

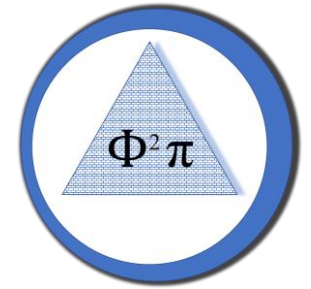
Thermoelectric Optimizer – SPB Model App

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October 2021

Hamilton ON Canada


$$\Phi^2 \pi$$

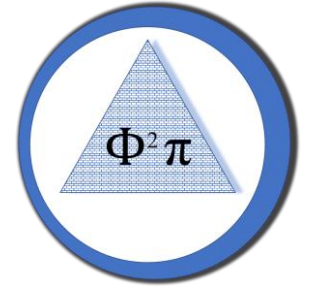


Introduction

Welcome to the Thermoelectric Optimizer App.

The App is based on the single-parabolic band model and can compute using empirical parameters such as Seebeck coefficient and mobility:

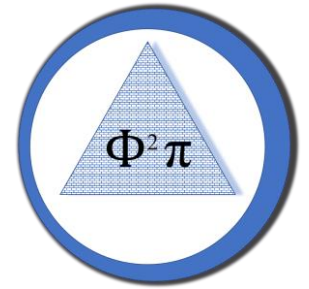
- Electrical thermal conductivity
- Seebeck coefficient, mobility, Lorenz number, and thermoelectric figure of merit as function of the charge carrier concentration
- Thermoelectric figure of merit as function of charge carrier concentration and temperature
- Optimized charge carrier concentration and thermoelectric figure of merit as function of temperature versus experimental data



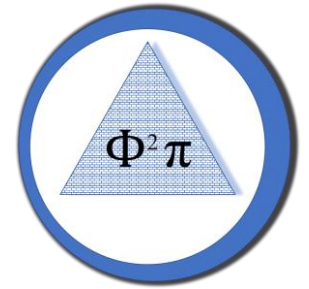
Introduction

- SPB model assumes that the effective mass does not change with carrier concentration (i.e., single parabolic band) and that the electron transport is limited by a single scattering mechanism:
 - Acoustic Deformation Potential (ADP) → vibrations of atoms reduce the mobility of the charge carriers
 - Polar Optical Phonon (POP) → charge carriers are scattered of the electric field of polar atoms (**material needs to be hetero-polar**)
- or
- Ionized Impurity (IMP) → charge carriers are scattered by the ionization of the lattice (i.e., unbalanced local charge near a crystal impurity)

Installation



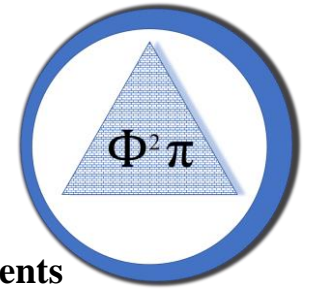
- Download the executable (i.e., Thermoelectric Optimizer.exe), the example .csv files (i.e. Example_SPB.csv) , and the icon (i.e., icon_spb.ico)
- Create a new folder and move all files in the folder (please note that temporary files will be save in the folder as well)
- Please note that the App won't work if the icon is not in the same folder than the executable (.csv file can be in a different folder)



Starting the program

- Double-click of the executable and a window will open (not included in the later version)
- Don't worry if the warning appears in the window:
MatplotlibDeprecationWarning: The MATPLOTLIBDATA environment variable was deprecated in Matplotlib 3.1 and will be removed in 3.3. `exec(bytecode, module.__dict__)`
- The opening of the App takes some time depending on your processor

Start Window – Input Parameters



Input parameters from experiments

A : Compound name (required)

B : Temperature in K (required)
(Temperature should be above 1 and below 10,000 K)

C : Seebeck Coefficient in $\mu\text{V K}^{-1}$ (required; only positive values)
(Seebeck coefficient should be above 0.1 and below $1,500 \mu\text{V K}^{-1}$)

D : Hall Carrier Concentration in cm^{-3} (not required; only positive values)
(Carrier Concentration should be above $1\text{E}12$ and below $1\text{E}24 \text{cm}^{-3}$)

E : Hall Mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (not required)
(Mobility should be above 0.01 and below $10,000 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)

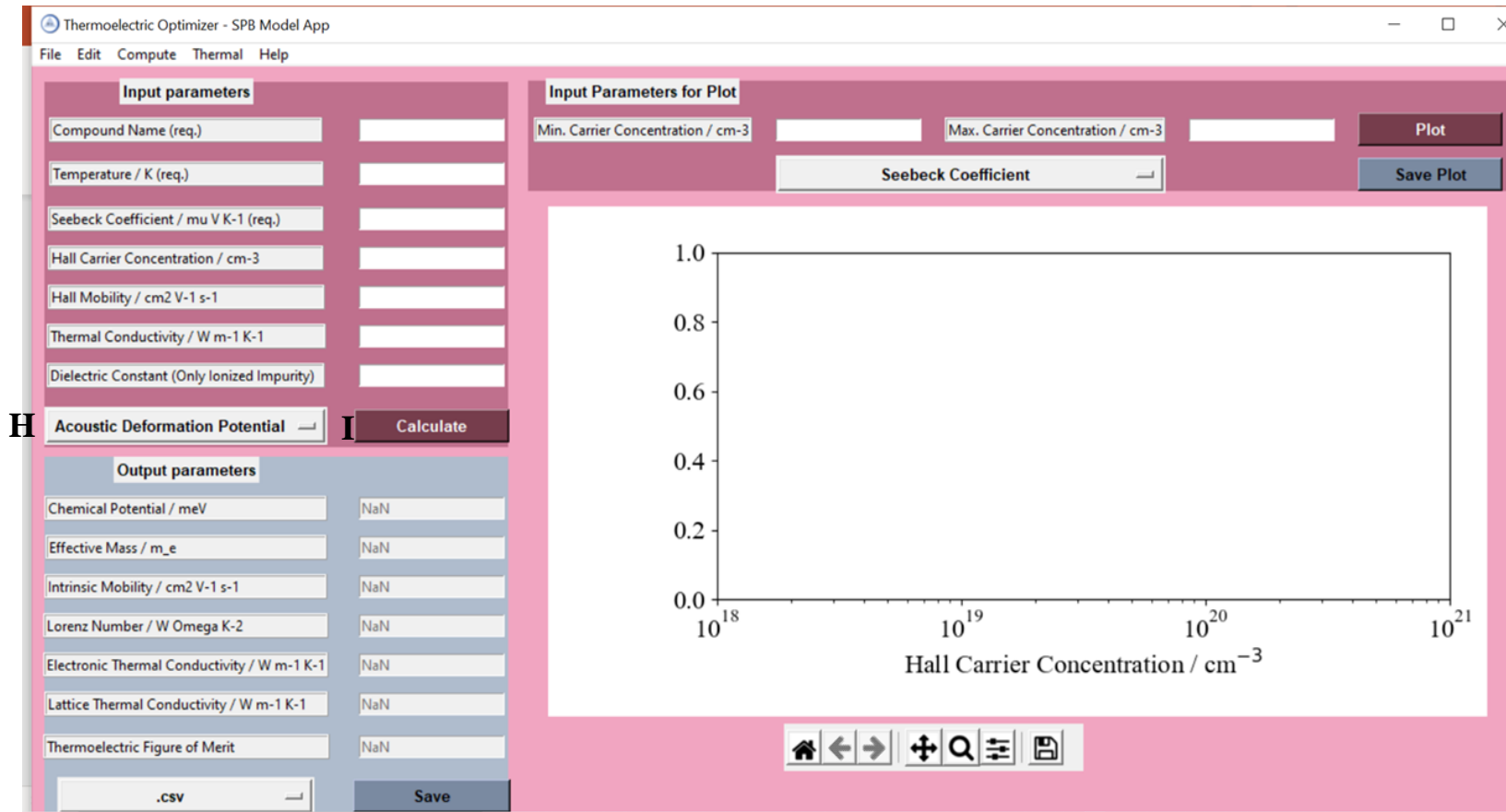
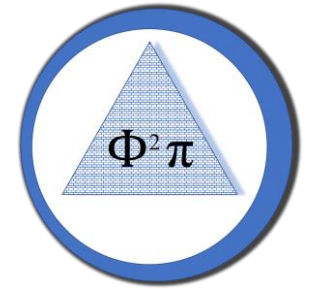
F : Total thermal Conductivity in $\text{W m}^{-1} \text{K}^{-1}$ (not required)
(Thermal Conductivity should be above 0 and below 10,000 $\text{W m}^{-1} \text{K}^{-1}$)

G : Dielectric Constant (unitless) (not required)
(Dielectric Constant should be above 1 and below 100,000)

Red is required to press 'Calculate' and 'Plot'. Green is not required.; only to compute certain parameters

* (req.) means required

Start Window – Calculation

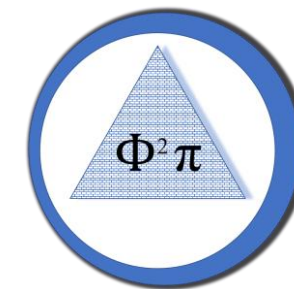


H : Choose the scattering mechanism (5)

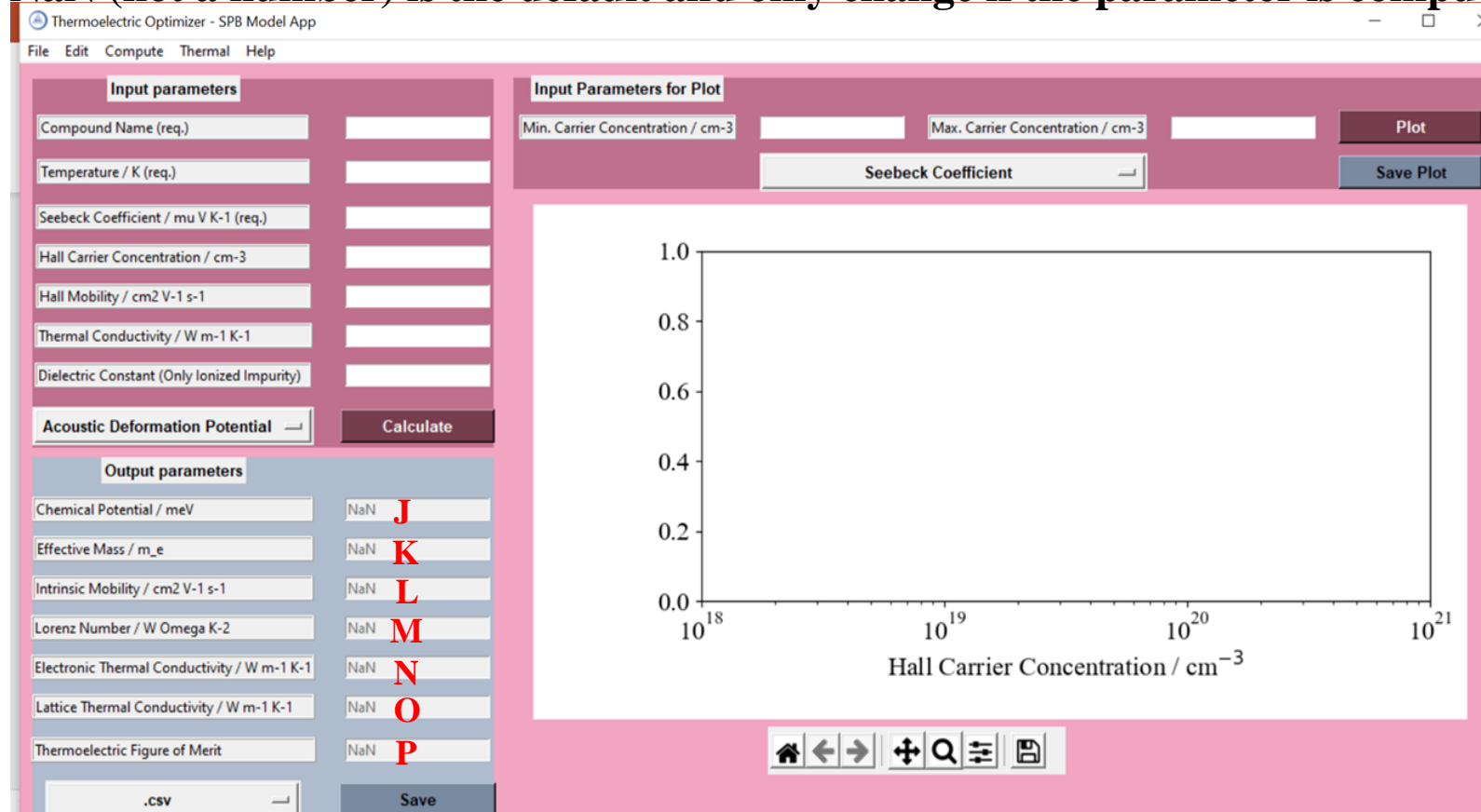
- **Acoustic Deformation Potential**
- **Polar Optical Phonon**
- **Ionized Impurity**
 - **Brooks-Herring (with screening)**
 - **Requires Dielectric Constant**
 - **Takes a long time which increases with increasing Seebeck Coefficient**
- **Polar Optical Phonon (Fermi)**
 - **Slight overestimation at high Carrier Concentration**
- **Ionized Impurity (Fermi)**
 - **Conwell-Weisskopf (without screening)**
 - **No Dielectric Constant required**
 - **Fast**
 - **Overestimation at high Carrier Concentration**

I : Calculate the properties below (make sure required fields have a value)

Start Window – Output Parameters



NaN (not a number) is the default and only change if the parameter is computed



J : Chemical Potential in meV (Computed from the Seebeck coefficient) *

K : Effective mass in m_e (Computed from the Seebeck coefficient and Carrier Concentration)

L : Intrinsic Mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (Computed from the Seebeck coefficient, Carrier Concentration and Mobility)

M : Lorenz number in $\text{W } \Omega \text{ K}^{-2}$ (Computed from the Seebeck coefficient) *

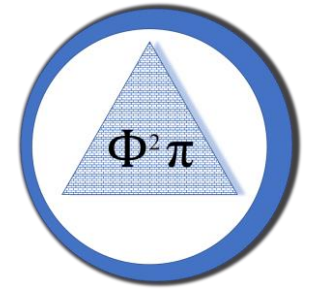
N : Electronic Thermal Conductivity in $\text{W m}^{-1} \text{K}^{-1}$ (Computed from the Seebeck coefficient, Carrier Concentration, and Mobility)

O : Lattice Thermal Conductivity in $\text{W m}^{-1} \text{K}^{-1}$ (Computed from the Seebeck coefficient, Carrier Concentration, Mobility, and Thermal Conductivity)

P : Thermoelectric Figure of Merit, zT (Computed from the Seebeck coefficient, Carrier Concentration, Mobility, and Thermal Conductivity)

* except Brooks-Herring Ionized Impurity Scattering which also requires Carrier Concentration and Dielectric Constant

Start Window – Save Information



Thermoelectric Optimizer - SPB Model App

File Edit Compute Thermal Help

Input parameters

Compound Name (req.)

Temperature / K (req.)

Seebeck Coefficient / $\mu\text{V K}^{-1}$ (req.)

Hall Carrier Concentration / cm^{-3}

Hall Mobility / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

Thermal Conductivity / $\text{W m}^{-1} \text{K}^{-1}$

Dielectric Constant (Only Ionized Impurity)

Acoustic Deformation Potential

Calculate

Output parameters

Chemical Potential / meV

Effective Mass / m_e

Intrinsic Mobility / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

Lorenz Number / $\text{W } \Omega \text{K}^{-2}$

Electronic Thermal Conductivity / $\text{W m}^{-1} \text{K}^{-1}$

Lattice Thermal Conductivity / $\text{W m}^{-1} \text{K}^{-1}$

Thermoelectric Figure of Merit

Input Parameters for Plot

Min. Carrier Concentration / cm^{-3} Max. Carrier Concentration / cm^{-3}

Seebeck Coefficient

Plot **Save Plot**

Q **R** **Save**

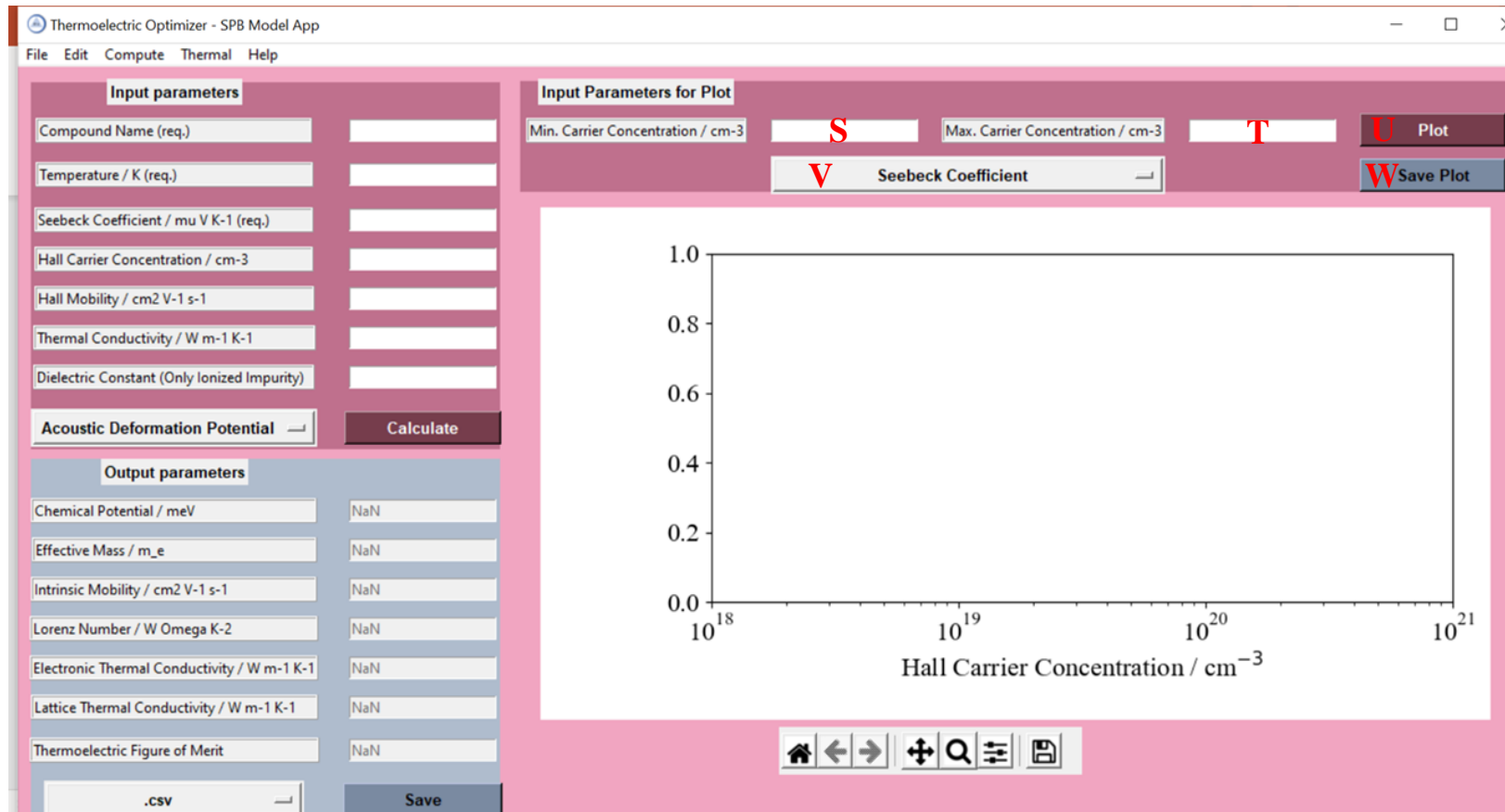
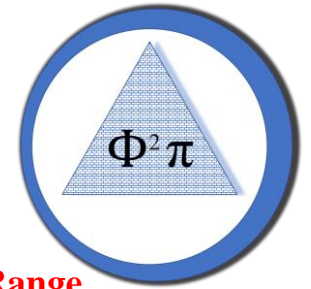
Q : Extension of File to save the above properties

- .csv (Comma delimited file) → Can be open with Excel
- .json (Json file) → Can be open with Python

R : Save Button

When the button ‘Calculate’ is pressed, a temporary file is produced and saved in the App folder. The information of the temporary file is used for the file to save to avoid that you change accidentally the input parameters and save the incorrect input parameters with the calculated parameters.

Start Window – Plot Information



Carrier Concentration Range

S : Minimum Carrier Concentration in cm^{-3}
(required; only positive values)

(Carrier Concentration should be above $1\text{E}12$ and below $1\text{E}24 \text{ cm}^{-3}$)

T : Maximum Carrier Concentration in cm^{-3}
(required; only positive values)

(Carrier Concentration should be above $1\text{E}12$ and below $1\text{E}24 \text{ cm}^{-3}$ and should be higher than minimum Carrier Concentration)

U : Plot button (Input parameters are required)
Create temporary file for the plot data

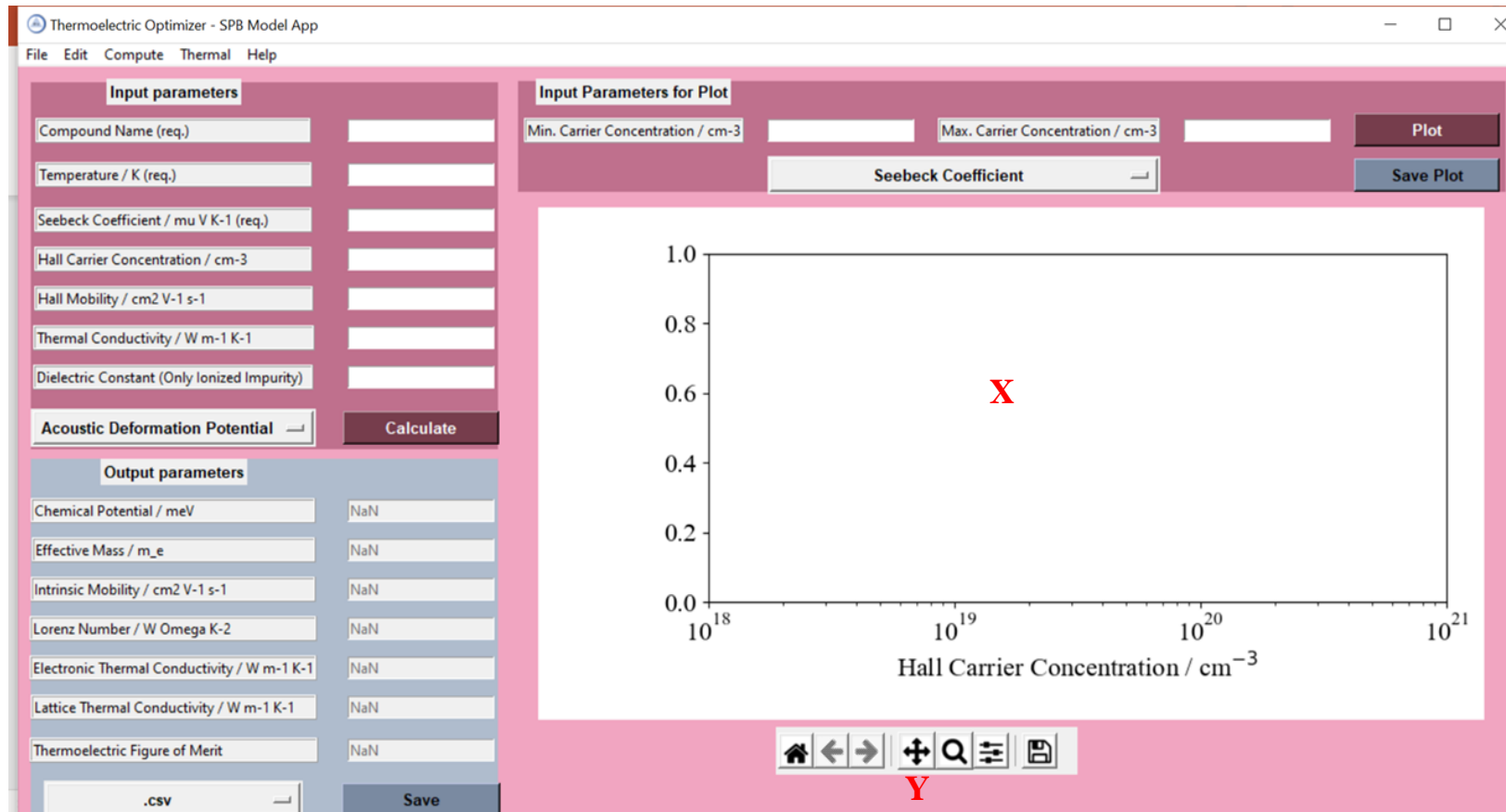
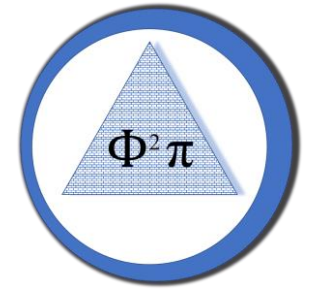
V : Plot Data on y-axis *

- Seebeck Coefficient (requires A, B, C, S, and T)
- Mobility (requires A, B, C, D, E, S, and T)
- Lorenz number (requires A, B, C, S, and T)
- Thermoelectric Figure of Merit (requires A, B, C, D, E, F, S, and T)

*** except Brooks-Herring Ionized Impurity Scattering which also requires Carrier Concentration and Dielectric Constant**

W : Save Button (save data of the plot with the extension which is set in R)

Start Window



X : Plot

Y : (from left to right)

House : Original Plot

Arrow left : Go to last step (if you zoomed in)

Arrow right : Go one step forward (if you went back)

Cross : Left-click → move graph

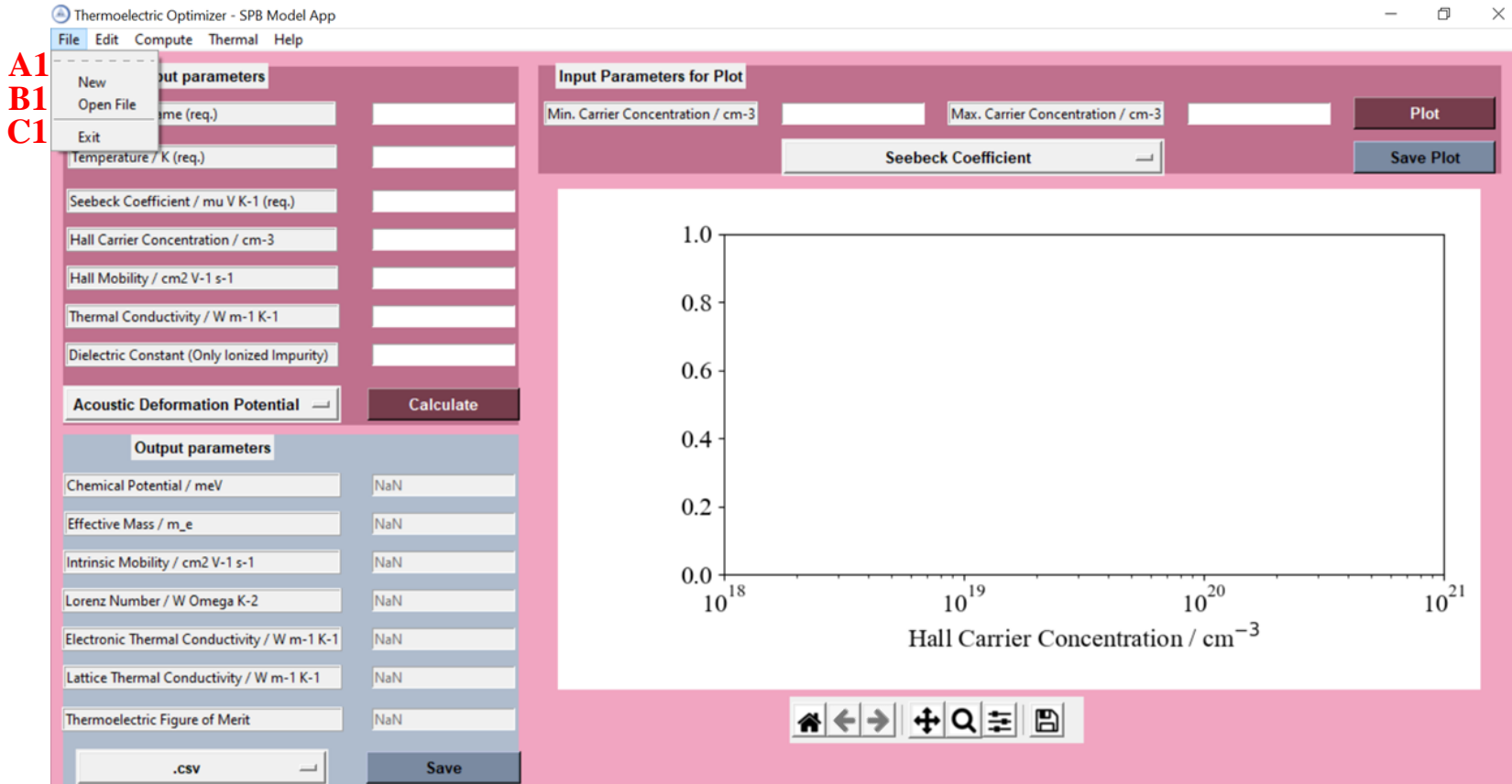
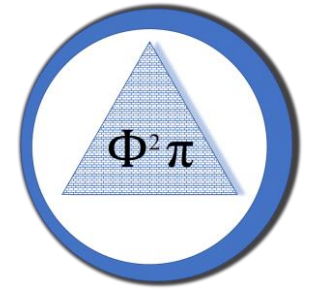
Right-click → zoom in

Magnifying glass : Zoom in

Shifters : No effect

Disk : Save the plot

File Menu



A1 : New

- Remove all temporary files
- Clean Plot
- Remove all data

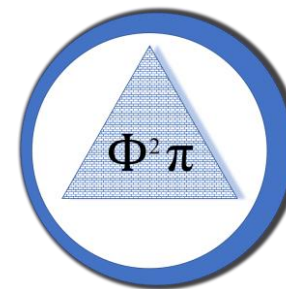
B1: Open File

- Open .csv file (see next slide)

C1: Exit

- Close the App
- Remove all temporary files

Open File



Seebeck Coefficient
in $\mu\text{V K}^{-1}$ → needs to
be positive

Carrier Concentration
in cm^{-3} → needs to be
positive

Thermal Conductivity
in $\text{W m}^{-1} \text{K}^{-1}$

Compound
Name

Temperature
in K

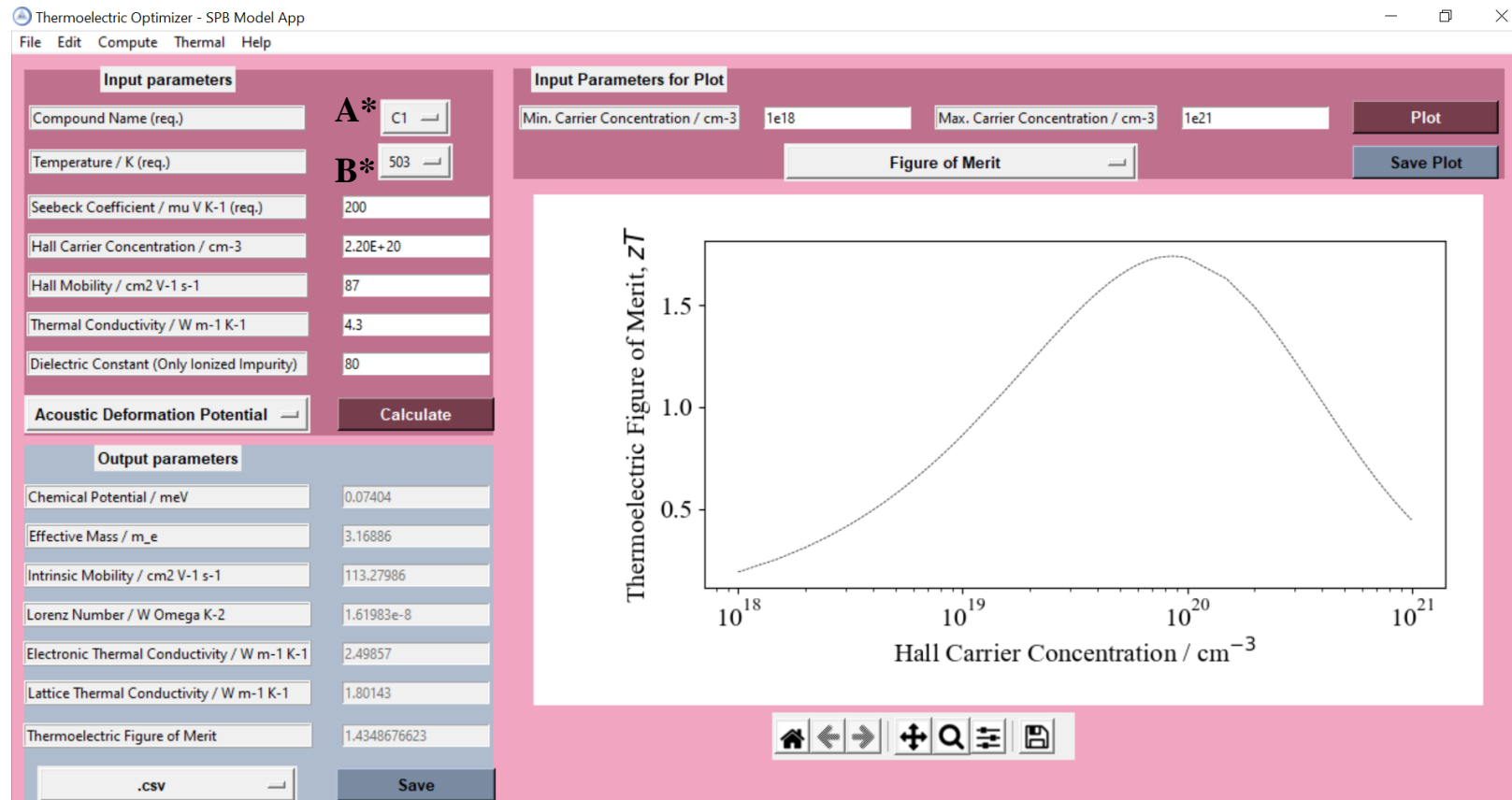
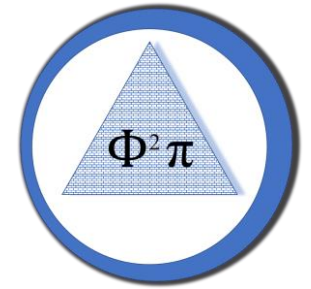
Mobility in
 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

Dielectric Constant

Example CSV file
(It needs to be in
this order and no
empty rows; empty
values are fine but
you need at least
a name, temperature
and Seebeck
coefficient for each
row; marked in red)

	A	B	C	D	E	F	G	H	I
1	Compound	Temperature / K	Seebeck Coefficient / $\mu\text{V K}^{-1}$	Carrier Concentration / cm^{-3}	Mobility / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$	Thermal Conductivity / $\text{W m}^{-1} \text{K}^{-1}$	Dielectric Constant		
2	A1	300	140	$3.00\text{E}+19$	80	3.4	200		
3	A1	400	180	$3.60\text{E}+19$	60	2.7	200		
4	A1	600	220	$3.90\text{E}+19$	34	2.1	200		
5	B1	450	35	$3.00\text{E}+21$	10	12	10		
6	C1	303	98	$1.00\text{E}+20$	112	5	80		
7	C1	403	145	$2.00\text{E}+20$	97	4.6	80		
8	C1	503	200	$2.20\text{E}+20$	87	4.3	80		
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									
21									

Uploaded Data

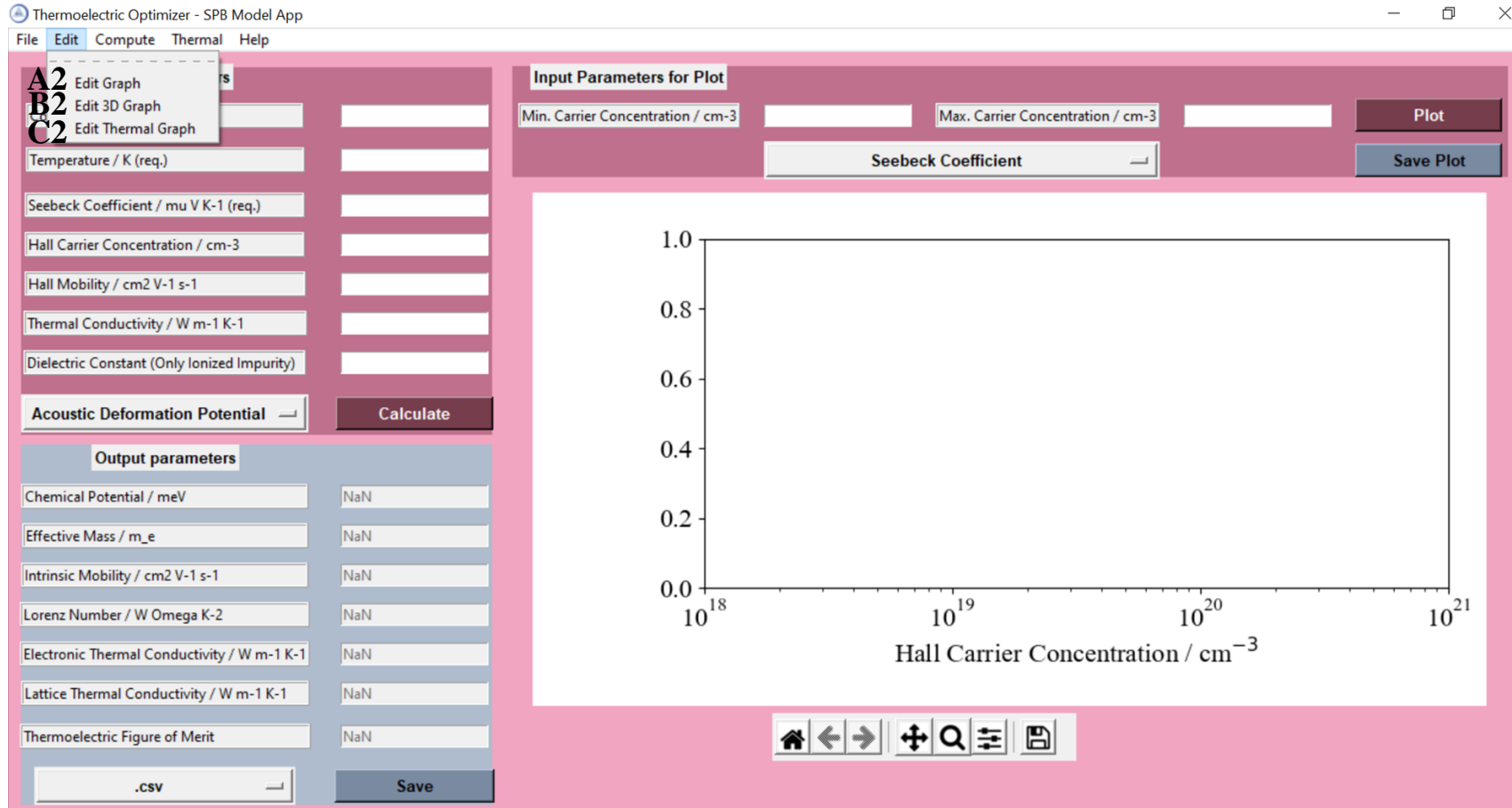
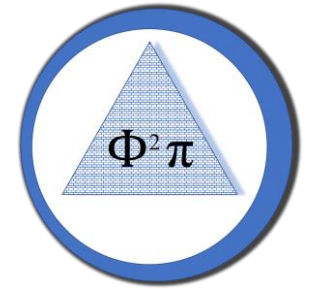


A* : List of Compound names
B* : List of Temperatures for the Corresponding Compound

Changing the compound will update the temperature list and the Seebeck Coefficient, Carrier Concentration, Mobility, Thermal Conductivity and Dielectric Constant

(The same for changing the temperature)

Edit Menu



A2 : Edit Graph

- Edit the graph on the first window and optimized graphs (see later)
- Other font, font size, or reposition it

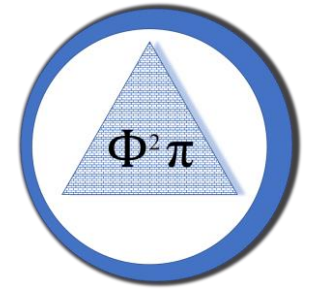
B2 : Edit 3D Graph

- Edit the graph for the 3D plot
- Other font, font size, or change the surface to a 3D grid

C2 : Edit Thermal Graph

- Edit the graph for the thermal plots
- Other font, font size, or reposition it

Edit Graph



Thermoelectric Optimizer - SPB Model App

Change font for figure

Font Size: 16 **A_Graph** Font: Times New Roman **B_Graph**

Change dimensions for figure

Figure Width: 8 **C_Graph** Figure Height: 4.3 **D_Graph**

Plot Start x: 0.18 **E_Graph** Plot Width x: 0.78 **F_Graph**

Plot Start y: 0.23 **G_Graph** Plot Width y: 0.68 **H_Graph**

Resolution / dpi: 100 **I_Graph** Close window

A_Graph : Font Size

B_Graph : Font (Choose certain fonts) *

C_Graph : Width of the figure

D_Graph : Height of the figure

E_Graph : x-point where the plot starts in the figure

F_Graph : Width of the plot

G_Graph : y-point where the plot starts in the figure

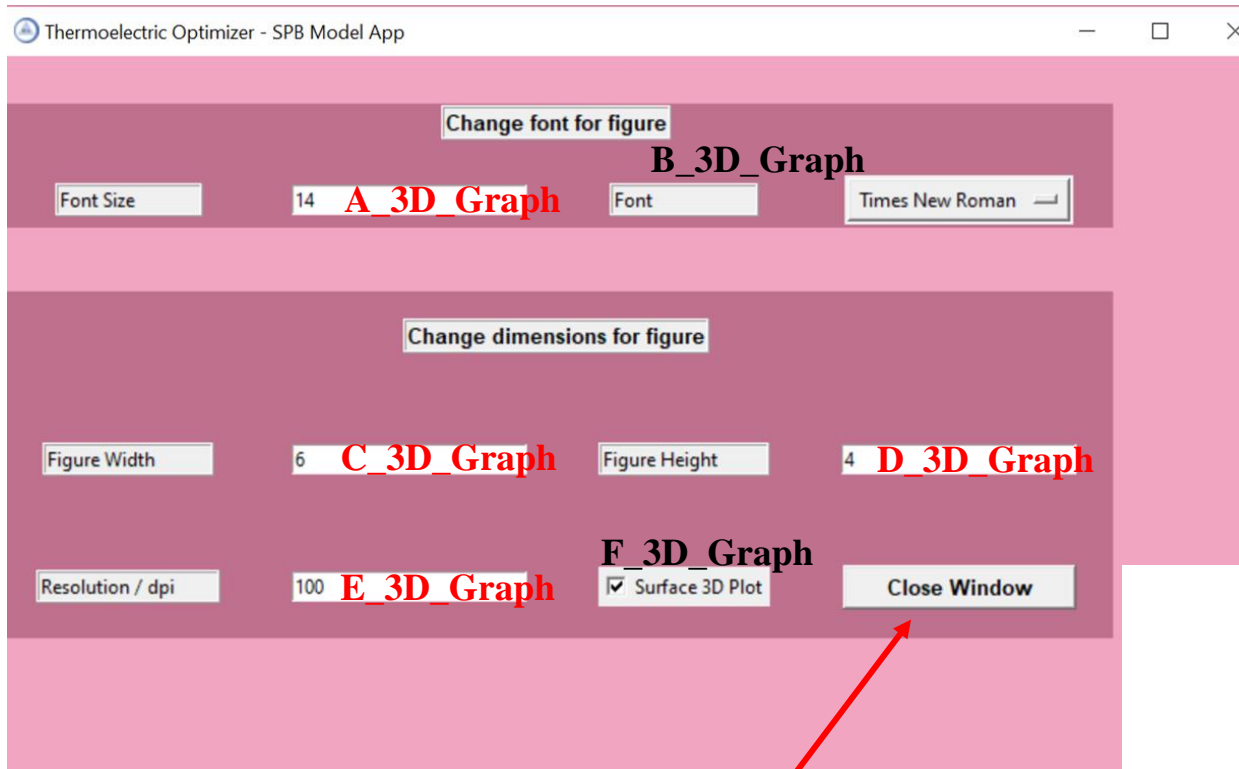
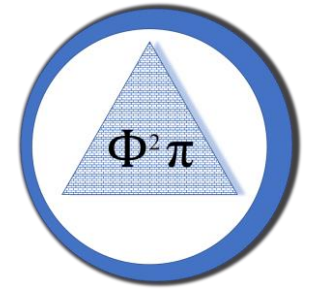
H_Graph : Height of the plot

I_Graph : resolution in dpi (change in resolution will change size in figures)

*** For more fonts, please send me an email**

**Close the
window
(produce an
empty graph)**

Edit Graph 3D



Close the
Window

* For more fonts, please send me an email

A_3D_Graph : Font Size

B_3D_Graph : Font (Choose selected fonts) *

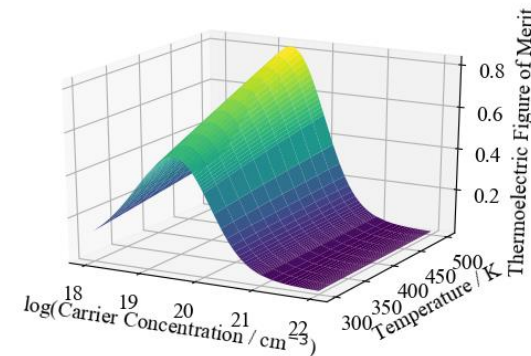
C_3D_Graph : Width of the 3D figure

D_3D_Graph : Height of the 3D figure

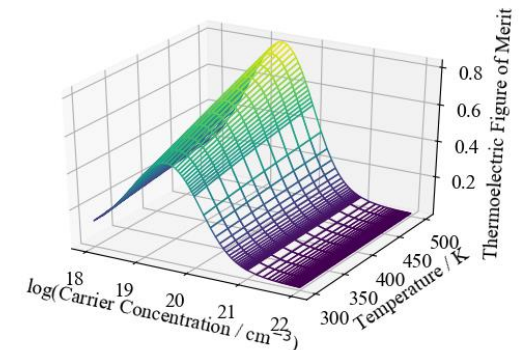
E_3D_Graph : resolution of the graph (change figure size)

F_3D_Graph : Change between a surface or wired 3D Figure

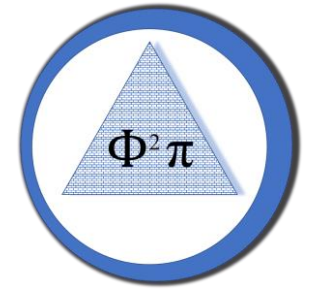
Surface:



Wired:



Edit Thermal Graph



Thermoelectric Optimizer - SPB Model App

Change font for figure

Font Size: 16 **A_Graph** Font: Times New Roman **B_Graph**

Change dimensions for figure

Figure Width: 6 **C_Graph** Figure Height: 3 **D_Graph**

Plot Start x: 0.25 **E_Graph** Plot Width x: 0.7 **F_Graph**

Plot Start y: 0.2 **G_Graph** Plot Width y: 0.7 **H_Graph**

Resolution / dpi: 100 **I_Graph** Close window

A_Graph : Font Size

B_Graph : Font (Choose certain fonts) *

C_Graph : Width of the figure

D_Graph : Height of the figure

E_Graph : x-point where the plot starts in the figure

F_Graph : Width of the plot

G_Graph : y-point where the plot starts in the figure

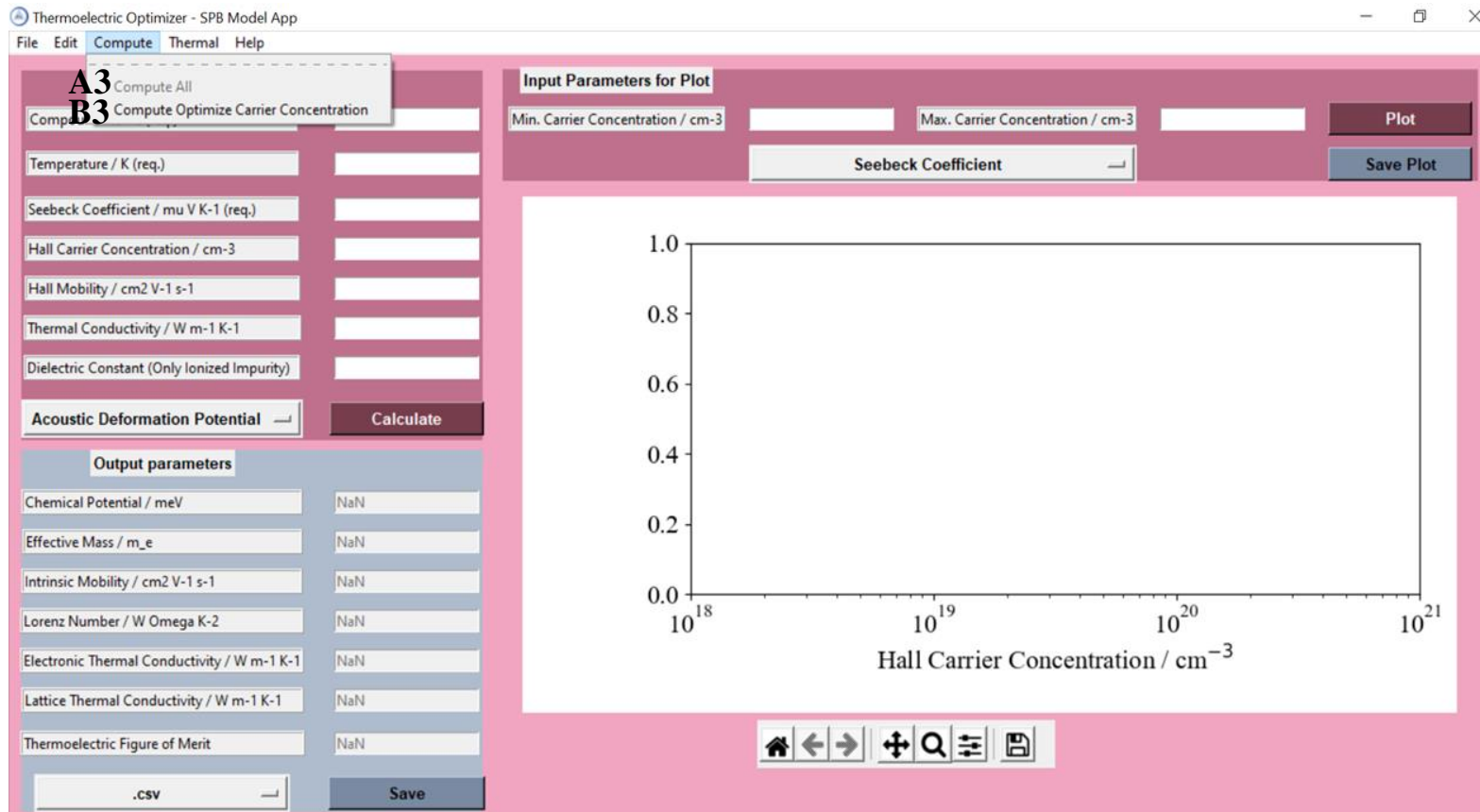
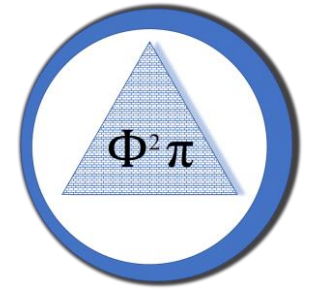
H_Graph : Height of the plot

I_Graph : resolution in dpi (change in resolution will change size in figures)

*** For more fonts, please send me an email**

**Close the
window
(produce an
empty graph)**

Compute Menu



A3 : Compute All (enabled when a file was open)

- Compute all the properties of a .csv file
- If Minimum and Maximum Carrier Concentration are given, compute all the properties as a function of Carrier Concentration
- Save computed data in a folder → each compound/temperature pair has its own file

B3 : Compute Optimize Carrier Concentration

- Compute the Thermoelectric Figure of Merit as a function of Carrier Concentration and Temperature
- Compute Optimized Carrier Concentration and the corresponding Optimized Thermoelectric Figure of Merit

Compute Optimized Carrier Concentration

Thermoelectric Optimizer - SPB Model App

Provide polynomial fitting coefficients of all thermoelectric parameters

Seebeck Coefficient Coefficients / $\mu\text{V K}^{-1}$ 1 **A_Opt** *T⁰

Hall Carrier Concentrations Coefficients / cm^{-3} 1 **B_Opt** *T⁰

Hall Mobility Coefficients / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ 1 **C_Opt** *T⁰

Thermal Conductivity Coefficients / $\text{W m}^{-1} \text{K}^{-1}$ 1 **D_Opt** *T⁰

Temperature range / K Min. T Max. T Step T

Hall Carrier Concentration range / cm^{-3} Min. nH Max. nH

Acoustic Deformation Potential 3D plot Exp. Plot Opt. Plot Plot .csv Save Close Window

A_Opt: Temperature-dependent Seebeck Coefficient in $\mu\text{V K}^{-1}$ described by polynomial to the fifth order

For example: $S = 100 * T^0 + 0.8 * T^1 + -1\text{E-}5 * T^2 \rightarrow$ Change List to 3 and write 100, 0.8, and -1E-5 in the three fields

B_Opt: Temperature-dependent Carrier Concentration cm^{-3} described by polynomial to the fifth order

C_Opt: Temperature-dependent Mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ described by polynomial to the fifth order

D_Opt: Temperature-dependent Thermal Conductivity in $\text{W m}^{-1} \text{K}^{-1}$ described by polynomial to the fifth order

Compute Optimized Carrier Concentration

Thermoelectric Optimizer - SPB Model App

Provide polynomial fitting coefficients of all thermoelectric parameters

Seebeck Coefficient Coefficients / $\mu\text{V K}^{-1}$ * T^0

Hall Carrier Concentrations Coefficients / cm^{-3} * T^0

Hall Mobility Coefficients / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ * T^0

Thermal Conductivity Coefficients / $\text{W m}^{-1} \text{K}^{-1}$ * T^0

Temperature range / K **E_Opt** **F_Opt** **G_Opt**

Hall Carrier Concentration range / cm^{-3} **H_Opt** **I_Opt**

Acoustic Deformation Potential

☐ 3D plot ☐ Exp. Plot ☐ Opt. Plot

E_Opt: Minimum Temperature in K (above 1 and below 10,000 K)

F_Opt: Maximum Temperature in K (above 1 and below 10,000 K and above Minimum Temperature)

G_Opt: Temperature Step in K (above 1 and below 100 K)

H_Opt: Temperature-dependent Thermal Conductivity in $\text{W m}^{-1} \text{K}^{-1}$ described by polynomial to the fifth order

Compute Optimized Carrier Concentration

Thermoelectric Optimizer - SPB Model App

Provide polynomial fitting coefficients of all thermoelectric parameters

Seebeck Coefficient Coefficients / $\mu\text{V K}^{-1}$ 1 $\ast T^0$

Hall Carrier Concentrations Coefficients / cm^{-3} 1 $\ast T^0$

Hall Mobility Coefficients / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ 1 $\ast T^0$

Thermal Conductivity Coefficients / $\text{W m}^{-1} \text{K}^{-1}$ 1 $\ast T^0$

Temperature range / K Min. T Max. T Step T

Hall Carrier Concentration range / cm^{-3} Min. nH Max. nH

J_Opt **K_Opt** **L_Opt** **M_Opt**

Acoustic Deformation Potential 3D plot Exp. Plot Opt. Plot Plot .csv Save Close Window

J_Opt: Choose the scattering mechanism (5)

- Acoustic Deformation Potential
- Polar Optical Phonon
- Ionized Impurity
- Polar Optical Phonon (Fermi)
- Ionized Impurity (Fermi)

K_Opt: Create a 3D plot (Temperature, Carrier Concentration and Thermoelectric Figure of Merit)

L_Opt: Create experimental Carrier Concentration vs Temperature and experimental Thermoelectric Figure of Merit vs Temperature

M_Opt: Create optimized Carrier Concentration vs Temperature and optimized Thermoelectric Figure of Merit vs Temperature

(If both are clicked, the experimental Carrier Concentration and Thermoelectric Figure of Merit are compared to the optimized values)

Compute Optimized Carrier Concentration

Thermolectric Optimizer - SPB Model App

Provide polynomial fitting coefficients of all thermoelectric parameters

Seebeck Coefficient Coefficients / $\mu\text{V K}^{-1}$ 1 T^0

Hall Carrier Concentrations Coefficients / cm^{-3} 1 T^0

Hall Mobility Coefficients / $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ 1 T^0

Thermal Conductivity Coefficients / $\text{W m}^{-1} \text{K}^{-1}$ 1 T^0

Temperature range / K Min. T Max. T Step T

Hall Carrier Concentration range / cm^{-3} Min. nH Max. nH

Acoustic Deformation Potential ☐ 3D plot ☐ Exp. Plot ☐ Opt. Plot

N_Opt Plot O_Opt .csv P_Opt Save Close Window

Close the Window

N_Opt : Plot the data for the corresponding plots (K, L, or M)

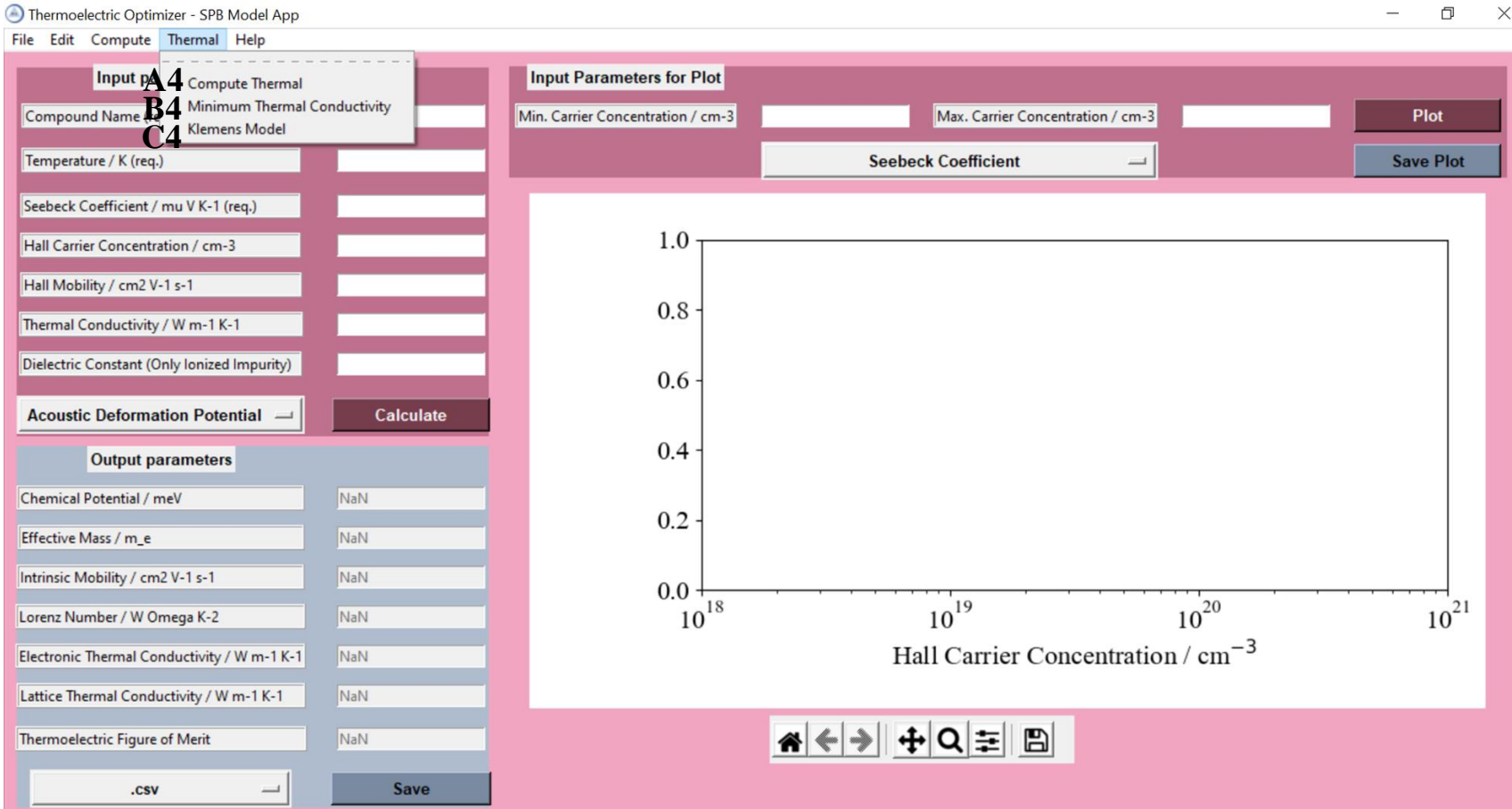
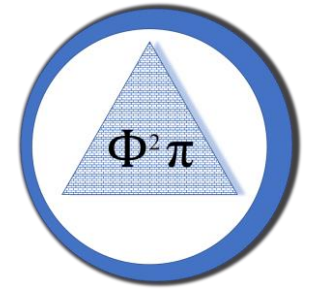
O_Opt : Choose the format to save the computed data (experimental versus optimized data)

- .csv file (Excel format)
- .json file (Python format)

P_Opt : Save button

Important: If the data is plotted, the main window can decrease (if the App is using in Microsoft Windows). You can change it by going → Display Settings → Change the size of text, apps, and other items to 100%

Thermal Menu



A4 : Compute Thermal

- Upload total thermal conductivity data
- Compute the electronic and phononic contributions using different scattering mechanisms
- Save computed data in a folder

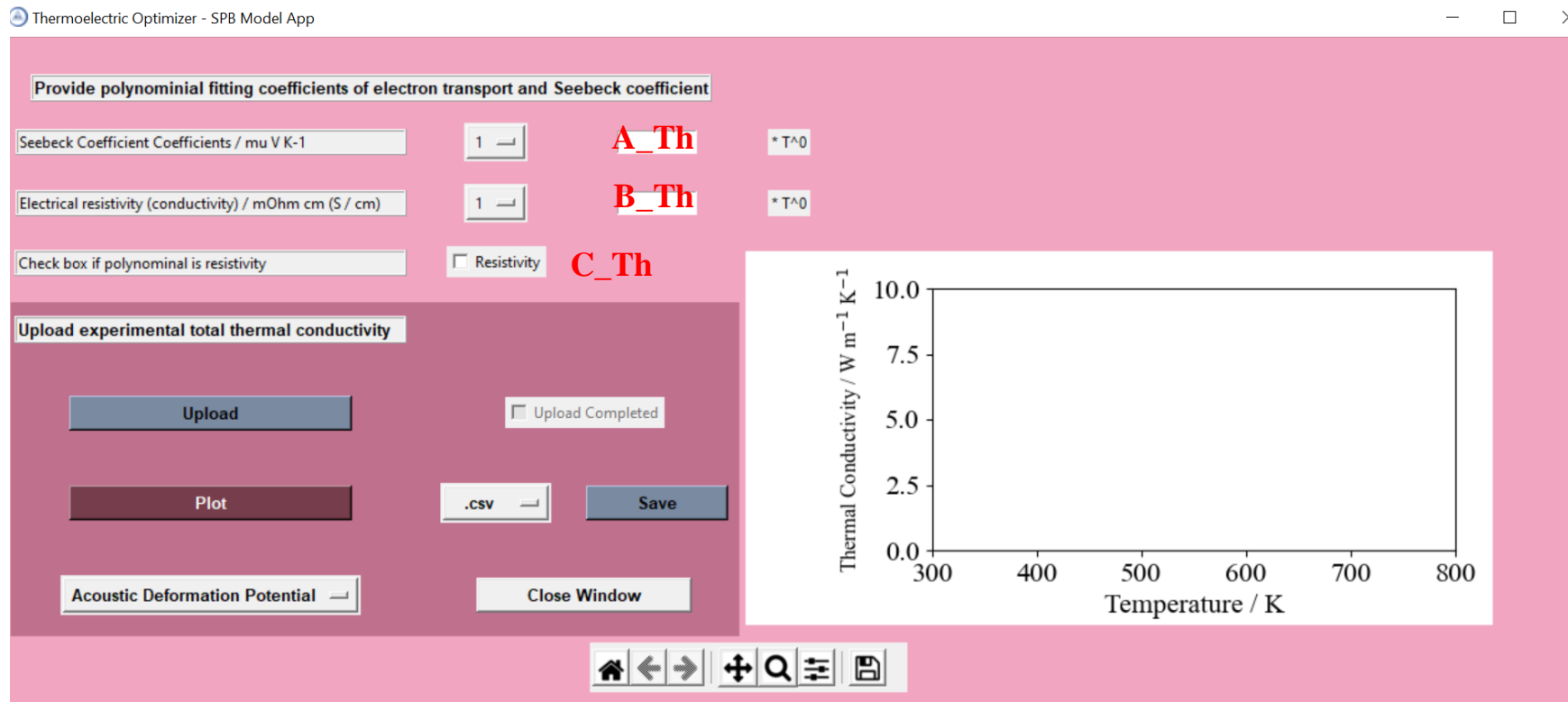
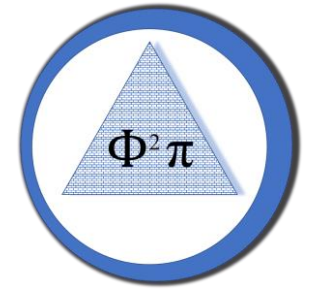
B4 : Minimum Thermal Conductivity

- Compute the minimum thermal conductivity at high temperature or as function of temperature
- Different models can be applied
- Save computed data

C4 : Klemens Model

- Compute the phononic contribution of the thermal conductivity for different dopings
- Find the optimum concentration between two compounds to lower the lattice thermal conductivity

Compute Thermal



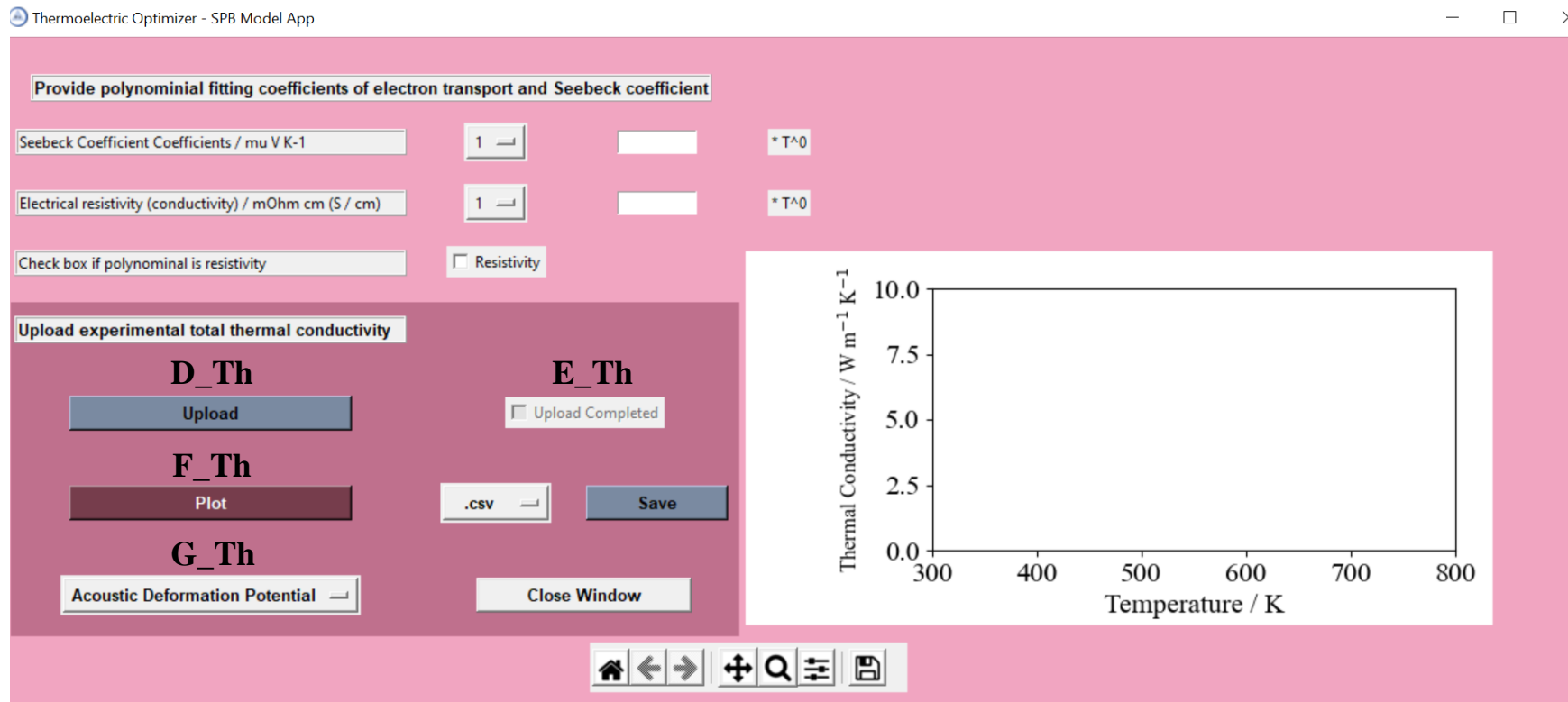
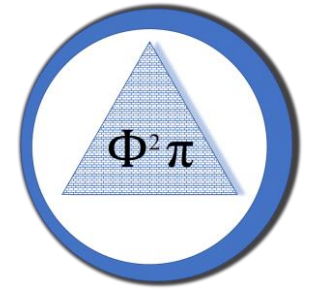
A_Th : Temperature-dependent Seebeck Coefficient in $\mu\text{V K}^{-1}$ described by polynomial to the fifth order

For example: $S = 100 * T^0 + 0.8 * T^1 + -1\text{E-}5 * T^2 \rightarrow$ Change List to 3 and write 100, 0.8, and -1E-5 in the three fields

B_Th : Temperature-dependent electrical resistivity in $\text{m}\Omega \text{ cm}$ (if box is clicked) or electrical conductivity in S cm^{-1} described by polynomial to the fifth order

C_Th : Checkbox. If checked electron transport data is resistivity; if not, electron transport data is electrical conductivity.

Compute Thermal



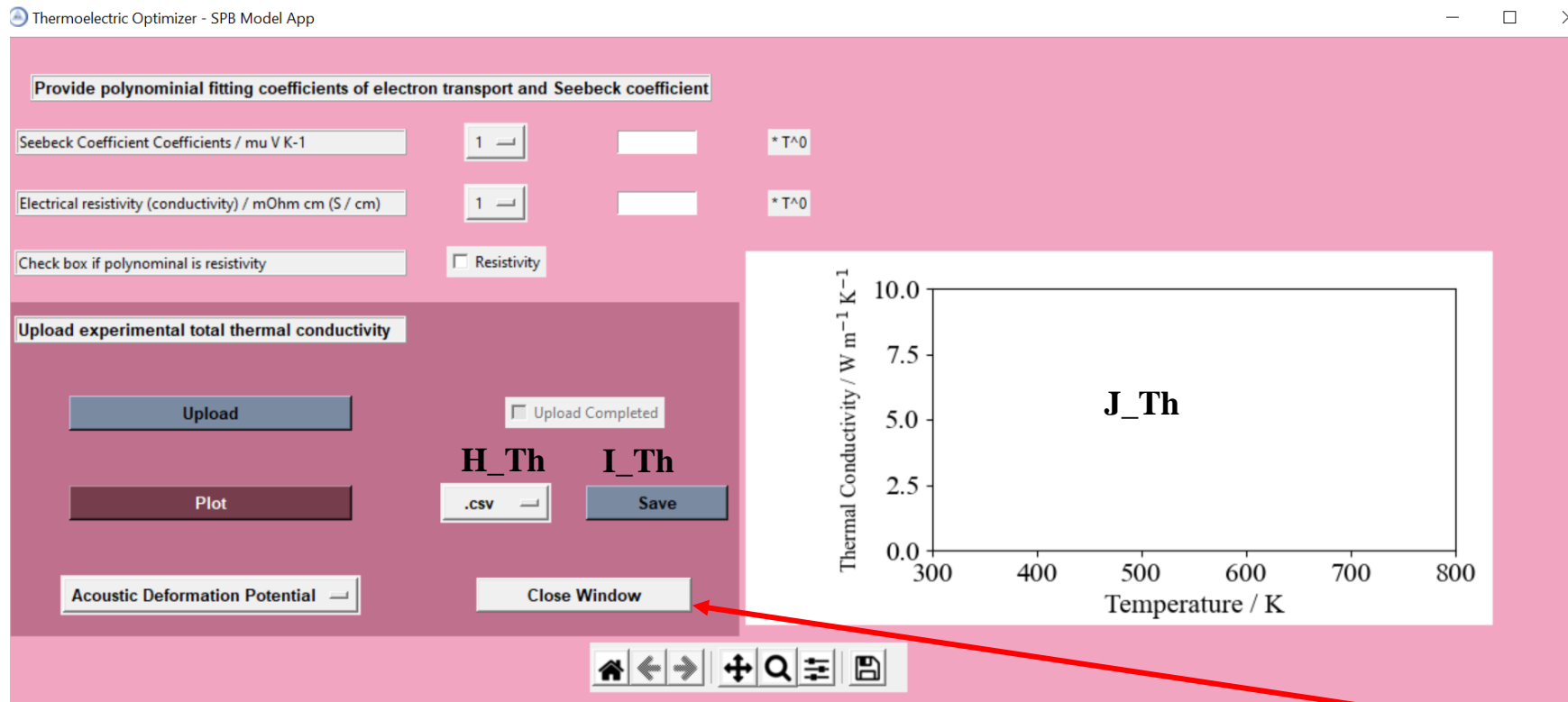
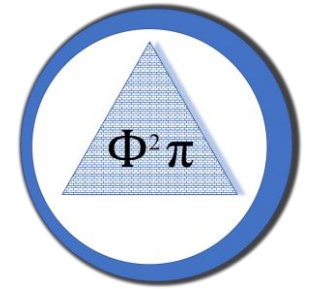
D_Th : Upload thermal data; see Thermal.csv as example (x data named temperature; y data named thermal)

E_Th : If checkbox is checked, a file was successfully upload

F_Th : Plot the data for the total thermal conductivity as well as electronic and phononic contributions.

G_Th : Choose the scattering mechanism (5); see page 22.

Compute Thermal



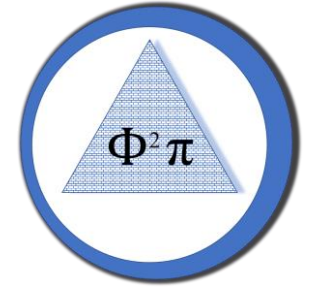
H_Th : Choose the format to save the computed data

- .csv file (Excel format)
- .json file (Python format)

I_Th : Save button

J_Th : Graph to show the thermal conductivity → can be changed under Edit → Edit Thermal Graph.

Close the Window



Upload Thermal File

Example Thermal.csv file
(It can only two columns
with the names:

- **temperature in K**
- **Thermal in $\text{W m}^{-1} \text{K}^{-1}$**

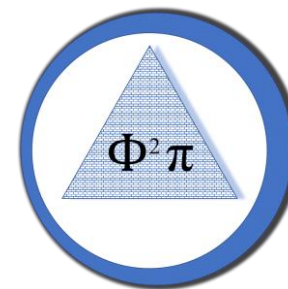
in the first row)

Temperature
in K

Total Thermal Conductivity
in $\text{W m}^{-1} \text{K}^{-1}$

	A	B	C	D	E	F	G	H	I
1	temperature	thermal							
2	300	3.5							
3	350	3.25							
4	400	3							
5	450	2.75							
6	500	2.5							
7	550	2.25							
8	600	2							
9	650	1.75							
10	700	1.5							
11	750	1.25							
12	800	1							
13									
14									
15									

Minimum Thermal Conductivity



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / Å ³ (req.)	A_MT		
Number of atoms per unit cell (req.)	B_MT	Mass density / g cm ⁻³ (req.)	C_MT
Longitudinal speed of sound / m s ⁻¹	D_MT	Bulk modulus / Pa	F_MT
Transverse speed of sound / m s ⁻¹	E_MT	Shear modulus / Pa	G_MT

Temperature range / K

Debye temperature / K		Temperature step / K	
Minimum temperature / K		Maximum temperature / K	

Output parameters

Cahill-Pohl

Minimum thermal conductivity / W m⁻¹ K⁻¹

Output Temperature

Cahill-Pohl

.csv

A_MT : Unit Cell Volume in Å³ (required)

B_MT : Number of atoms per unit cell (required)

C_MT : Mass density in g cm⁻³ (required)

D_MT : Longitudinal speed of sound in m s⁻¹

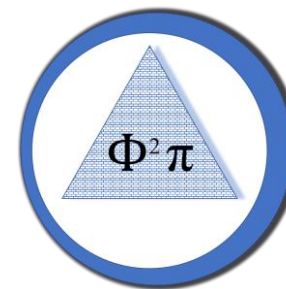
E_MT : Transverse speed of sound in m s⁻¹

F_MT : Bulk modulus in Pa

G_MT : Shear modulus in Pa

(You need to provide longitudinal and transverse speed of sound OR bulk and shear modulus)

Minimum Thermal Conductivity



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / Å ³ (req.)			
Number of atoms per unit cell (req.)		Mass density / g cm ⁻³ (req.)	
Longitudinal speed of sound / m s ⁻¹		Bulk modulus / Pa	
Transverse speed of sound / m s ⁻¹		Shear modulus / Pa	

Temperature range / K

Debye temperature / K	H_MT	Temperature step / K	I_MT
Minimum temperature / K	J_MT	Maximum temperature / K	K_MT

Output parameters

Cahill-Pohl

Minimum thermal conductivity / W m⁻¹ K⁻¹

Output Temperature

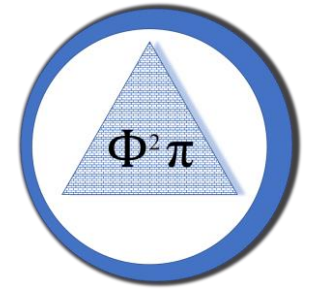
Cahill-Pohl

.csv

H_MT : Debye temperature in K
(can be inserted or it will be
calculated from the longitudinal
and transverse speed of sound
OR the bulk and shear modulus)
I_MT : Temperature step in K
(required for the plot)
J_MT : Minimum temperature in
K (required for the plot)
K_MT : Maximum temperature
in K (required for the plot)

Minimum thermal conductivity is
plotted from the minimum to the
maximum temperature with a
temperature step

Minimum Thermal Conductivity



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / A3 (req.)			
Number of atoms per unit cell (req.)		Mass density / g cm-3 (req.)	
Longitudinal speed of sound / m s-1		Bulk modulus / Pa	
Transverse speed of sound / m s-1		Shear modulus / Pa	

Temperature range / K

Debye temperature / K		Temperature step / K	
Minimum temperature / K		Maximum temperature / K	

Output parameters

Cahill-Pohl **L_MT**

Minimum thermal conductivity / W m-1 K-1

M_MT

N_MT

Output Temperature

Cahill-Pohl

.csv

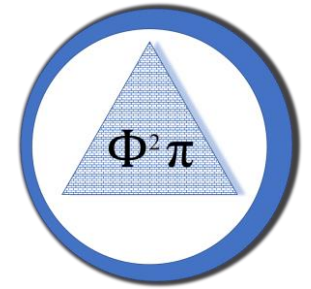
L_MT : Five (5) different models to compute the minimum thermal conductivity in $\text{W m}^{-1} \text{K}^{-1}$

- Cahill-Pohls
- Pohls
- Dynamic
- Diffusion
- Clarke

(see next slide)

M_MT : Calculate the minimum thermal conductivity in $\text{W m}^{-1} \text{K}^{-1}$ using the input parameters and the model

N_MT : Minimum temperature in $\text{W m}^{-1} \text{K}^{-1}$



Minimum Thermal Conductivity

Models used:

Cahill-Pohl: D. G. Cahill and R. O. Pohl, “Lattice Vibrations and Heat Transport in Crystals and Glasses,” Annual Review of Physical Chemistry, 39, 93–121, 1988.

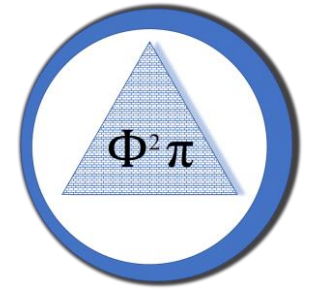
Pohls: J.-H. Pohls, M. B. Johnson, and M. A. White, “Origins of ultralow thermal conductivity in bulk [6,6]-phenyl-C61-butyric acid methyl ester (PCBM),” Physical Chemistry Chemical Physics, 18, 1185–1190, 2016.

Dynamic: J.-H. Pohls et al., "Metal phosphides as potential thermoelectric materials," Journal of Materials Chemistry C 5, 12441-12456, 2017.

Diffusive: M. T. Agne, R. Hanus and G. Jeffrey Snyder, "Minimum thermal conductivity in the context of diffuson-mediated thermal transport," Energy Environ. Sci. 11, 609-616, 2018.

Clarke: D. R. Clarke, "Materials selection guidelines for low thermal conductivity thermal barrier coatings," Surf. Coat. Technol. 163, 67—74, 2003.

Minimum Thermal Conductivity



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / A ³ (req.)			
Number of atoms per unit cell (req.)		Mass density / g cm ⁻³ (req.)	
Longitudinal speed of sound / m s ⁻¹		Bulk modulus / Pa	
Transverse speed of sound / m s ⁻¹		Shear modulus / Pa	

Temperature range / K

Debye temperature / K		Temperature step / K	
Minimum temperature / K		Maximum temperature / K	

Output parameters

Cahill-Pohl

Minimum thermal conductivity / W m⁻¹ K⁻¹

O_MT

Cahill-Pohl

Q_MT

.csv

Output Temperature

P_MT

R_MT

O_MT : Three (3) different models to compute the minimum thermal conductivity in W m⁻¹ K⁻¹ as function of temperature

- Cahill-Pohls
- Pohls
- Diffusion

P_MT : Plot the minimum thermal conductivity in W m⁻¹ K⁻¹ as function of temperature

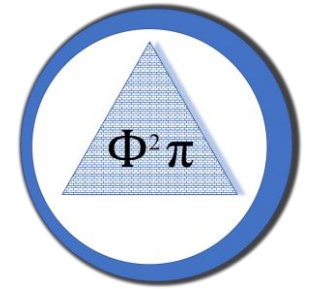
N_MT : Choose the format to save the computed data

- .csv file (Excel format)
- .json file (Python format)

R_MT : Save button

Close the Window

Klemens Model



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / Å ³ (req.)	A_KM	Unit cell volume / Å ³ (doped)	
Number of atoms per unit cell (req.)	B_KM	Number of atoms per unit cell (doped)	
Longitudinal speed of sound / m s ⁻¹ (req.)	C_KM	Longitudinal speed of sound / m s ⁻¹ (doped)	
Transverse speed of sound / m s ⁻¹ (req.)	D_KM	Transverse speed of sound / m s ⁻¹ (doped)	
Lattice thermal conductivity / W m ⁻¹ K ⁻¹ (req.)	E_KM	Lattice thermal conductivity / W m ⁻¹ K ⁻¹ (doped)	

Site(s)	Molar Mass	Radius	Fraction

Output parameters

Lattice thermal conductivity / W m⁻¹ K⁻¹

Calculate

Plot as function of fraction

Plot

.csv Save

Close Window

Parameters of the undoped sample

A_KM : Unit Cell Volume in Å³ (required)

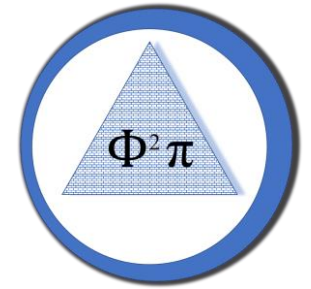
B_KM : Number of atoms per unit cell (required)

C_KM : Longitudinal speed of sound in m s⁻¹ (required)

D_KM : Transverse speed of sound in m s⁻¹ (required)

E_KM : Lattice thermal conductivity in W m⁻¹ K⁻¹ (required)

Klemens Model



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / Å ³ (req.)		Unit cell volume / Å ³ (doped)	F_KM
Number of atoms per unit cell (req.)		Number of atoms per unit cell (doped)	G_KM
Longitudinal speed of sound / m s ⁻¹ (req.)		Longitudinal speed of sound / m s ⁻¹ (doped)	H_KM
Transverse speed of sound / m s ⁻¹ (req.)		Transverse speed of sound / m s ⁻¹ (doped)	I_KM
Lattice thermal conductivity / W m ⁻¹ K ⁻¹ (req.)		Lattice thermal conductivity / W m ⁻¹ K ⁻¹ (doped)	J_KM

Site(s)	Molar Mass	Radius	Fraction

Output parameters

Lattice thermal conductivity / W m⁻¹ K⁻¹

Calculate

Plot as function of fraction

Plot

.csv Save

Close Window

Parameters of the doped sample (only for the plot)

F_KM : Unit Cell Volume in Å³
G_KM : Number of atoms per unit cell

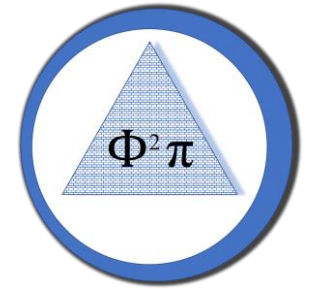
H_KM : Longitudinal speed of sound in m s⁻¹

I_KM : Transverse speed of sound in m s⁻¹

J_KM : Lattice thermal conductivity in W m⁻¹ K⁻¹

P. G. Klemens, “The thermal conductivity of dielectric solids at low temperatures.” Proc. Royal Soc. London - ser. A 1951, 208, 108.

Klemens Model



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / A3 (req.)		Unit cell volume / A3 (doped)	
Number of atoms per unit cell (req.)		Number of atoms per unit cell (doped)	
Longitudinal speed of sound / m s-1 (req.)		Longitudinal speed of sound / m s-1 (doped)	
Transverse speed of sound / m s-1 (req.)		Transverse speed of sound / m s-1 (doped)	
Lattice thermal conductivity / W m-1 K-1 (req.)		Lattice thermal conductivity / W m-1 K-1 (doped)	

Output parameters

Lattice thermal conductivity / W m-1 K-1

Calculate

Plot as function of fraction

Plot

.csv Save

Close Window

Site(s)	Molar Mass	Radius	Fraction
K_KM	L_KM	M_KM	N_KM

K_KM : Site should be an integer (e.g., 1, 2, 3 – choose at least two atoms on the same site; you can choose multiple sites)

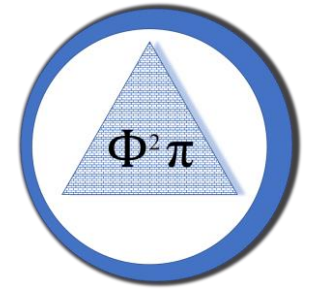
L_KM : Molar Mass (unit does not matter as long as it is consistent)

M_KM : Radius (ionic) (unit does not matter as long as it is consistent)

N_KM : Fraction should be between 0 and 1 and the sum of all fractions on the same site should be maximum 1

(For the plot, only the first two rows are considered)

Klemens Model



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / A3 (req.)		Unit cell volume / A3 (doped)	
Number of atoms per unit cell (req.)		Number of atoms per unit cell (doped)	
Longitudinal speed of sound / m s-1 (req.)		Longitudinal speed of sound / m s-1 (doped)	
Transverse speed of sound / m s-1 (req.)		Transverse speed of sound / m s-1 (doped)	
Lattice thermal conductivity / W m-1 K-1 (req.)		Lattice thermal conductivity / W m-1 K-1 (doped)	

Output parameters

Lattice thermal conductivity / W m-1 K-1

Calculate

Plot as function of fraction

Plot

.csv Save

Close Window

Site(s)	Molar Mass	Radius	Fraction
K_KM	L_KM	M_KM	N_KM

K_KM : Site should be an integer (e.g., 1, 2, 3 – choose at least two atoms on the same site; you can choose multiple sites)

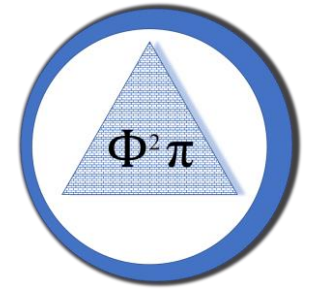
L_KM : Molar Mass (unit does not matter as long as it is consistent)

M_KM : Radius (ionic) (unit does not matter as long as it is consistent)

N_KM : Fraction should be between 0 and 1 and the sum of all fractions on the same site should be maximum 1

(For the plot, only the first two rows are considered)

Klemens Model



Thermoelectric Optimizer - SPB Model App

Input parameters

Unit cell volume / A3 (req.)		Unit cell volume / A3 (doped)	
Number of atoms per unit cell (req.)		Number of atoms per unit cell (doped)	
Longitudinal speed of sound / m s-1 (req.)		Longitudinal speed of sound / m s-1 (doped)	
Transverse speed of sound / m s-1 (req.)		Transverse speed of sound / m s-1 (doped)	
Lattice thermal conductivity / W m-1 K-1 (req.)		Lattice thermal conductivity / W m-1 K-1 (doped)	

Site(s)	Molar Mass	Radius	Fraction

Output parameters

Lattice thermal conductivity / W m-1 K-1

O_KM **P_KM**

Calculate

Plot as function of fraction

Q_KM

Plot

R_KM **S_KM**

.csv Save

Close Window

Close the
Window

O_KM : Calculate the lattice thermal conductivity in $\text{W m}^{-1} \text{K}^{-1}$ for different doping elements and levels

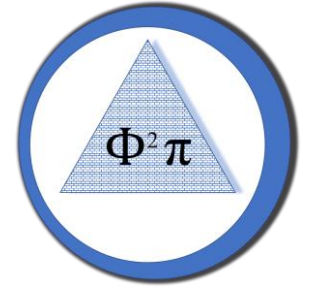
P_KM : Lattice thermal conductivity in $\text{W m}^{-1} \text{K}^{-1}$ for different doping elements and levels

Q_KM : Plot lattice thermal conductivity as function of fraction of the second row of elements to indicate the lowest thermal conductivities (e.g., of solid solutions)

R_KM : Choose the format to save the computed data

S_MT : Save button

Questions?



- If you have questions or concerns or find some errors, please send me an email: Jan.Poehls@Dal.ca
- Thank you for choosing the Thermoelectric Optimizer based on Scattering-dependent SPB Model App