Transport Properties of Graphene on Hexagonal Boron Nitride

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MSE 690

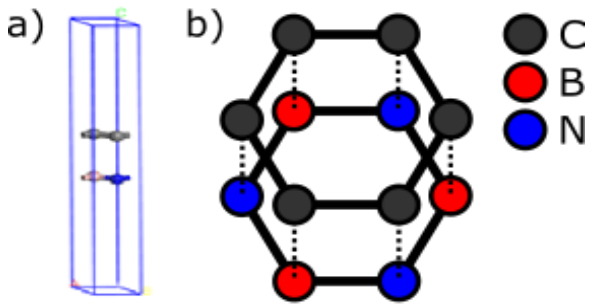
PROF. ALE STRAHAN

Work Flow

Step 1

Input Structure

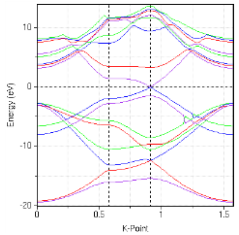
- Atomic Structure (Fractional or Cartesian)
- Cell Vectors (Å)

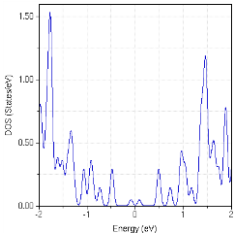


Step 2

DFT Calculations (DFT MatProp)

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

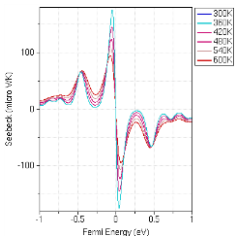


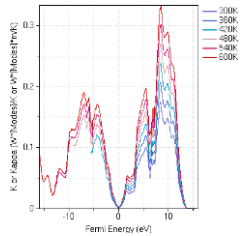


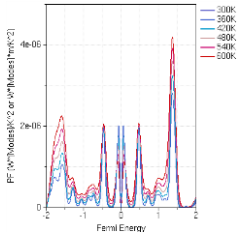
Step 3

Landauer Transport (LanTraP)

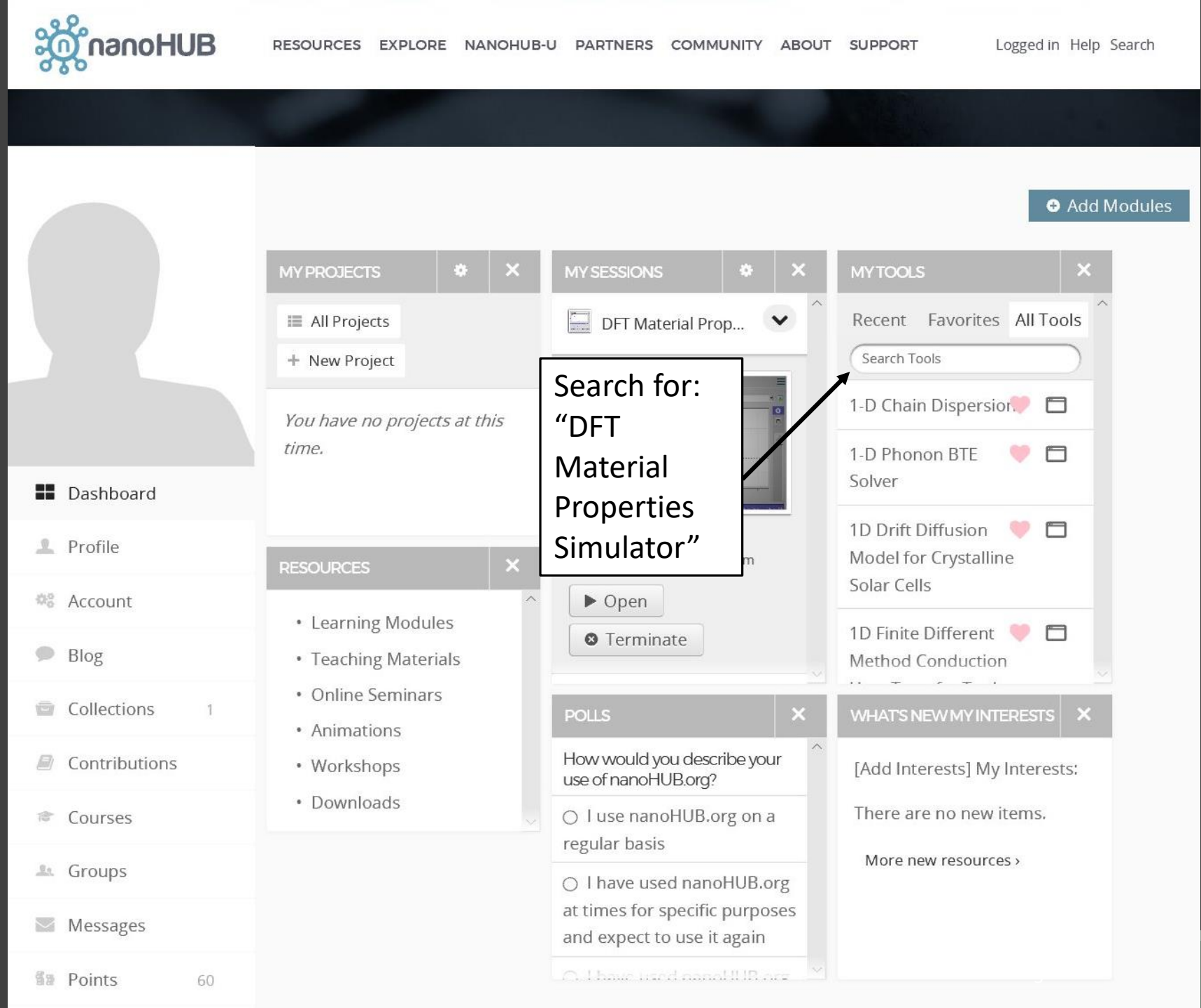
- Seebeck Coefficient (S)
- Conductivity (σ)
- Power Factor (PF)







First Part: DFT



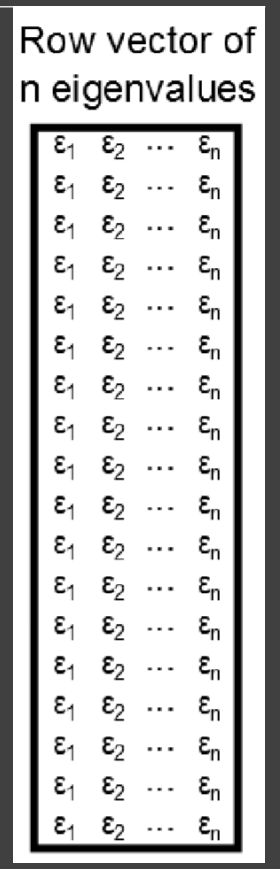
Density Functional Theory (DFT)

Objectives:

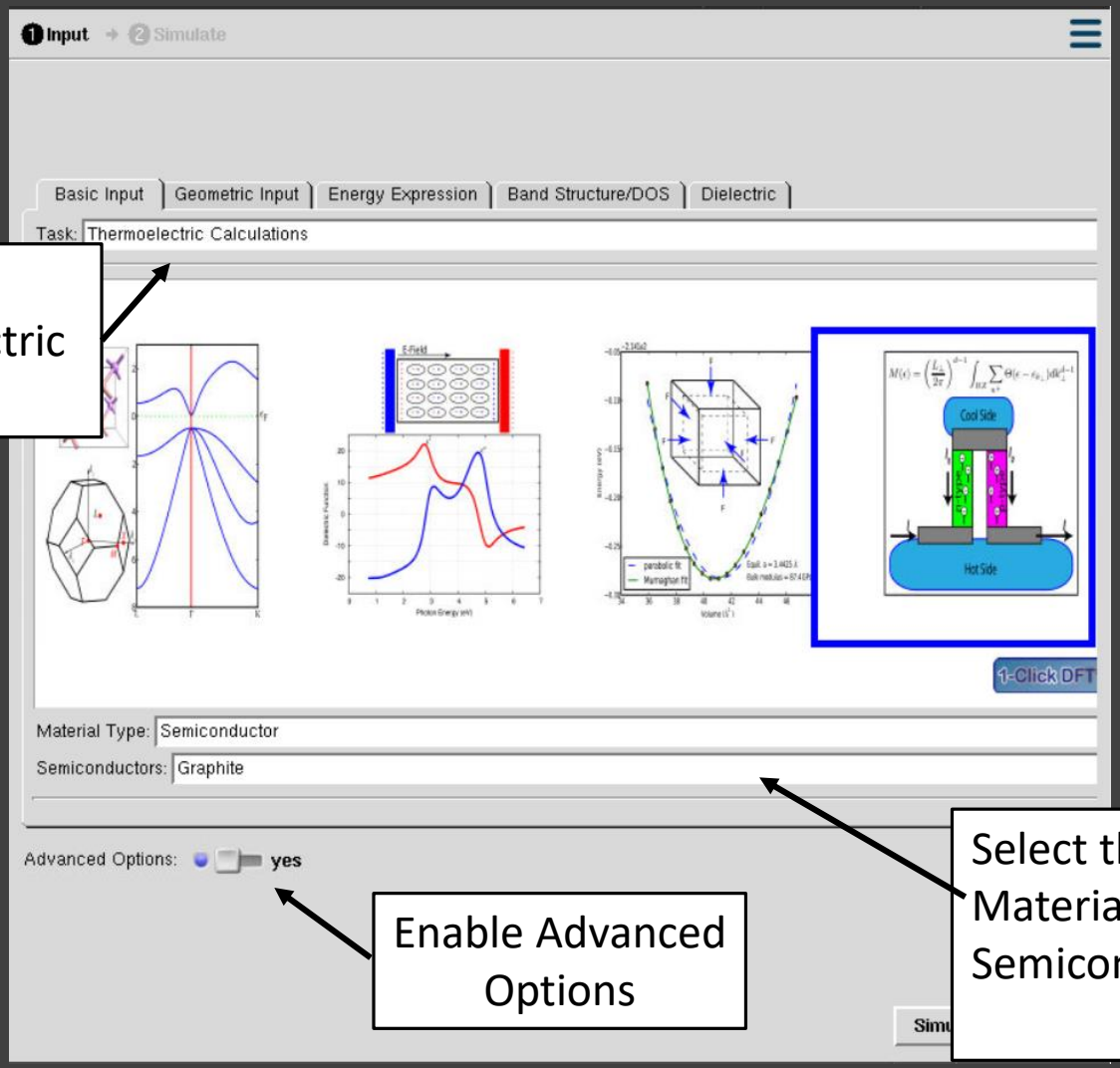
- Compute the band diagrams and electronic density of states for the G-hBN Bilayer
- Obtain input file to work with LanTraP

Approach:

- Perform DFT calculations using the Local Density Approximation (LDA)



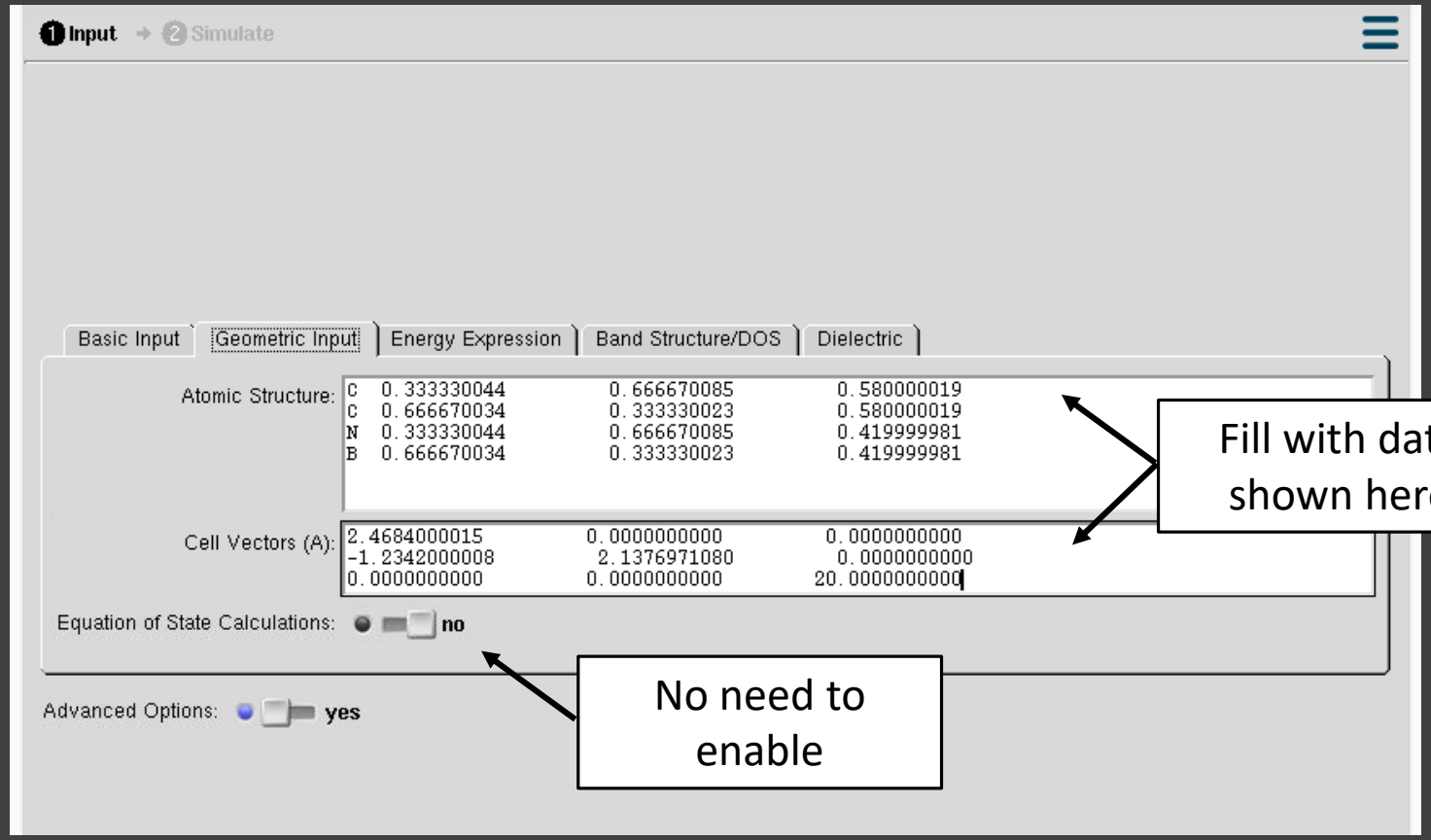
Define Basic Inputs



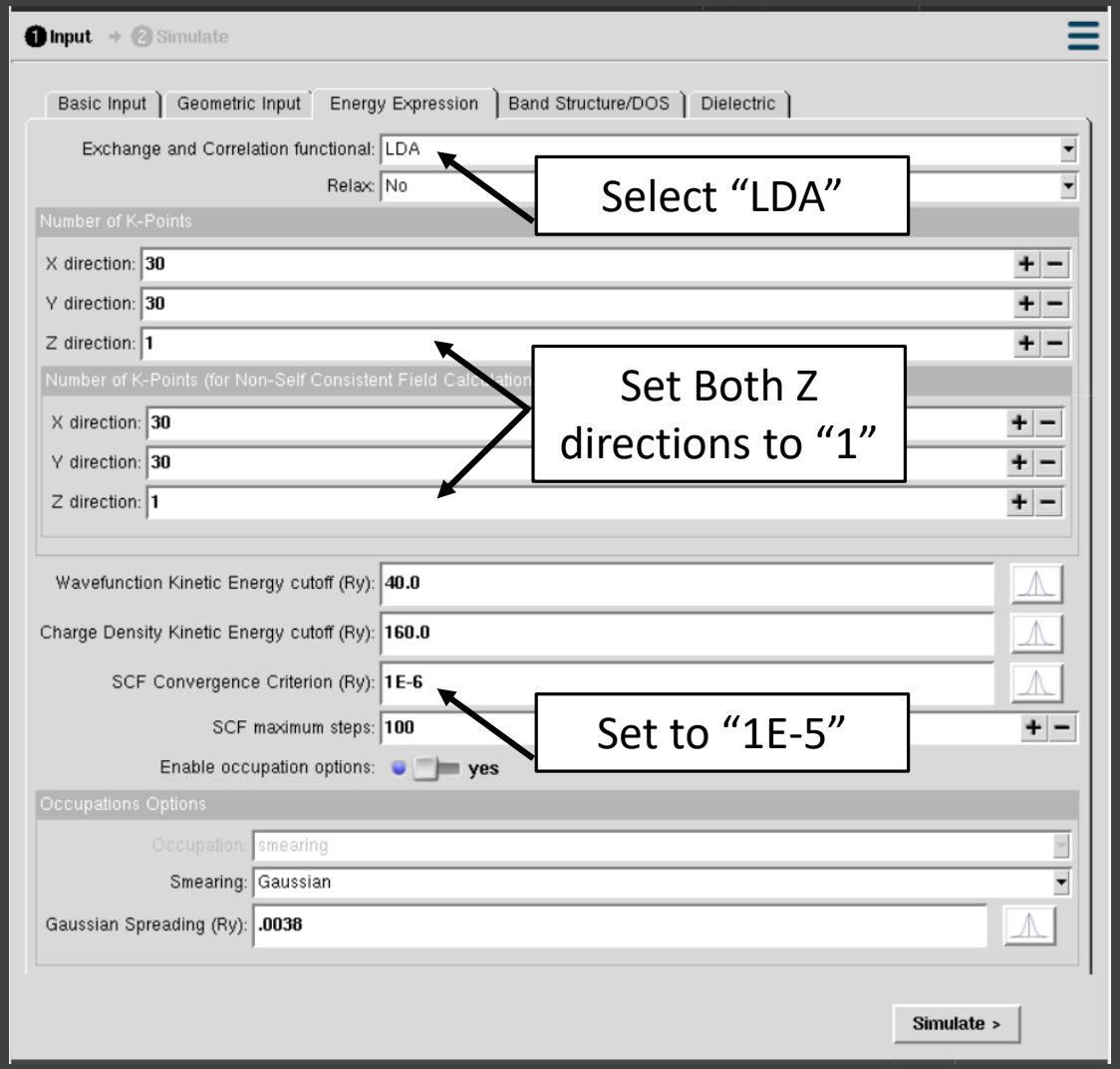
Select: "Thermoelectric Calculations"

Enable Advanced Options

Select the following:
Material Type: Semiconductor
Semiconductors: Graphite

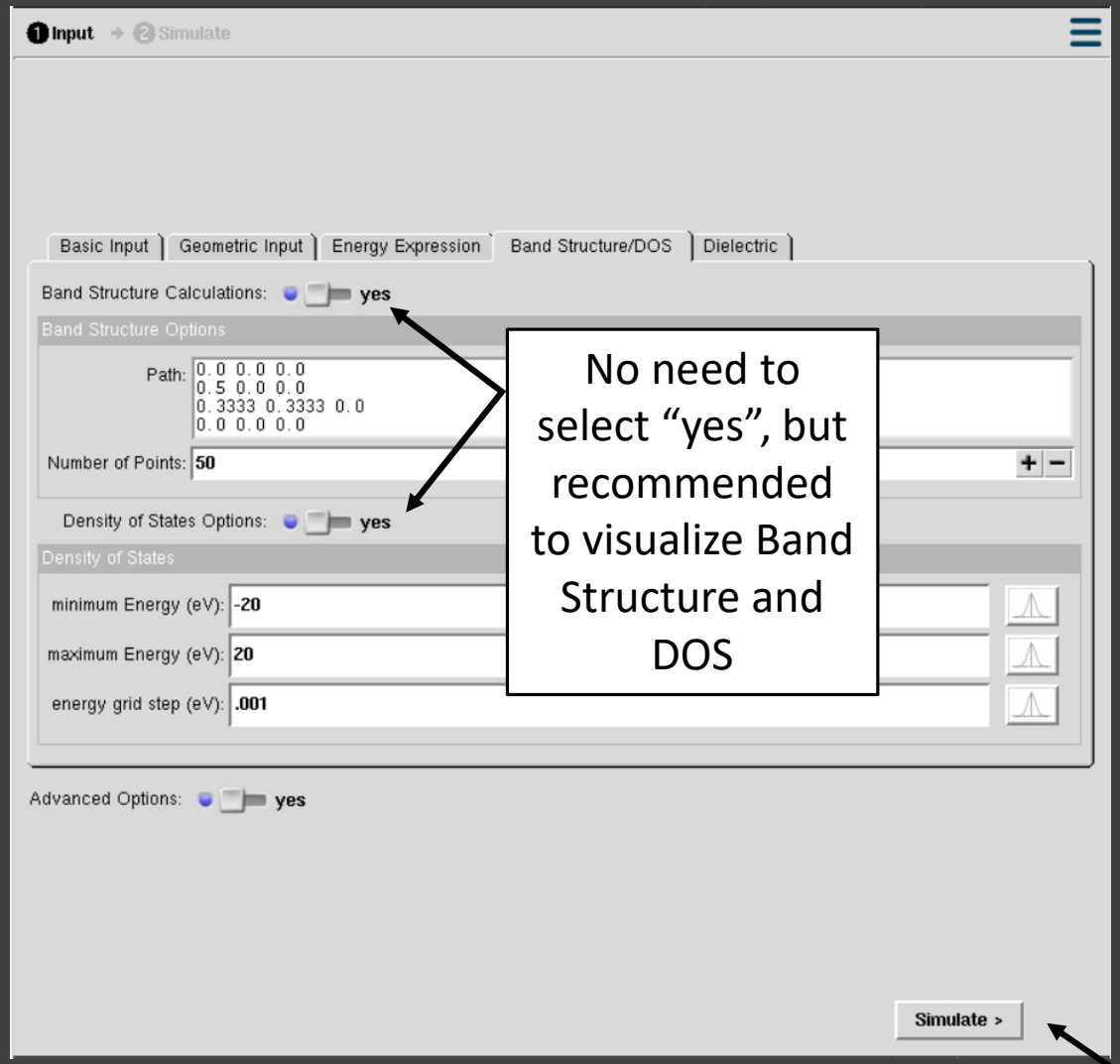


Define Geometric Input



Energy Expression

Final Step and RUN



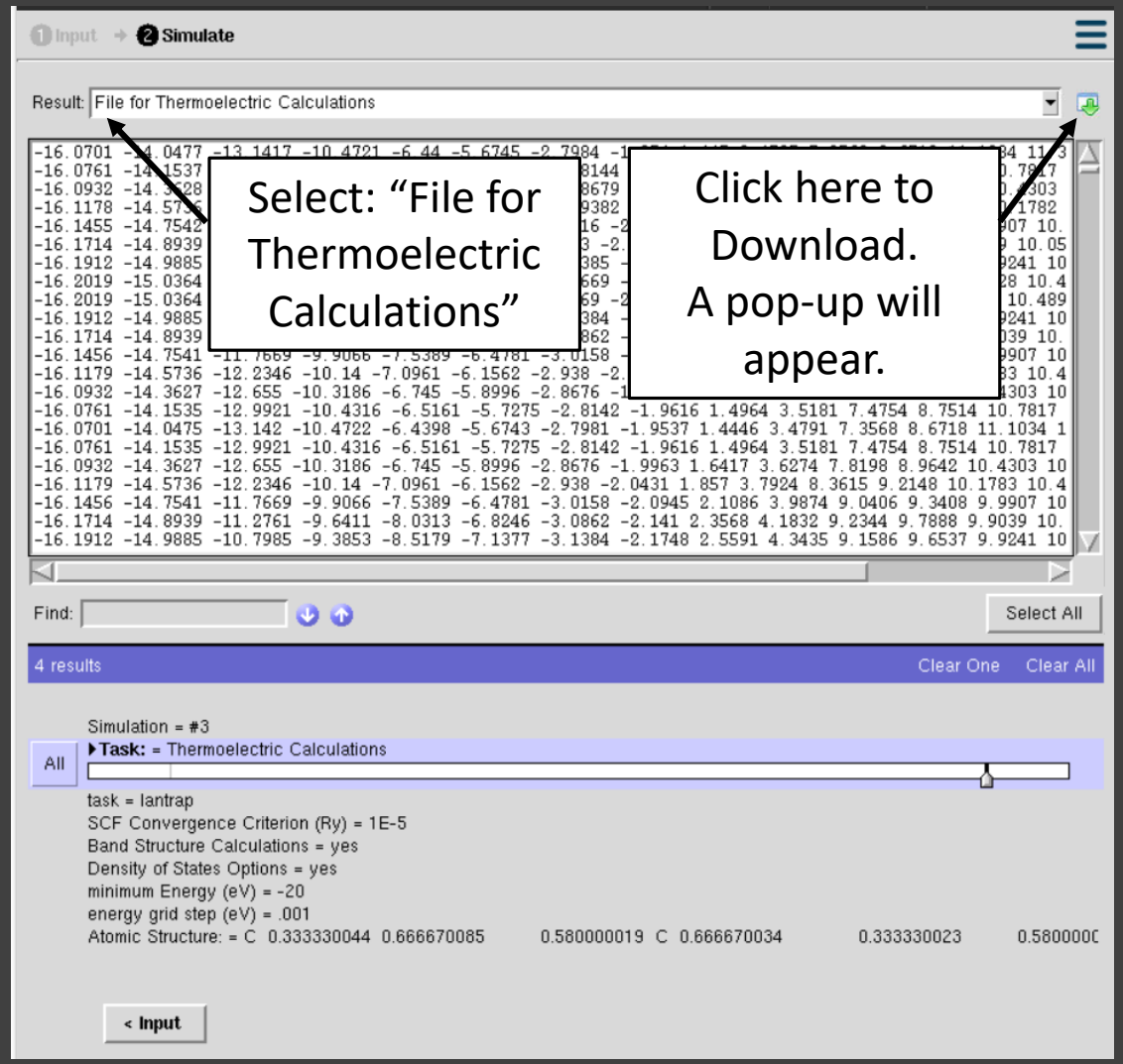
No need to select “yes”, but recommended to visualize Band Structure and DOS

Press “Simulate to Begin”

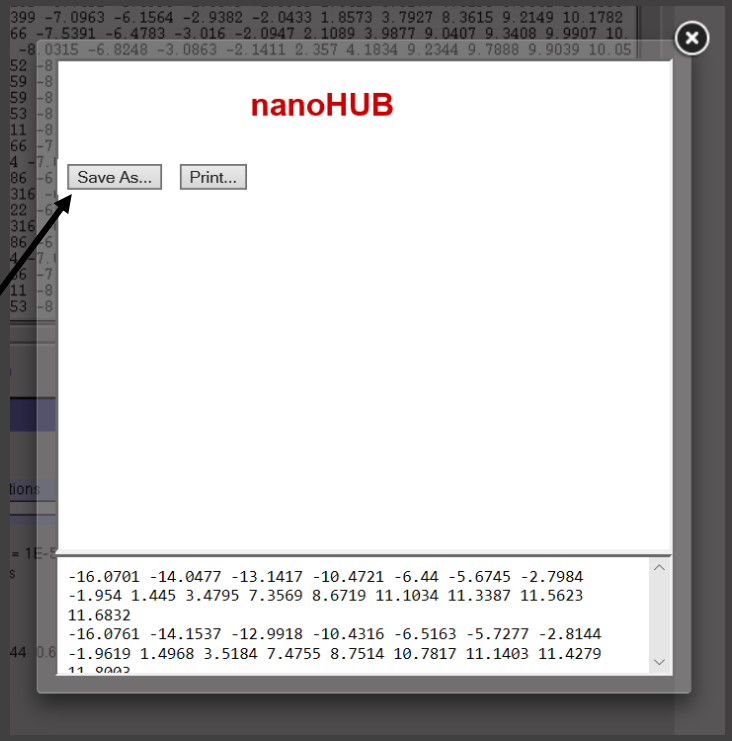
Be Warned: Simulation may take more than 30 Mins.

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

Obtaining Input File



Save File on your Computer

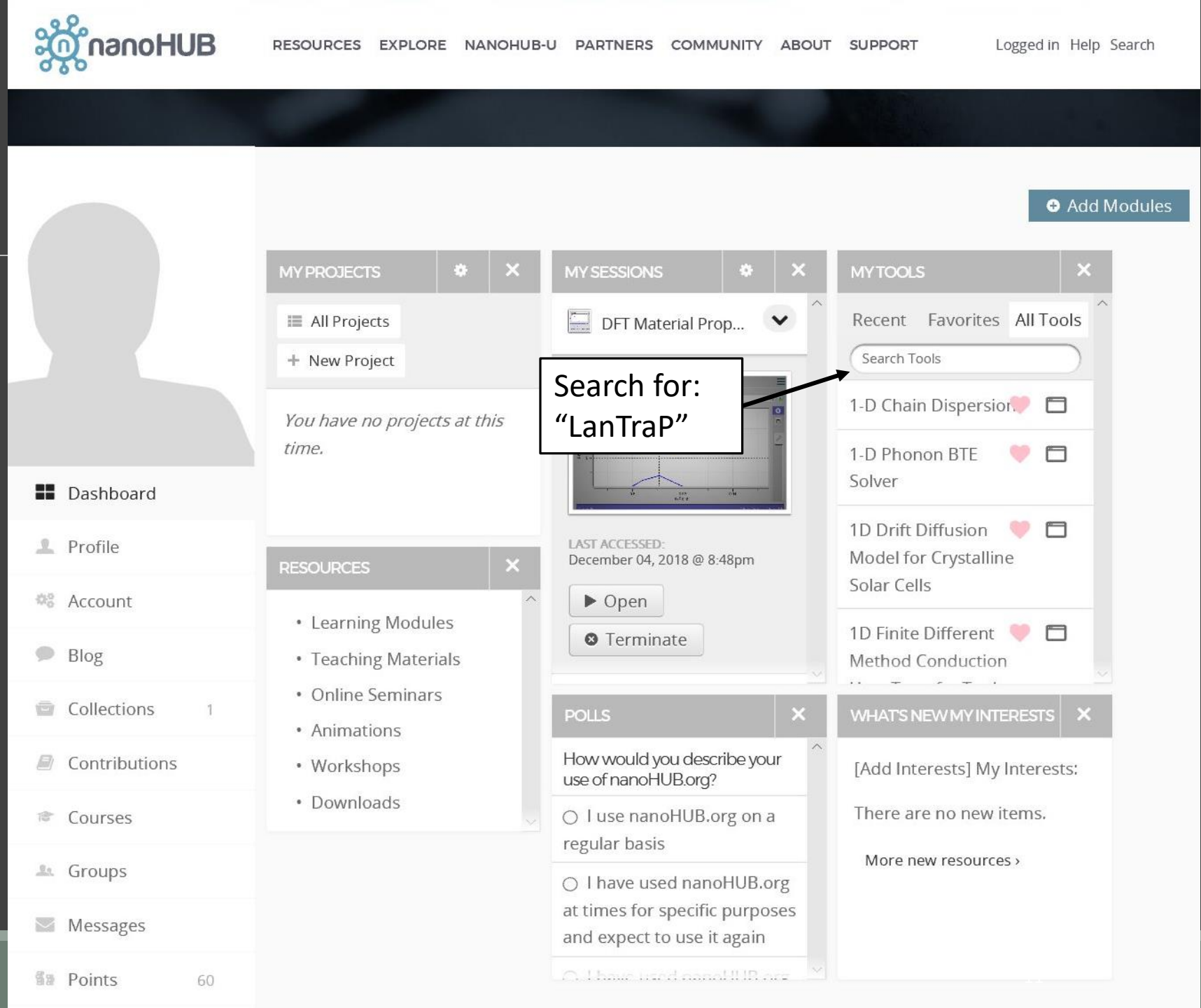


LanTraP

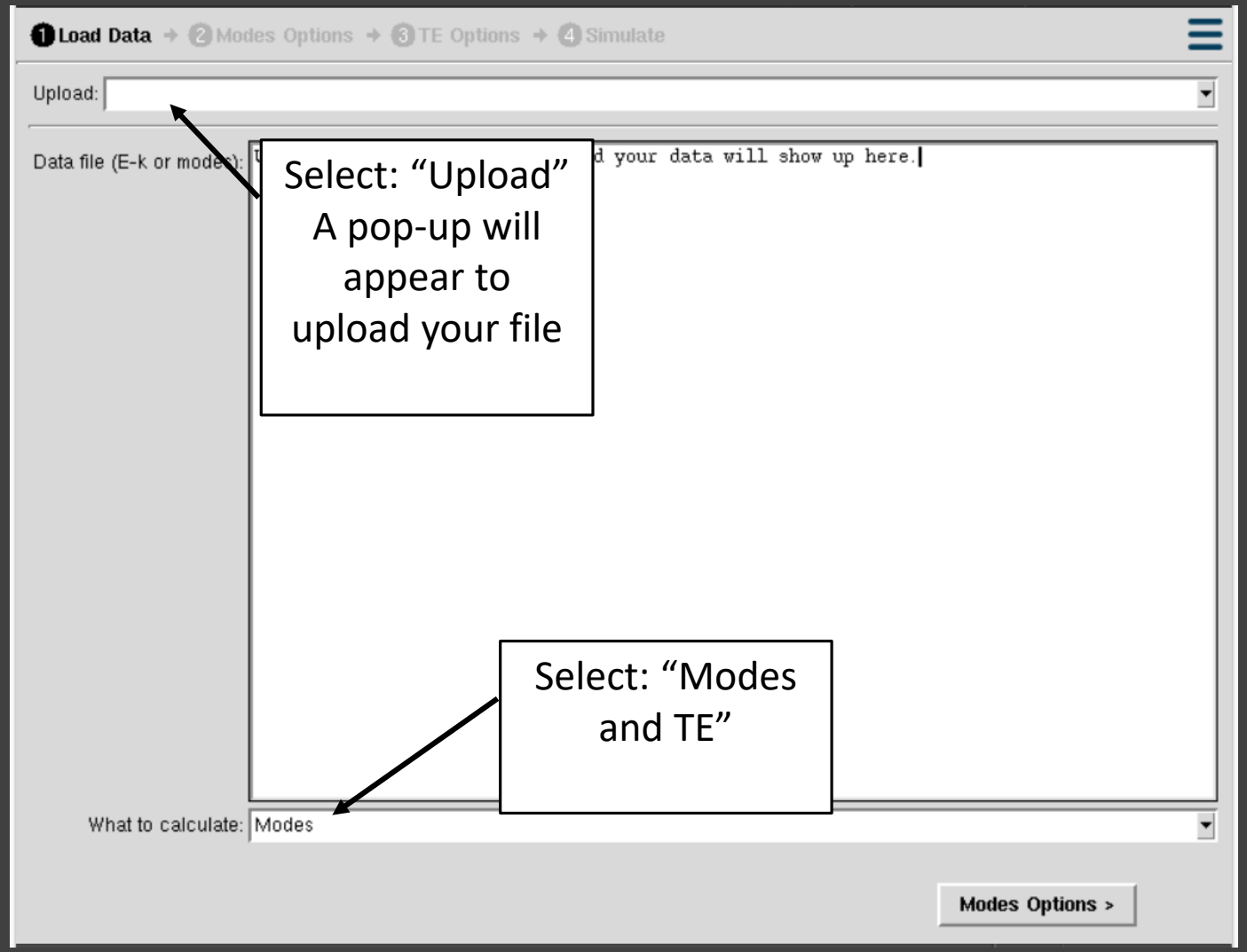
Objectives:

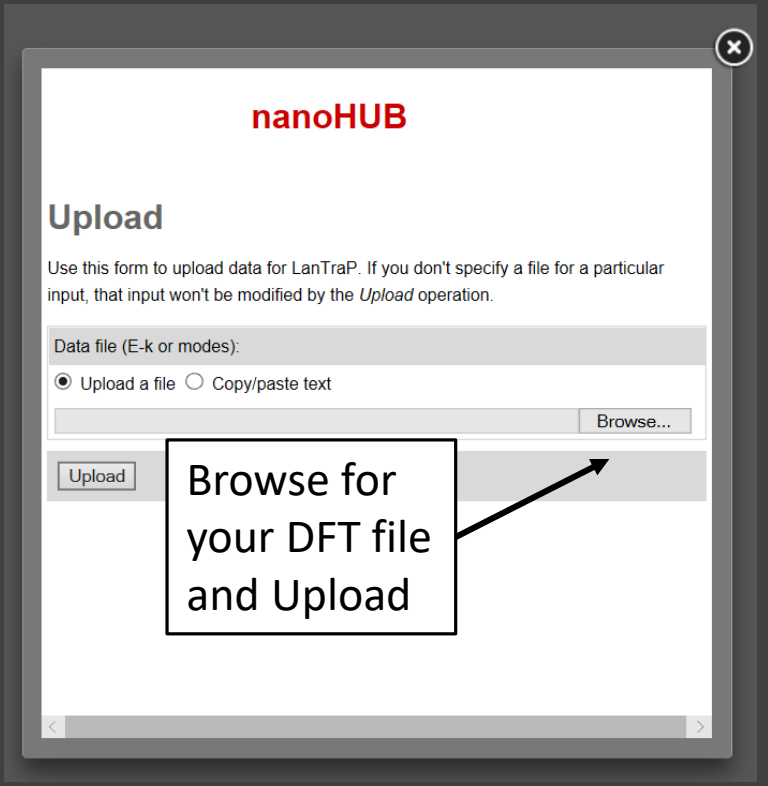
- Determine the Transport Properties of G-hBN bilayer.
  - Seebeck Coefficient (S)
  - Conductivity (σ)
  - Power Factor (PF)

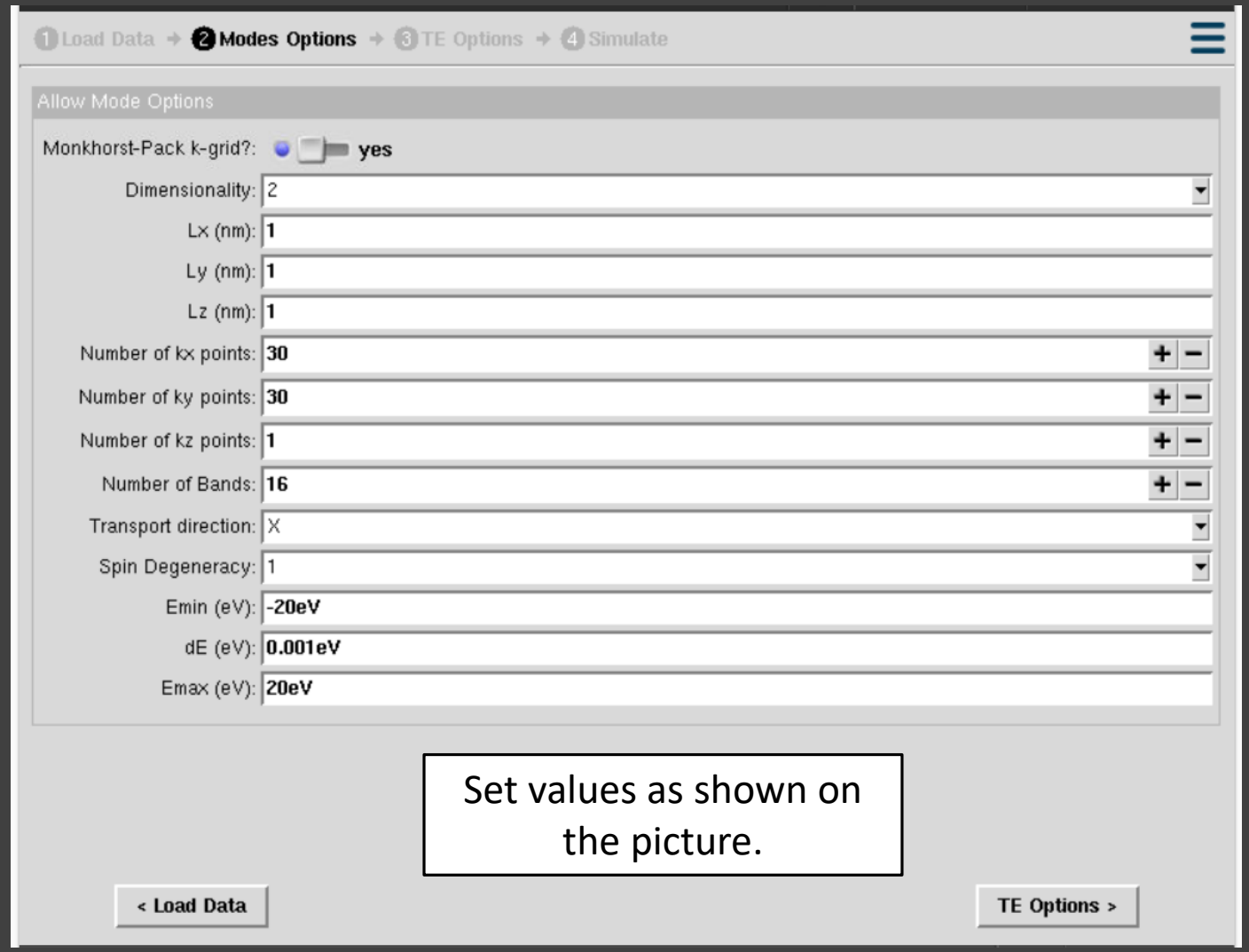
Second Part: LanTraP



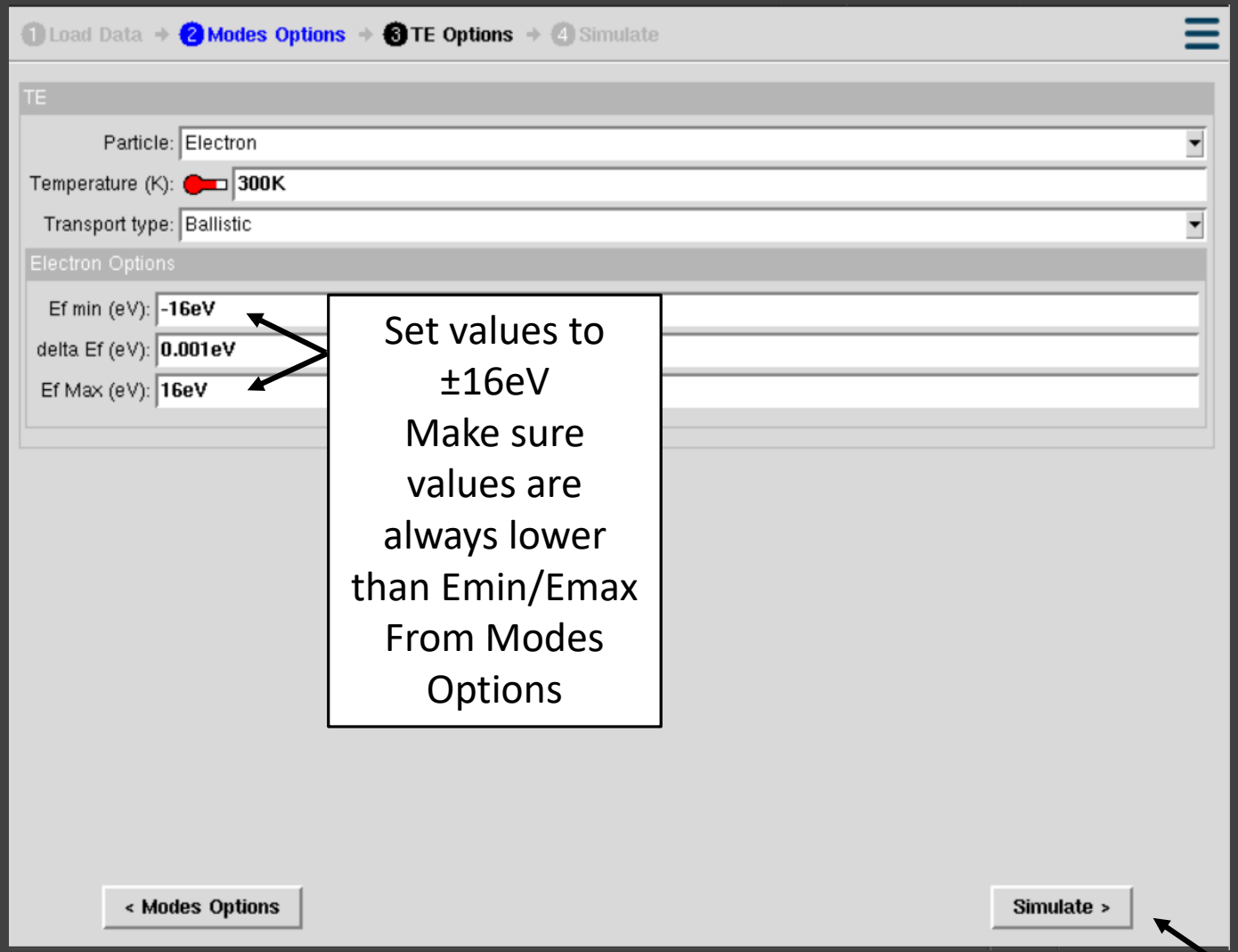
Upload Input File







Modes Options

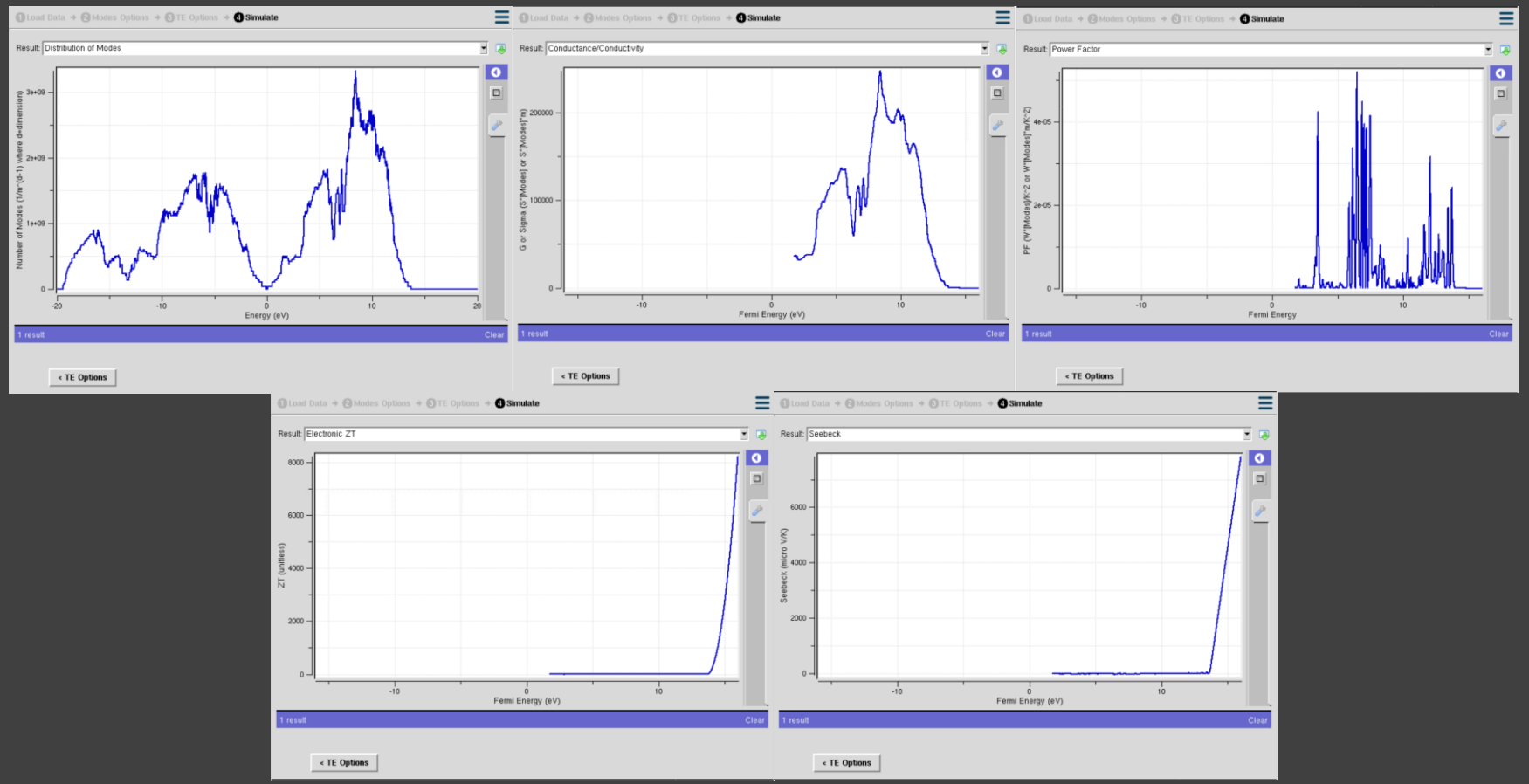


Set values to ±16eV
Make sure values are always lower than Emin/Emax From Modes Options

Press “Simulate to Begin”

TE Options

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