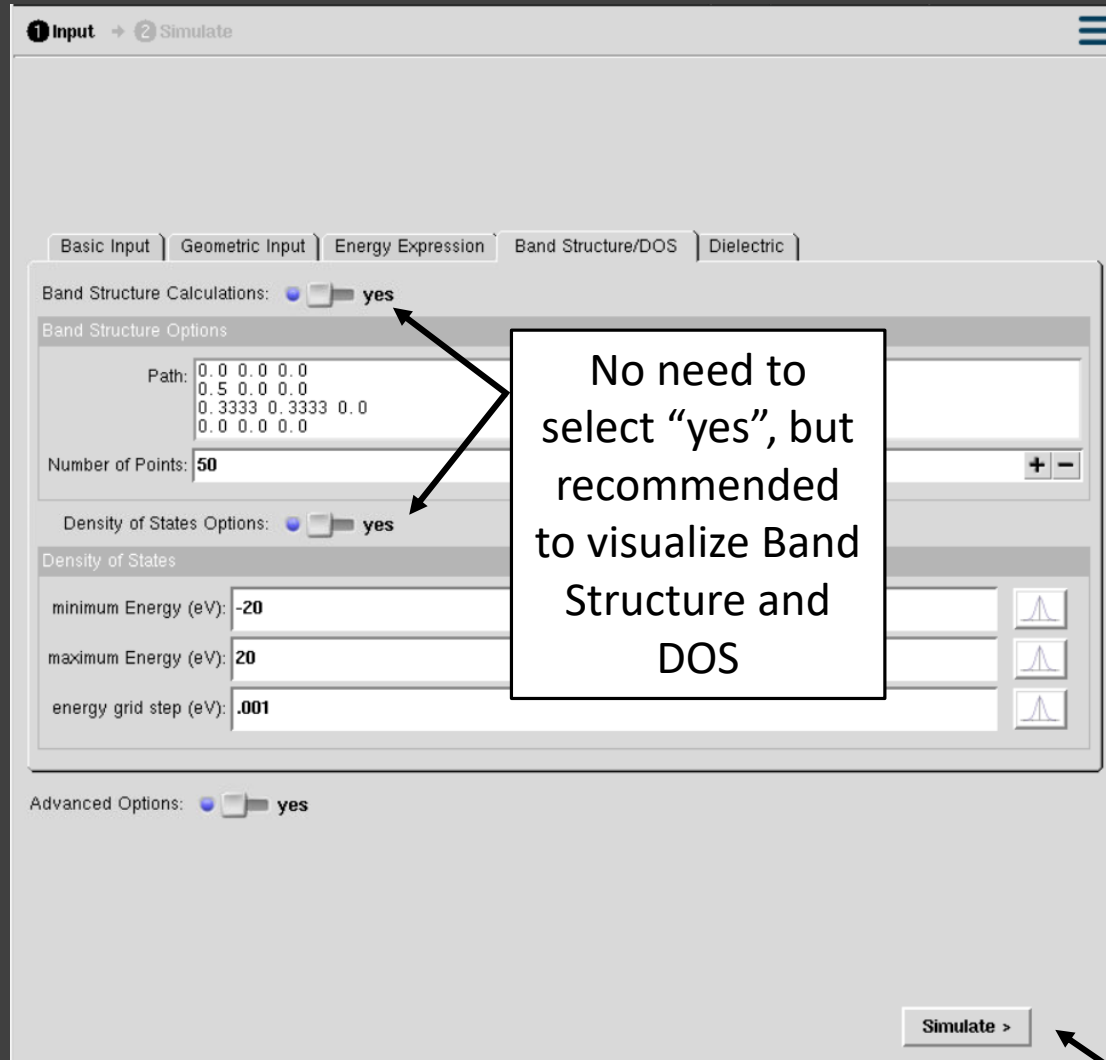
Simulate >

Select "LDA"

Set Both Z directions to "1"

Set to "1E-5"

Energy Expression



No need to select “yes”, but recommended to visualize Band Structure and DOS

Press “Simulate to Begin”

Final Step and RUN

Be Warned: Simulation may take more than 30 Mins.

For a more in-Depth tutorial into Band Structure and DOS, consult Shukai Yao’s presentation.

1 Input → 2 Simulate

Result: File for Thermoelectric Calculations

Select: "File for Thermoelectric Calculations"

Click here to Download. A pop-up will appear.

```

-16.0701 -14.0477 -13.1417 -10.4721 -6.44 -5.6745 -2.7984 -1.9537 1.4466 3.4791 7.3568 8.6718 11.1034 1
-16.0761 -14.1537 -12.9921 -10.4316 -6.5161 -5.7275 -2.8142 -1.9616 1.4964 3.5181 7.4754 8.7514 10.7817
-16.0932 -14.3627 -12.655 -10.3186 -6.745 -5.8996 -2.8676 -1.9963 1.6417 3.6274 7.8198 8.9642 10.4303 10
-16.1178 -14.5716 -11.7669 -9.9066 -7.5389 -6.4781 -3.0158 -2.0945 2.1086 3.9874 9.0406 9.3408 9.9907 10
-16.1455 -14.7542 -11.2761 -9.6411 -8.0313 -6.8246 -3.0862 -2.141 2.3568 4.1832 9.2344 9.7888 9.9039 10
-16.1714 -14.8939 -10.7985 -9.3853 -8.5179 -7.1377 -3.1384 -2.1748 2.5591 4.3435 9.1586 9.6537 9.9241 10
-16.1912 -14.9885 -10.1034 1 -11.7669 -9.9066 -7.5389 -6.4781 -3.0158 -2.0945 2.1086 3.9874 9.0406 9.3408 9.9907 10
-16.2019 -15.0364 -10.4316 -6.5161 -5.7275 -2.8142 -1.9616 1.4964 3.5181 7.4754 8.7514 10.7817
-16.2019 -15.0364 -10.4316 -6.5161 -5.7275 -2.8142 -1.9616 1.4964 3.5181 7.4754 8.7514 10.7817
-16.1912 -14.9885 -10.1034 1 -11.7669 -9.9066 -7.5389 -6.4781 -3.0158 -2.0945 2.1086 3.9874 9.0406 9.3408 9.9907 10
-16.1714 -14.8939 -10.7985 -9.3853 -8.5179 -7.1377 -3.1384 -2.1748 2.5591 4.3435 9.1586 9.6537 9.9241 10
-16.1456 -14.7541 -11.7669 -9.9066 -7.5389 -6.4781 -3.0158 -2.0945 2.1086 3.9874 9.0406 9.3408 9.9907 10
-16.1179 -14.5736 -12.2346 -10.14 -7.0961 -6.1562 -2.938 -2.0431 1.857 3.7924 8.3615 9.2148 10.1783 10.4
-16.0932 -14.3627 -12.655 -10.3186 -6.745 -5.8996 -2.8676 -1.9963 1.6417 3.6274 7.8198 8.9642 10.4303 10
-16.0761 -14.1535 -12.9921 -10.4316 -6.5161 -5.7275 -2.8142 -1.9616 1.4964 3.5181 7.4754 8.7514 10.7817
-16.0701 -14.0475 -13.142 -10.4722 -6.4398 -5.6743 -2.7981 -1.9537 1.4466 3.4791 7.3568 8.6718 11.1034 1
-16.0761 -14.1535 -12.9921 -10.4316 -6.5161 -5.7275 -2.8142 -1.9616 1.4964 3.5181 7.4754 8.7514 10.7817
-16.0932 -14.3627 -12.655 -10.3186 -6.745 -5.8996 -2.8676 -1.9963 1.6417 3.6274 7.8198 8.9642 10.4303 10
-16.1179 -14.5736 -12.2346 -10.14 -7.0961 -6.1562 -2.938 -2.0431 1.857 3.7924 8.3615 9.2148 10.1783 10.4
-16.1456 -14.7541 -11.7669 -9.9066 -7.5389 -6.4781 -3.0158 -2.0945 2.1086 3.9874 9.0406 9.3408 9.9907 10
-16.1714 -14.8939 -11.2761 -9.6411 -8.0313 -6.8246 -3.0862 -2.141 2.3568 4.1832 9.2344 9.7888 9.9039 10
-16.1912 -14.9885 -10.7985 -9.3853 -8.5179 -7.1377 -3.1384 -2.1748 2.5591 4.3435 9.1586 9.6537 9.9241 10

```

Find:

4 results

Simulation = #3

Task: Thermoelectric Calculations

task = lantrap
 SCF Convergence Criterion (Ry) = 1E-5
 Band Structure Calculations = yes
 Density of States Options = yes
 minimum Energy (eV) = -20
 energy grid step (eV) = .001
 Atomic Structure: = C 0.333330044 0.666670085 0.580000019 C 0.666670034 0.333330023 0.5800000

Obtaining Input File

Save File on your Computer

nanoHUB

```

-16.0701 -14.0477 -13.1417 -10.4721 -6.44 -5.6745 -2.7984
-1.954 1.445 3.4795 7.3569 8.6719 11.1034 11.3387 11.5623
11.6832
-16.0761 -14.1537 -12.9918 -10.4316 -6.5163 -5.7277 -2.8144
-1.9619 1.4968 3.5184 7.4755 8.7514 10.7817 11.1403 11.4279
11.6902

```


LanTraP

Objectives:

- Determine the Transport Properties of G-hBN bilayer.
 - Seebeck Coefficient (S)
 - Conductivity (σ)
 - Power Factor (PF)

Second Part: LanTraP

+ Add Modules



- Dashboard
- Profile
- Account
- Blog
- Collections 1
- Contributions
- Courses
- Groups
- Messages
- Points 60

MY PROJECTS ⚙️ ✕

All Projects

+ New Project

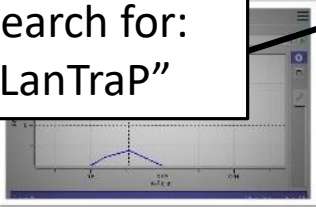
You have no projects at this time.

RESOURCES ✕

- Learning Modules
- Teaching Materials
- Online Seminars
- Animations
- Workshops
- Downloads

MY SESSIONS ⚙️ ✕

DFT Material Prop... ▼



LAST ACCESSED:
December 04, 2018 @ 8:48pm

▶ Open

✕ Terminate

POLLS ✕

How would you describe your use of nanoHUB.org?

I use nanoHUB.org on a regular basis

I have used nanoHUB.org at times for specific purposes and expect to use it again

MY TOOLS ✕

Recent Favorites All Tools

Search Tools

1-D Chain Dispersion ❤️ 🗑️

1-D Phonon BTE Solver ❤️ 🗑️

1D Drift Diffusion Model for Crystalline Solar Cells ❤️ 🗑️

1D Finite Different Method Conduction ❤️ 🗑️


WHAT'S NEW MY INTERESTS ✕

[Add Interests] My Interests:

There are no new items.

[More new resources >](#)

Search for:
"LanTraP"



1 Load Data → 2 Modes Options → 3 TE Options → 4 Simulate

Upload:

Data file (E-k or modes): [Placeholder: d your data will show up here.]

Select: "Upload"
A pop-up will appear to upload your file

Select: "Modes and TE"

What to calculate: Modes

Modes Options >

Upload Input File

nanoHUB

Upload

Use this form to upload data for LanTraP. If you don't specify a file for a particular input, that input won't be modified by the *Upload* operation.

Data file (E-k or modes):

Upload a file Copy/paste text

Browse for your DFT file and Upload

1 Load Data → 2 Modes Options → 3 TE Options → 4 Simulate

Allow Mode Options

Monkhorst-Pack k-grid?: yes

Dimensionality: 2

Lx (nm): 1

Ly (nm): 1

Lz (nm): 1

Number of kx points: 30 + -

Number of ky points: 30 + -

Number of kz points: 1 + -

Number of Bands: 16 + -

Transport direction: X

Spin Degeneracy: 1

Emin (eV): -20eV

dE (eV): 0.001eV

Emax (eV): 20eV

< Load Data

TE Options >

Set values as shown on the picture.

Modes Options

1 Load Data → 2 Modes Options → 3 TE Options → 4 Simulate

TE

Particle: Electron

Temperature (K): 300K

Transport type: Ballistic

Electron Options

Ef min (eV): -16eV

delta Ef (eV): 0.001eV

Ef Max (eV): 16eV

< Modes Options

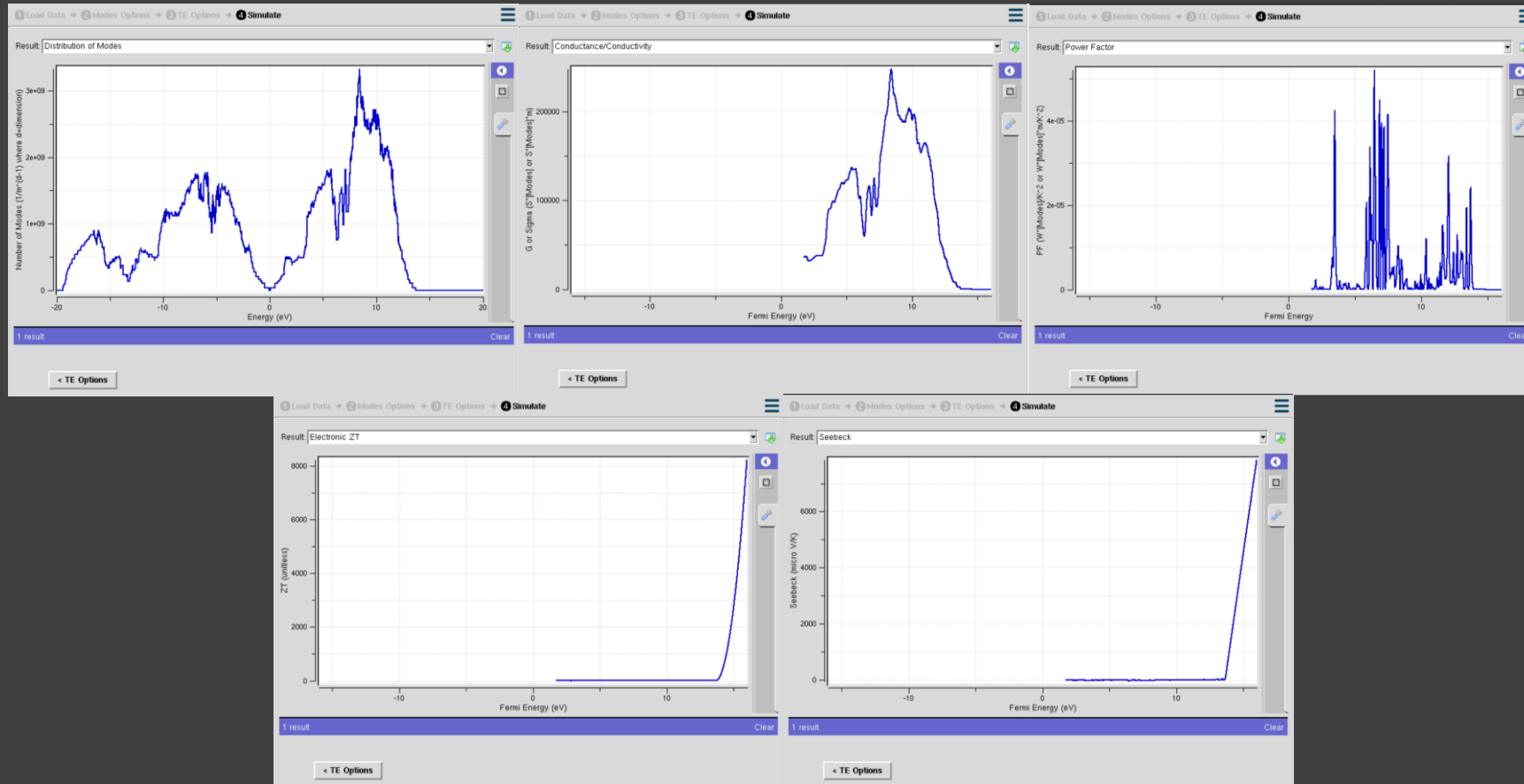
Simulate >

Set values to $\pm 16\text{eV}$
Make sure values are always lower than Emin/Emax From Modes Options

TE Options

Press "Simulate to Begin"

Visualizing Transport Properties



Further Work

- Study the effects of Interplanar Distance, Temperature, and layer stacking to the transport properties of materials.
- Study other 2D materials.
- Study Phonon ballistic transport