

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

Using DFT Materials Properties Simulator and Lantrap

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# Launch DFT Materials Properties Simulator in NanoHUB

1 Input → 2 Simulate

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

Task: Thermoelectric Calculations

Material Type: Semiconductor

Semiconductors: Si(Diamond)

Advanced Options:  yes

Simulate >

Choose Thermoelectric Calculations to obtain LanTrap friendly data

Choose Semiconductor

Turn on Advanced Options

# Geometry Input

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

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

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




Exchange and Correlation functional: GGA  
Relax: No

Number of K-Points


X direction: 25 + -  
Y direction: 25 + -  
Z direction: 1 + -

Number of K-Points (for Non-Self Consistent Field Calculation)

X direction: 25 + -  
Y direction: 25 + -  
Z direction: 1 + -

Wavefunction Kinetic Energy cutoff (Ry): 40   
Charge Density Kinetic Energy cutoff (Ry): 160   
SCF Convergence Criterion (Ry): 1E-6   
SCF maximum steps: 100 + -  
Enable occupation options:  yes

Occupations Options

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

Enable mixing options:  no

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

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

Band Structure Calculations:   **yes**


Band Structure Options


Path:   
  
  
 → Along the path  $\Gamma$ , M, K,  $\Gamma$


Number of Points:  + - → Number of K points

Density of States Options:   **yes** → Calculate Density of States to directly read bandgap

Density of States

minimum Energy (eV):  

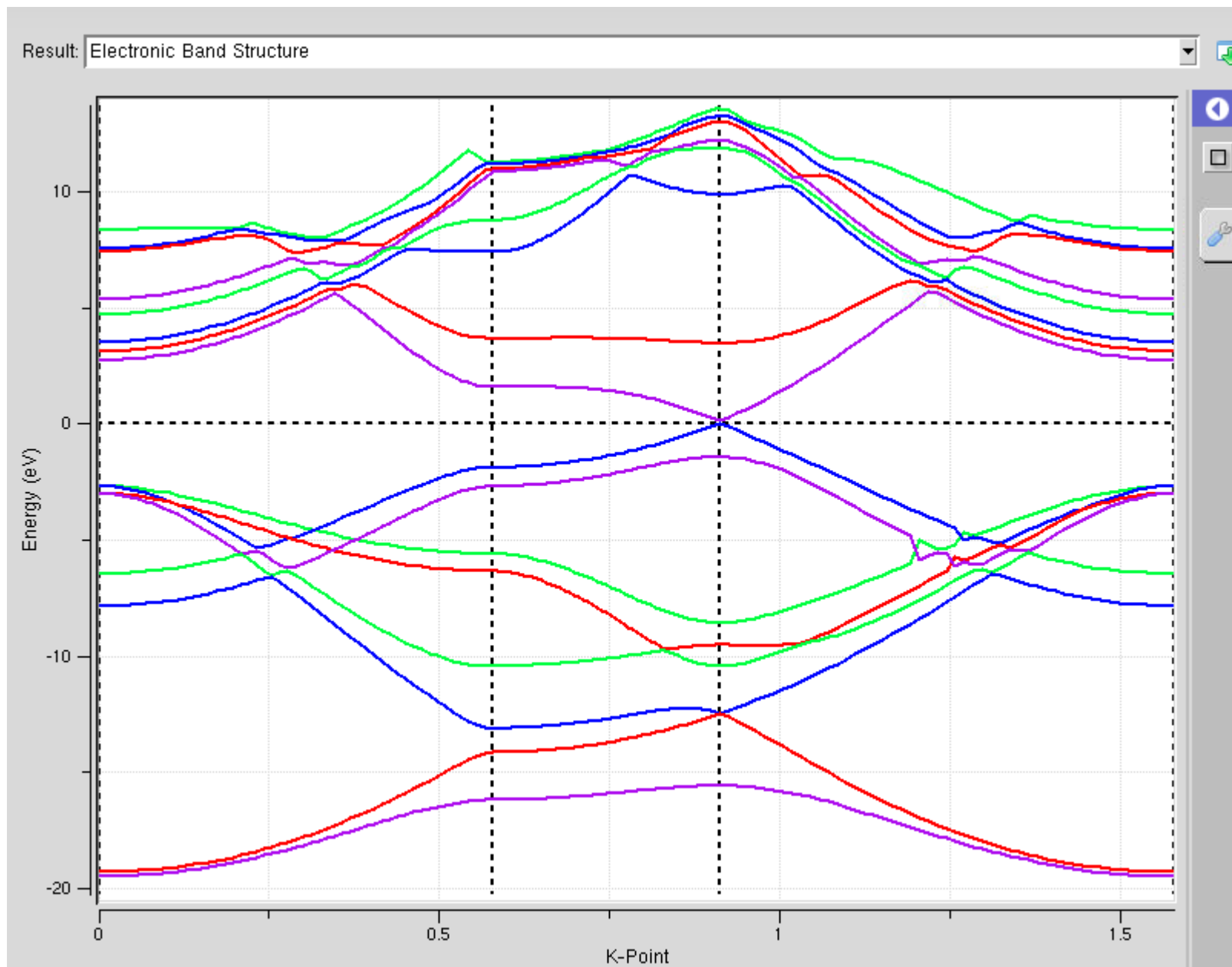
maximum Energy (eV):  

energy grid step (eV):  → To obtain accurate bandgap since the gap is very small 

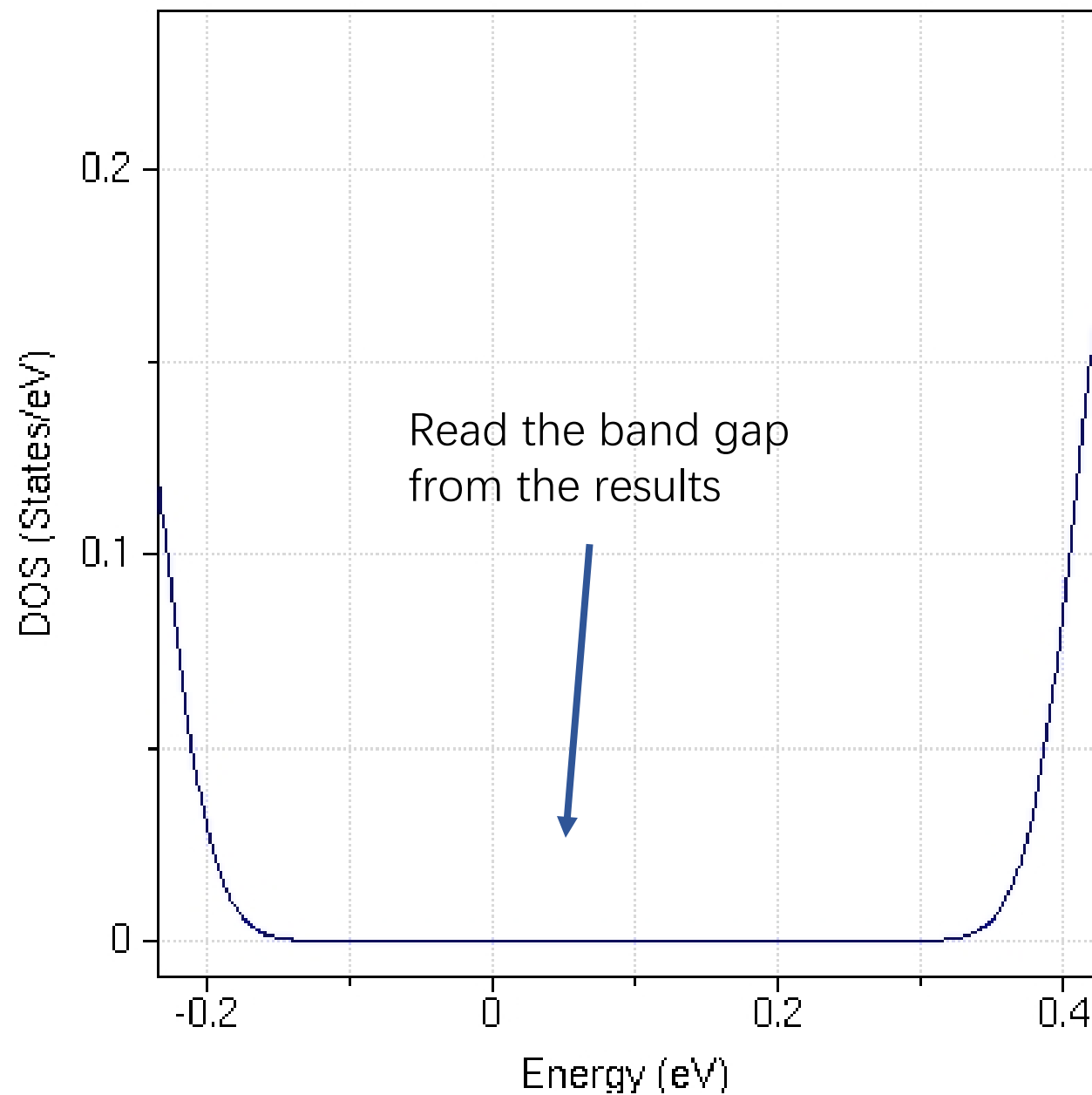
Advanced Options:   **yes**

Then click Simulate to start

# Result: Band Structure



# Result: Density of States



# Result: File for Thermoelectric Calculations

Result: File for Thermoelectric Calculations

```
-16.1923 -14.1422 -13.0956 -10.4188 -6.4747 -5.6904 -2.6644 -1.8538 1.6104 3.6856 7.573 8.9052 10.9154 11.0293
-16.1689 -14.221 -12.8585 -10.3248 -6.8205 -5.9519 -2.6289 -1.8124 1.6668 3.7421 8.0641 9.2542 10.5055 10.7607
-16.1613 -14.412 -12.3916 -10.1299 -7.327 -6.3276 -2.6374 -1.804 1.8346 3.8832 8.8245 9.6008 10.2214 10.3759 1
-16.1644 -14.5899 -11.8337 -9.8589 -7.9313 -6.7707 -2.6716 -1.8168 2.0607 4.0698 9.5304 9.8097 9.9946 10.2402
-16.1713 -14.7172 -11.2564 -9.5546 -8.5525 -7.1995 -2.7068 -1.8323 2.2747 4.2477 9.3992 9.7814 10.0902 10.8235
-16.1764 -14.7827 -10.7956 -9.3254 -9.0397 -7.5009 -2.7315 -1.8438 2.4061 4.3578 9.311 9.6722 10.011 10.77 11.
-16.1764 -14.7827 -10.7957 -9.3255 -9.0396 -7.5008 -2.7315 -1.8438 2.4061 4.3577 9.311 9.6722 10.011 10.77 11.
-16.1713 -14.7172 -11.2566 -9.5547 -8.5523 -7.1993 -2.7067 -1.8322 2.2745 4.2475 9.3992 9.7814 10.0902 10.8236
-16.1644 -14.5899 -11.834 -9.859 -7.931 -6.7705 -2.6715 -1.8166 2.0604 4.0695 9.5304 9.8099 9.9946 10.2402 10.
-16.1613 -14.412 -12.3918 -10.13 -7.3267 -6.3273 -2.6372 -1.8039 1.8342 3.8829 8.8246 9.6009 10.2214 10.3759 1
-16.169 -14.2209 -12.8588 -10.3249 -6.8202 -5.9516 -2.6287 -1.8122 1.6664 3.7418 8.0643 9.2543 10.5055 10.7607
-16.1924 -14.142 -13.096 -10.4188 -6.4744 -5.6901 -2.6642 -1.8536 1.6099 3.6852 7.5731 8.9053 10.9153 11.0293
-16.2334 -14.3194 -12.9525 -10.398 -6.3397 -5.5874 -2.7506 -1.9264 1.6895 3.7331 7.4087 8.7547 10.3368 10.6223
-16.2888 -14.6126 -12.5693 -10.2683 -6.4355 -5.6533 -2.8724 -2.0174 1.8997 3.8849 7.5921 8.8131 9.8187 10.0708
-16.3518 -14.895 -12.0784 -10.0455 -6.7448 -5.8825 -3.0184 -2.1282 2.2007 4.1134 8.0995 8.9074 9.4786 9.6427 1
-16.413 -15.1275 -11.5244 -9.7423 -7.2098 -6.2197 -3.1572 -2.2314 2.5444 4.3824 8.7207 8.915 9.2004 9.4295 10.
-16.4639 -15.2983 -10.9428 -9.3993 -7.7637 -6.6121 -3.2686 -2.3154 2.8695 4.6416 8.5436 8.946 9.2296 9.8846 10
-16.4974 -15.4025 -10.4038 -9.0922 -8.3003 -6.9602 -3.3422 -2.3698 3.1059 4.8324 8.4068 8.7892 9.1057 10.2418
-16.5091 -15.4372 -10.1339 -8.9547 -8.5713 -7.1146 -3.3665 -2.3879 3.1947 4.9048 8.3595 8.7362 9.0613 10.1972
-16.4974 -15.4025 -10.4037 -9.0922 -8.3004 -6.9603 -3.3422 -2.3698 3.106 4.8325 8.4068 8.7892 9.1057 10.2418 1
-16.4639 -15.2983 -10.9426 -9.3992 -7.7639 -6.6123 -3.2686 -2.3155 2.8697 4.6418 8.5436 8.946 9.2296 9.8845 10
-16.413 -15.1275 -11.5242 -9.7422 -7.2101 -6.22 -3.1573 -2.2315 2.5447 4.3826 8.7207 8.9149 9.2004 9.4295 10.2
-16.3517 -14.895 -12.0781 -10.0454 -6.7451 -5.8827 -3.0185 -2.1283 2.201 4.1137 8.0994 8.9074 9.4786 9.6427 10
-16.2887 -14.6127 -12.569 -10.2682 -6.4358 -5.6536 -2.8726 -2.0176 1.9001 3.8852 7.592 8.813 9.8187 10.0708 10
-16.2333 -14.3195 -12.9522 -10.3979 -6.34 -5.5877 -2.7508 -1.9266 1.6899 3.7335 7.4086 8.7546 10.3368 10.6223
-16.1689 -14.221 -12.8585 -10.3248 -6.8205 -5.9519 -2.6289 -1.8124 1.6668 3.7421 8.0641 9.2542 10.5055 10.7607
-16.0684 -13.9475 -12.9064 -10.2671 -7.366 -6.3643 -2.425 -1.6245 1.5477 3.6978 8.8079 9.8494 11.192 11.3614 1
-15.9926 -13.9264 -12.5908 -10.1103 -8.0126 -6.8472 -2.2861 -1.4834 1.5348 3.7345 9.7406 10.3918 11.0249 11.16
-15.9416 -14.0151 -12.0718 -9.8755 -8.698 -7.3434 -2.2037 -1.3878 1.5941 3.82 10.3961 10.7232 10.8506 11.0976
-15.913 -14.0903 -11.5373 -9.6235 -9.3179 -7.7569 -2.1665 -1.3351 1.6693 3.905 10.294 10.5361 10.7832 11.0358
-15.9039 -14.1177 -11.2584 -9.6344 -9.4891 -7.9394 -2.1544 -1.3198 1.7031 3.9404 10.2308 10.4459 10.7047 10.99
-15.913 -14.0903 -11.5375 -9.6236 -9.3177 -7.7568 -2.1664 -1.335 1.6691 3.9049 10.294 10.5361 10.7832 11.0358
-15.9417 -14.015 -12.0721 -9.8756 -8.6977 -7.3433 -2.2036 -1.3876 1.5938 3.8198 10.3961 10.7233 10.8507 11.097
-15.9926 -13.9263 -12.5911 -10.1104 -8.0124 -6.847 -2.2859 -1.4832 1.5344 3.7342 9.7408 10.3919 11.0249 11.167
-16.0685 -13.9473 -12.9067 -10.2672 -7.3658 -6.3641 -2.4248 -1.6242 1.5473 3.6974 8.808 9.8495 11.192 11.3614
-16.169 -14.2209 -12.8588 -10.3249 -6.8202 -5.9516 -2.6287 -1.8122 1.6664 3.7417 8.0643 9.2543 10.5055 10.7607
-16.2888 -14.6126 -12.5693 -10.2683 -6.4355 -5.6533 -2.8723 -2.0174 1.8997 3.8848 7.5921 8.8131 9.8187 10.0708
-16.4195 -14.9971 -12.1645 -10.1103 -6.265 -5.5187 -3.1413 -2.2371 2.2262 4.1144 7.4452 8.5471 9.2573 9.4746 9
-16.5496 -15.3347 -11.6843 -9.8586 -6.3244 -5.5532 -3.3985 -2.4447 2.6231 4.4131 7.6439 8.337 8.8508 9.0131 9.
```

Find:

Select All



Download the data of E-K diagram for thermoelectric calculation



# Launch LanTrap in NanoHUB

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

Upload:

Data file (E-k or modes):

```
-16.1923 -14.1422 -13.0956 -10.4188 -6.4747 -5.6904 -2.6644 -1.8538 1.6104 3.6856 7.573 8.9052 10.9154 11.0293 11.2252 11.3203
-16.1689 -14.221 -12.8585 -10.3248 -6.8205 -5.9519 -2.6289 -1.8124 1.6668 3.7421 8.0641 9.2542 10.5055 10.7607 11.1816 11.719
-16.1613 -14.412 -12.3916 -10.1299 -7.327 -6.3276 -2.6374 -1.804 1.8346 3.8832 8.8245 9.6008 10.2214 10.3759 10.9028 11.8188
-16.1644 -14.5899 -11.8337 -9.8589 -7.9313 -6.7707 -2.6716 -1.8168 2.0607 4.0698 9.5304 9.8097 9.9946 10.2402 10.9951 11.5338
-16.1713 -14.7172 -11.2564 -9.5546 -8.5525 -7.1995 -2.7068 -1.8323 2.2747 4.2477 9.3992 9.7814 10.0902 10.8235 11.0201 11.3132
-16.1764 -14.7827 -10.7956 -9.3254 -9.0397 -7.5009 -2.7315 -1.8438 2.4061 4.3578 9.311 9.6722 10.011 10.77 11.1717 11.715
-16.1764 -14.7827 -10.7957 -9.3255 -9.0396 -7.5008 -2.7315 -1.8438 2.4061 4.3577 9.311 9.6722 10.011 10.77 11.1717 11.715
-16.1713 -14.7172 -11.2566 -9.5547 -8.5523 -7.1993 -2.7067 -1.8322 2.2745 4.2475 9.3992 9.7814 10.0902 10.8236 11.0202 11.3132
-16.1644 -14.5899 -11.834 -9.859 -7.931 -6.7705 -2.6715 -1.8166 2.0604 4.0695 9.5304 9.8099 9.9946 10.2402 10.9952 11.5338
-16.1613 -14.412 -12.3918 -10.13 -7.3267 -6.3273 -2.6372 -1.8039 1.8342 3.8829 8.8246 9.6009 10.2214 10.3759 10.9028 11.8188
-16.169 -14.2209 -12.8588 -10.3249 -6.8202 -5.9516 -2.6287 -1.8122 1.6664 3.7418 8.0643 9.2543 10.5055 10.7607 11.1816 11.719
-16.1924 -14.142 -13.096 -10.4188 -6.4744 -5.6901 -2.6642 -1.8536 1.6099 3.6852 7.5731 8.9053 10.9153 11.0293 11.2252 11.3203
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-16.2888 -14.6126 -12.5693 -10.2683 -6.4355 -5.6533 -2.8724 -2.0174 1.8997 3.8849 7.5921 8.8131 9.8187 10.0708 10.5217 11.5811
-16.3518 -14.895 -12.0784 -10.0455 -6.7448 -5.8825 -3.0184 -2.1282 2.2007 4.1134 8.0995 8.9074 9.4786 9.6427 10.2039 11.1417
-16.413 -15.1275 -11.5244 -9.7423 -7.2098 -6.2197 -3.1572 -2.2314 2.5444 4.3824 8.7207 8.915 9.2004 9.4295 10.2654 10.8241
```

What to calculate:

Modes Options >

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!