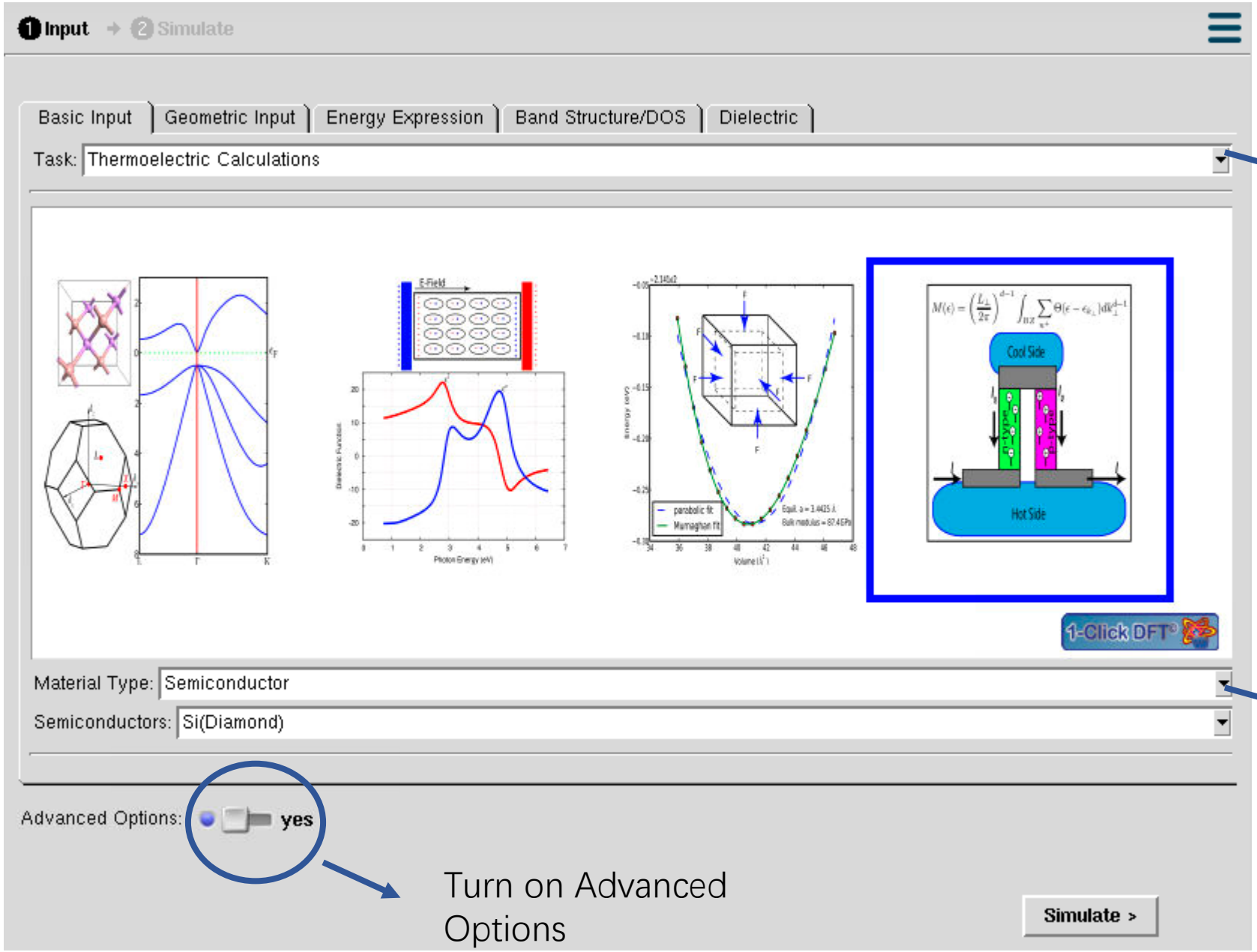
# Calculating the band structure and transport properties of Graphene-BN

Using DFT Materials Properties Simulator and Lantrap

Shukai Yao

# Launch DFT Materials Properties Simulator in NanoHUB

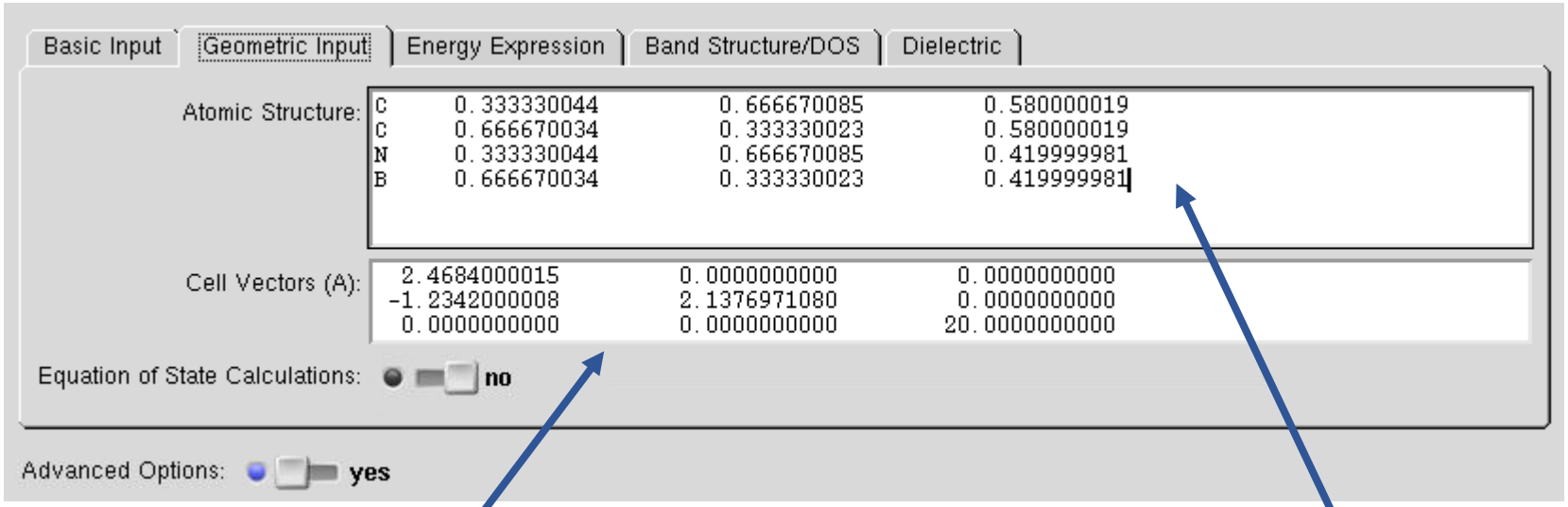



Choose Thermoelectric Calculations to obtain LanTrap friendly data

Choose Semiconductor

Turn on Advanced Options

# Geometry Input



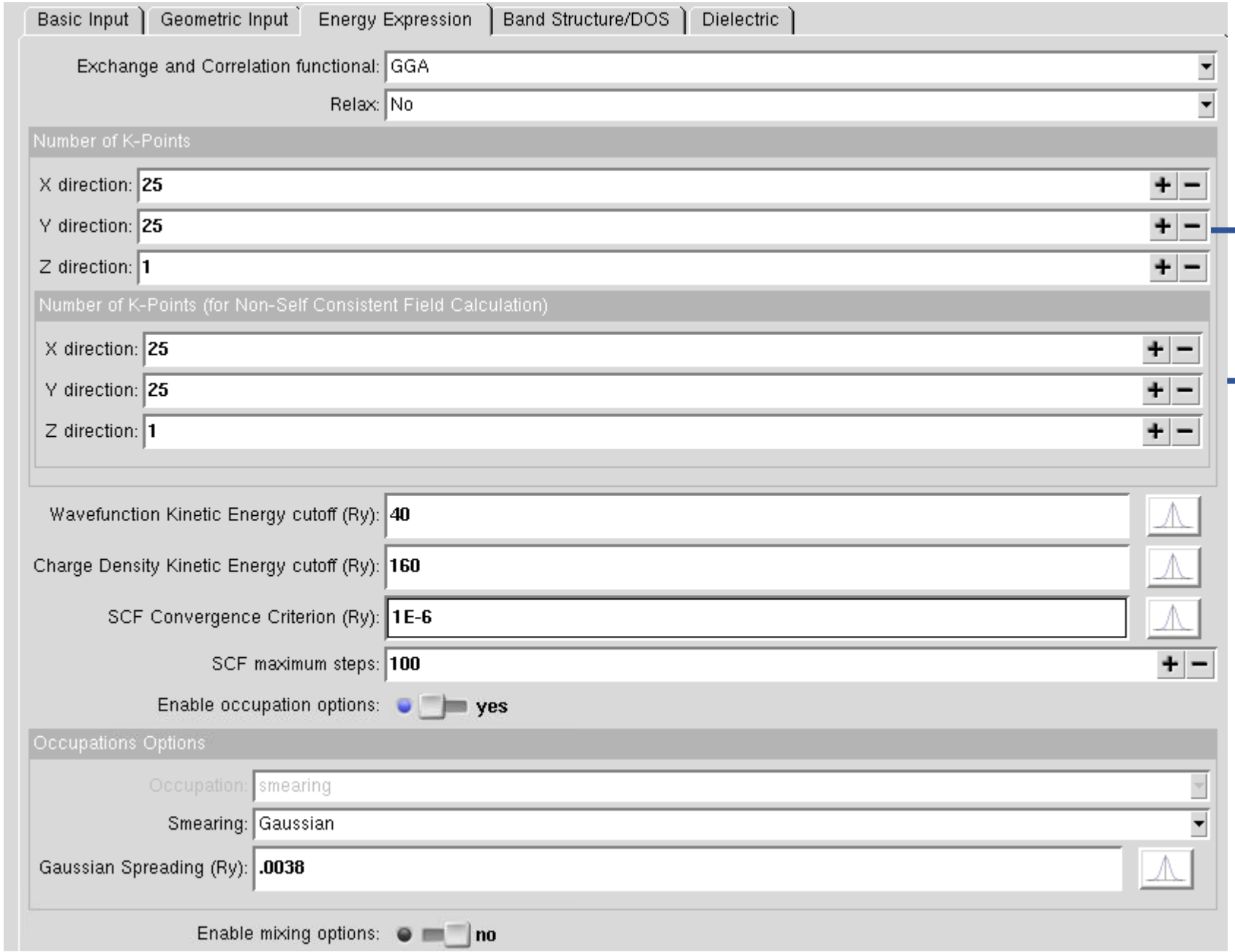

## Cell Vectors:

| | | |
|---|---|---|
| 2.4684000015 | 0.0000000000 | 0.0000000000 |
| -1.2342000008 | 2.1376971080 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 20.0000000000 |

## 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 |

# Energy Expression

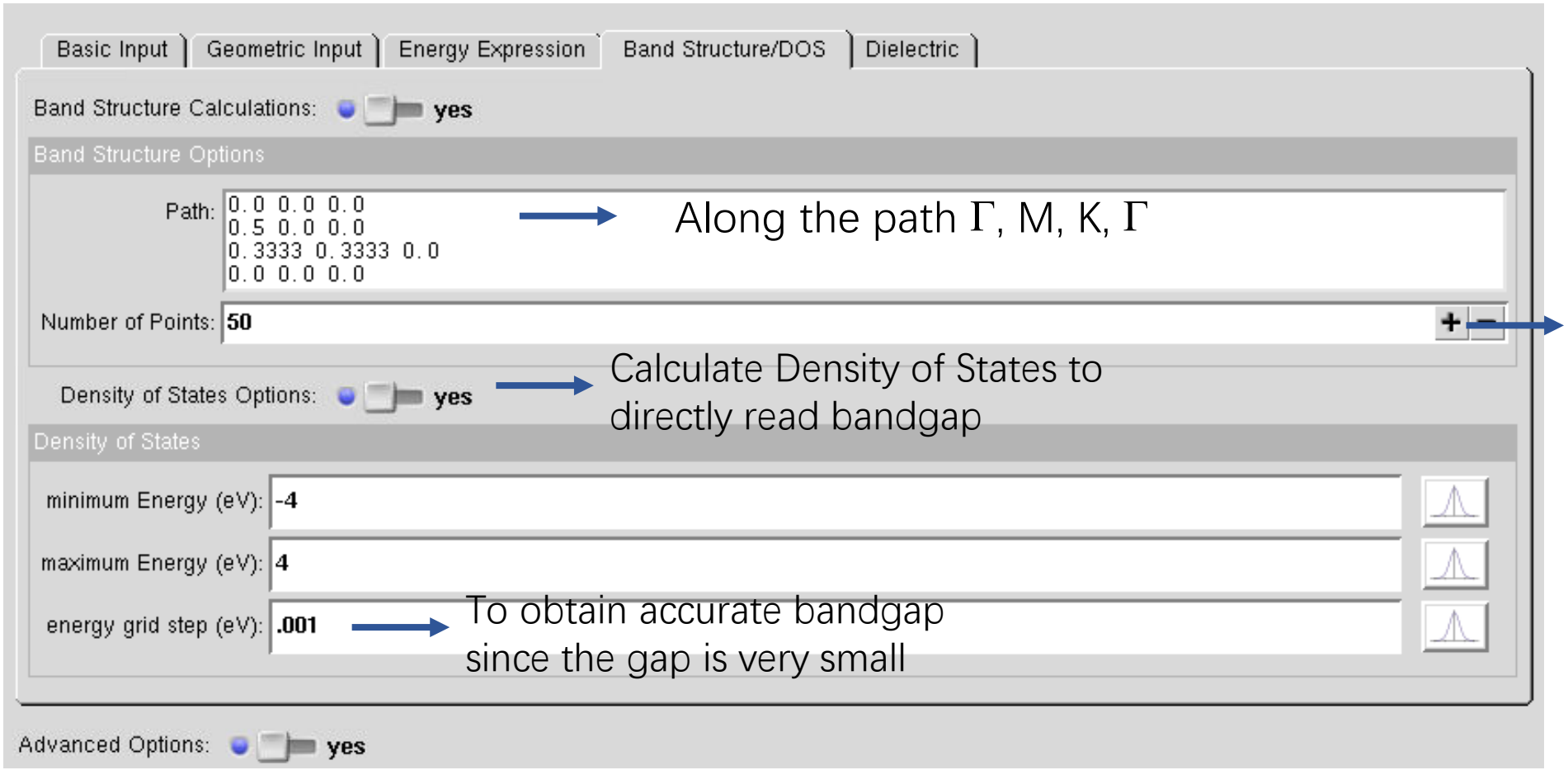



K mesh for self-consistent field calculation (Z direction is the non periodic direction)

K mesh for non self-consistent field calculation

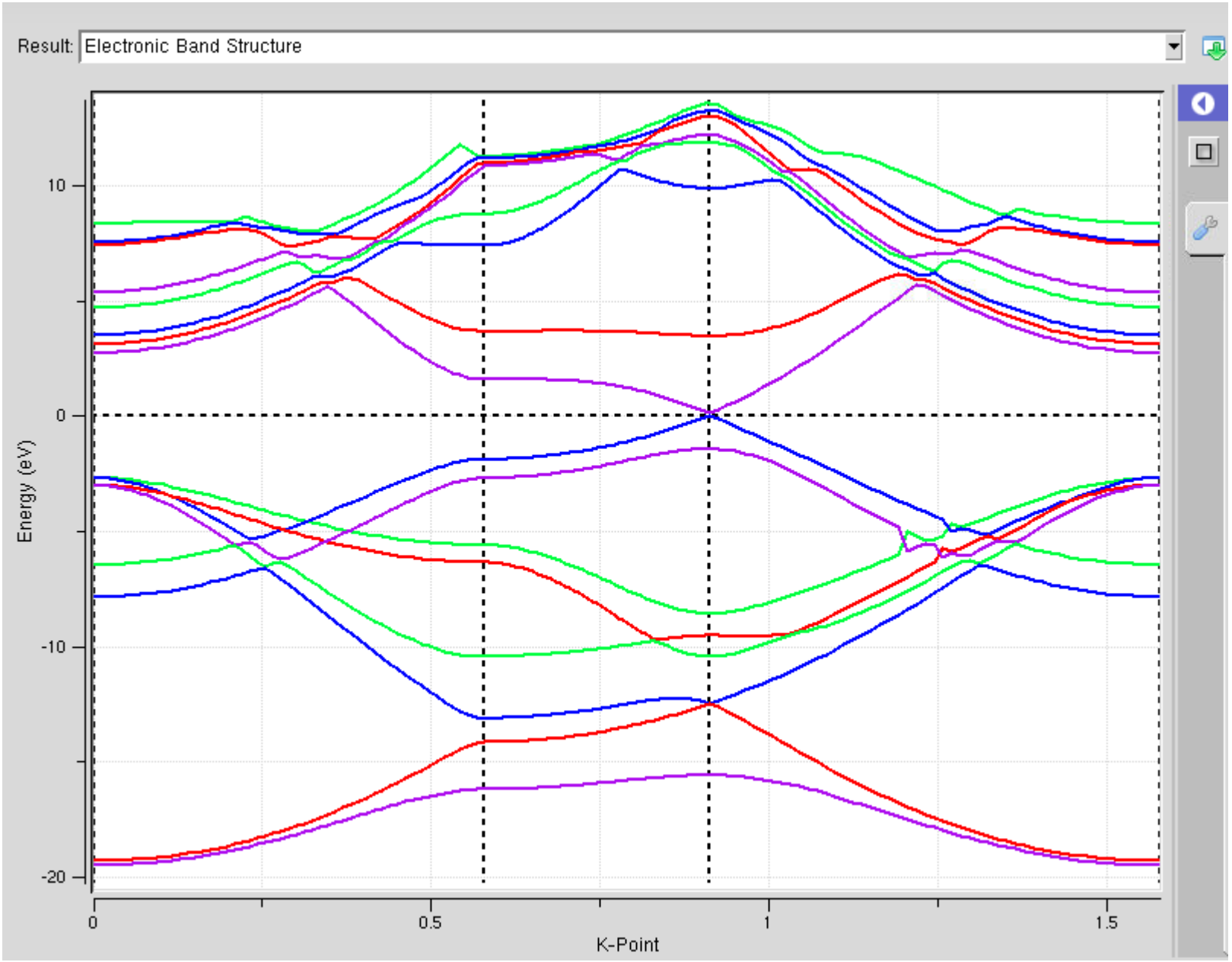
Energy cutoff, SCF convergence criterion, steps, smearing

# Band Structure Options

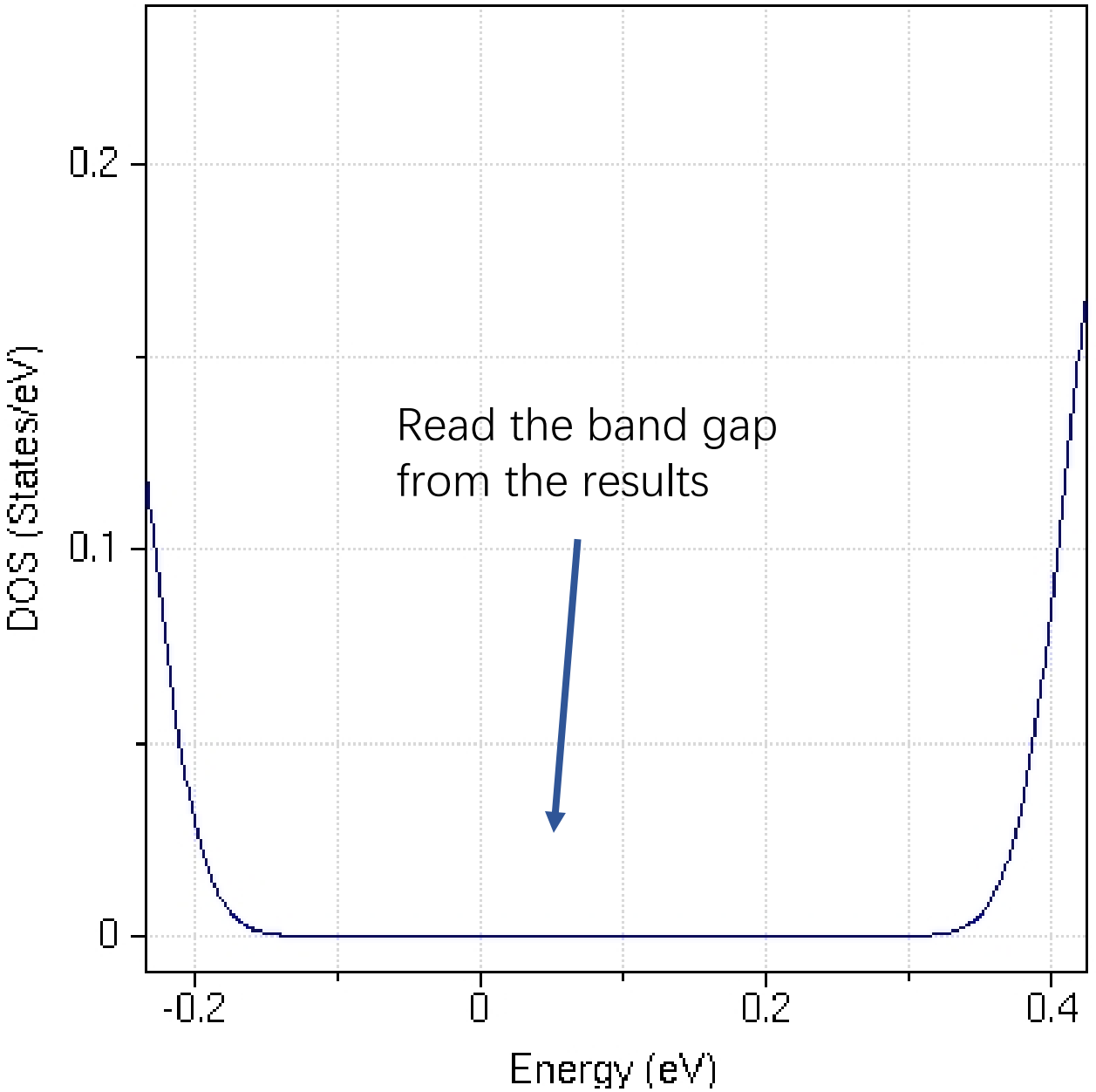



Then click Simulate to start

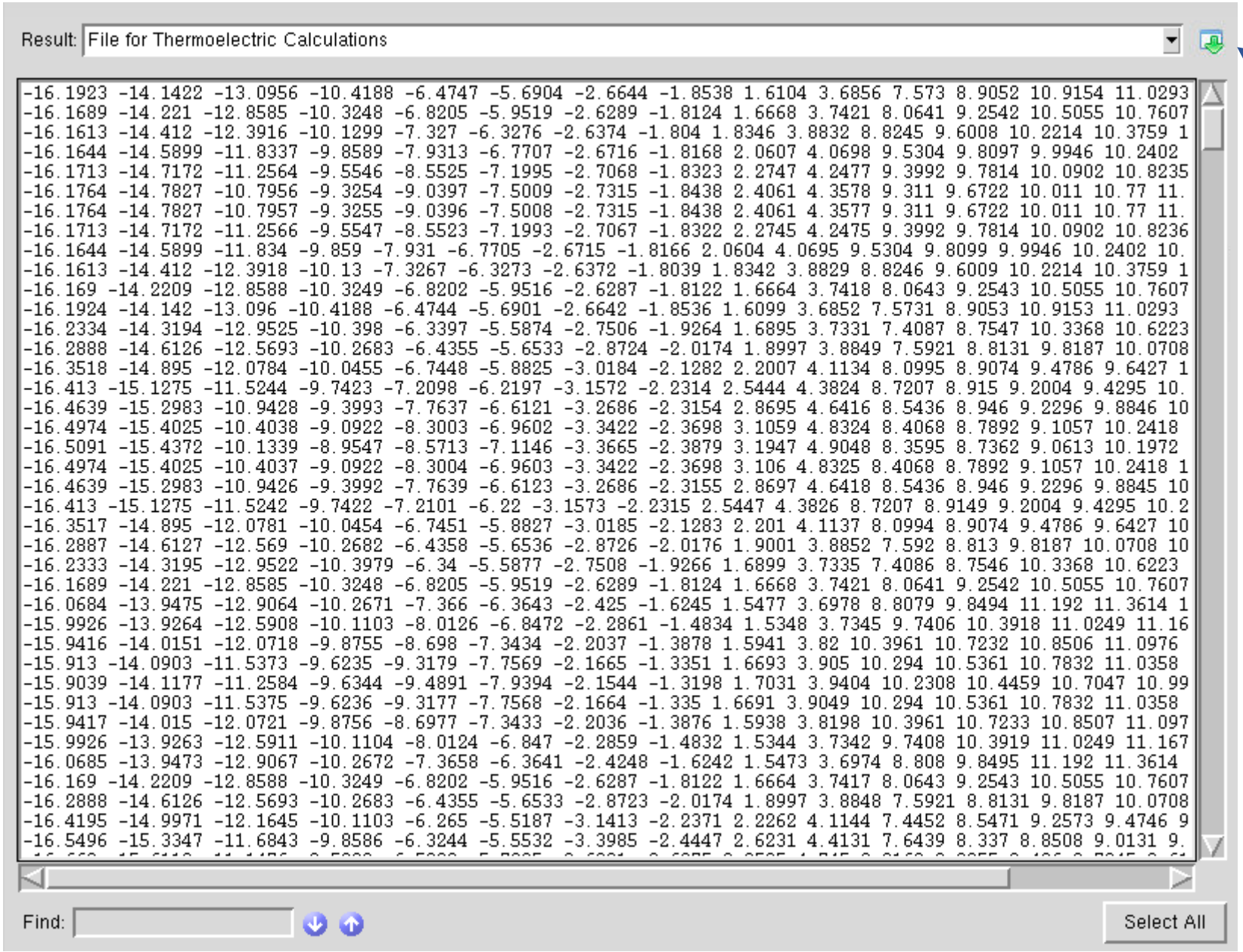
# Result: Band Structure



# Result: Density of States

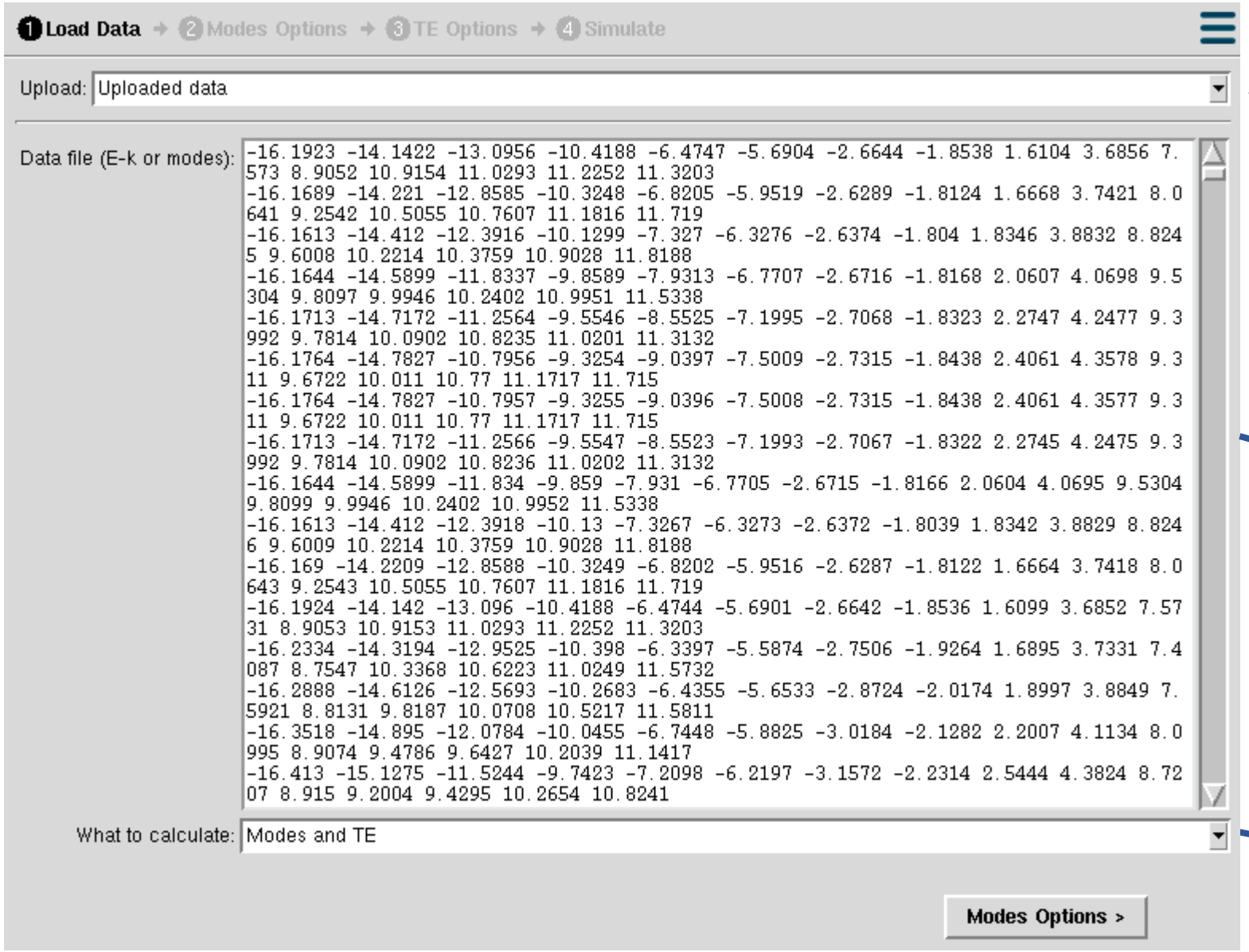


# Result: File for Thermoelectric Calculations




Download the data of E-K diagram for thermoelectric calculation

# Launch LanTrap in NanoHUB




Choose Uploaded data. Upload the E-K diagram data from last step

Data is uploaded

Choose Modes and TE

Then refer to the tutorial produced by my colleague Luis Regalado Bermejo, who focused on transport properties calculation using LanTrap!