Thermoelectric Optimizer – SPB Model App

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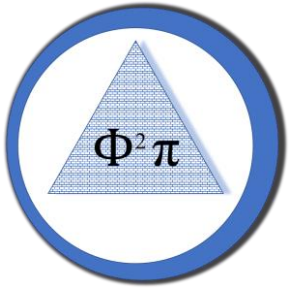
July 2020

Montreal QC Canada

Introduction

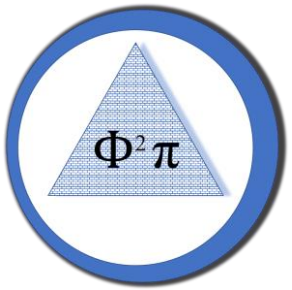


Welcome to the Thermoelectric Optimizer App.

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)

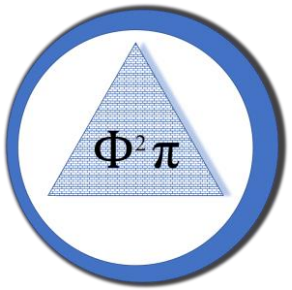
Installation

- Download all files (i.e., Thermoelectric Optimizer.py), the example .csv file (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 python file (.csv file can be in a different folder)

Starting the program

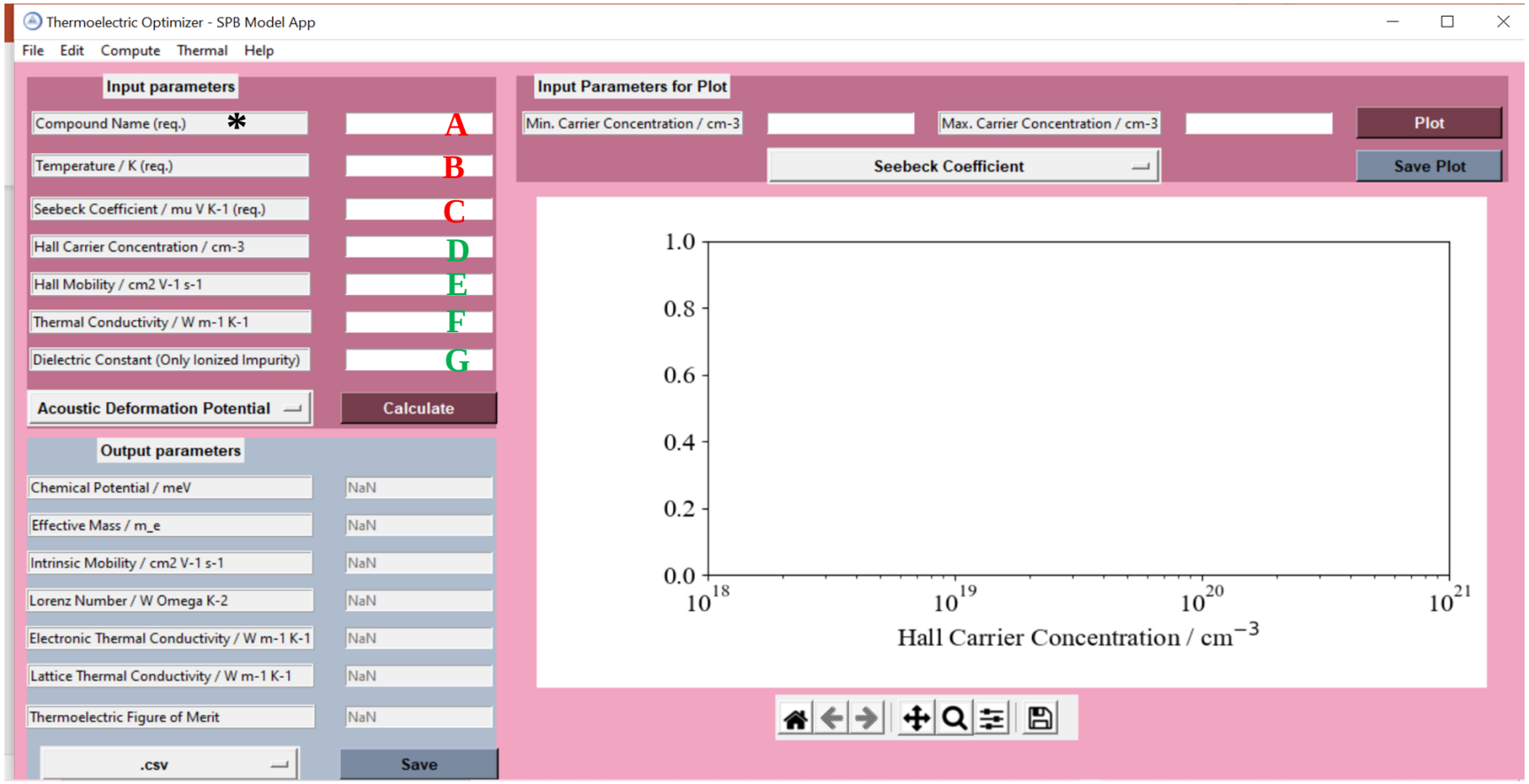


- If you haven’t download a Python 3.xx, please download it
  - Make sure that these packages are available:
    - tkinter, os, json, numpy, scipy, and matplotlib

- Open the App using command line: python Thermoelectric Optimizer.py

- 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 μV K^{-1}
(required; only positive values)
(Seebeck coefficient should be above 0.1 and below 1,500 μV K^{-1})

D : Hall Carrier Concentration in cm^{-3}
(not required; only positive values)
(Carrier Concentration should be above 1E12 and below 1E24 cm^{-3})

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

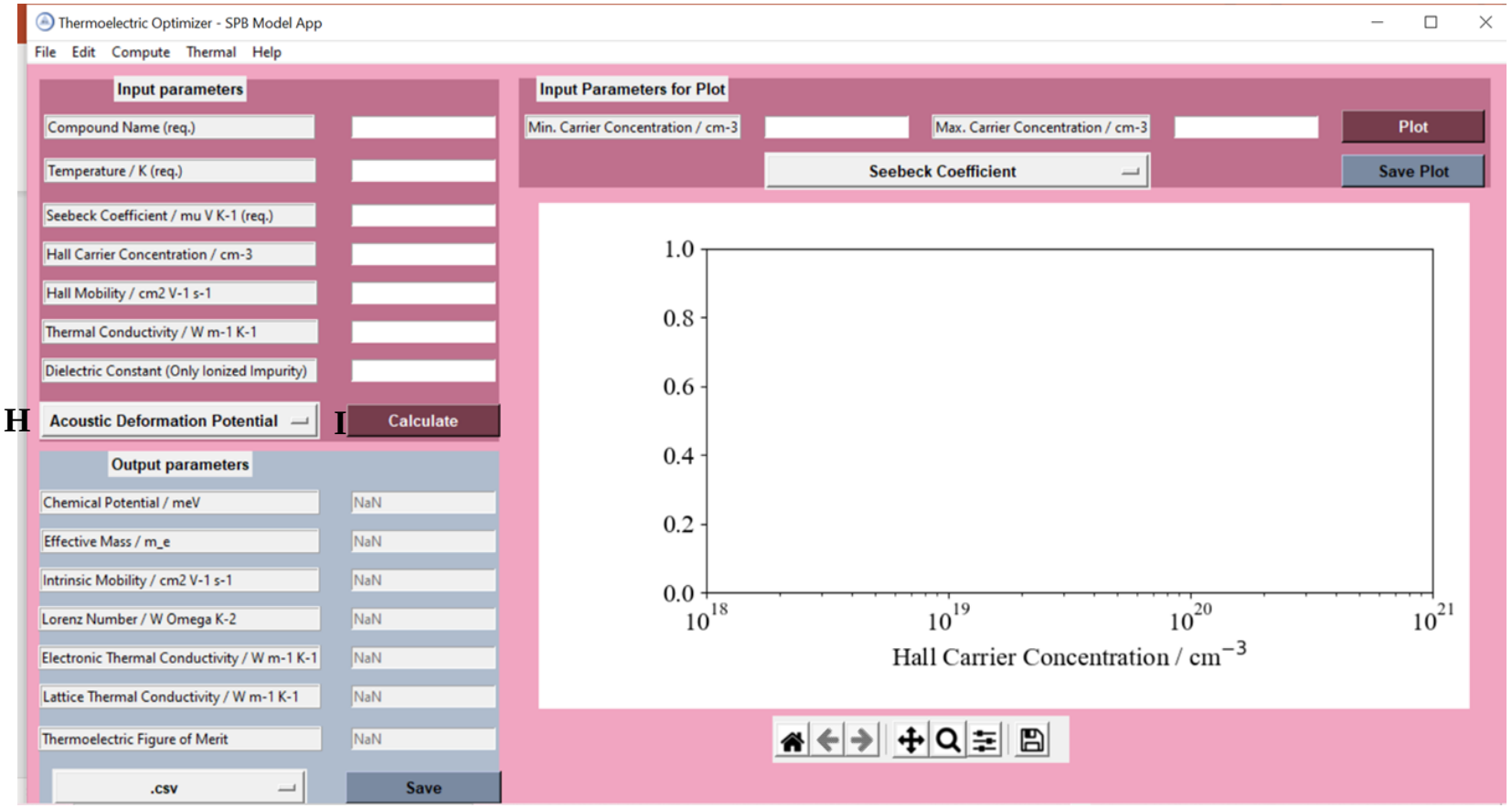
F : Total thermal Conductivity in W m^{-1} K^{-1}
(not required) (Thermal Conductivity should be above 0 and below 10,000 W m^{-1} K^{-1})

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



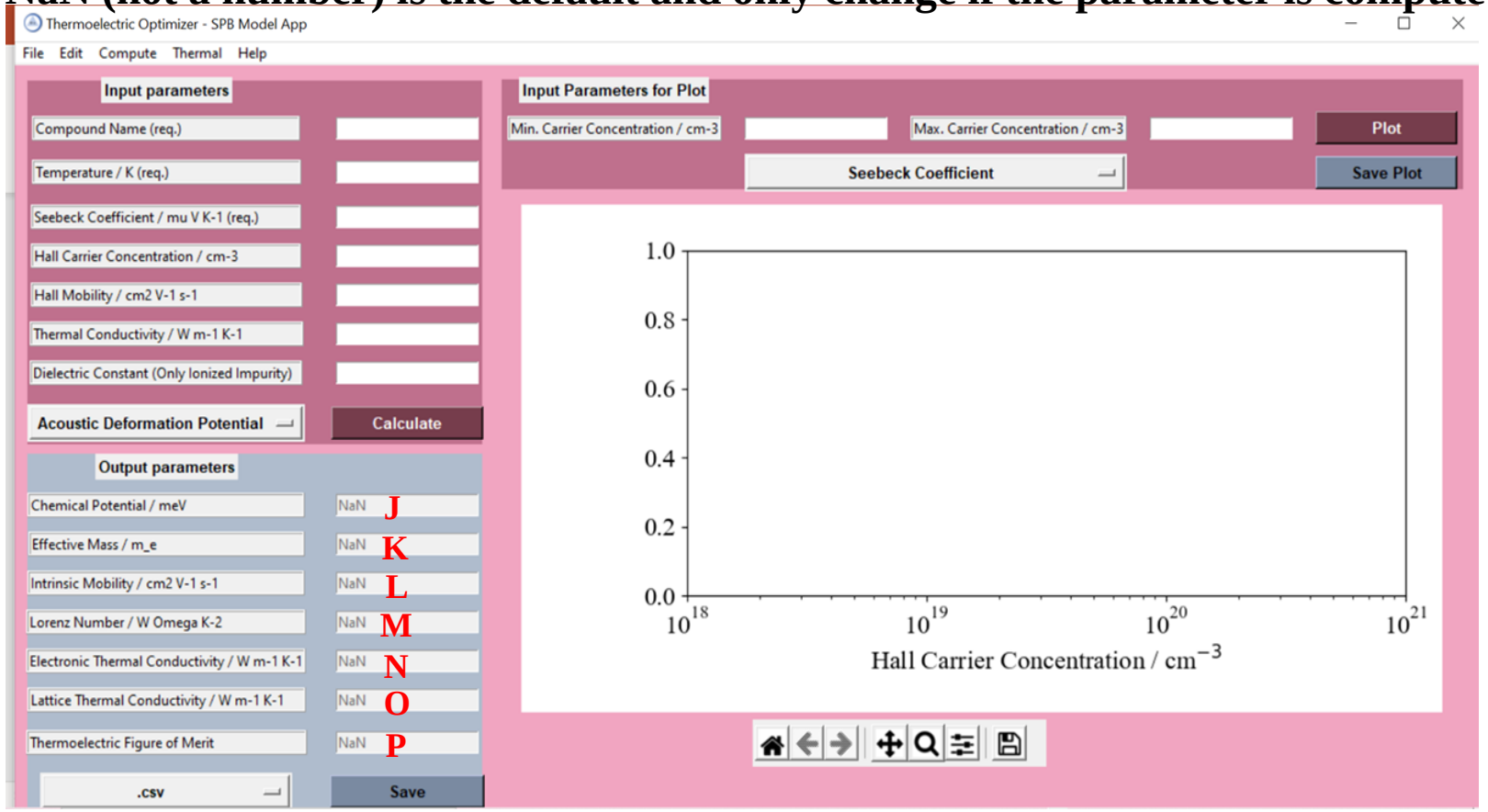
H : Choose the scattering mechanism (5)

- **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 $cm^2\ V^{-1}\ s^{-1}$ (Computed from the Seebeck coefficient, Carrier Concentration and Mobility)

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

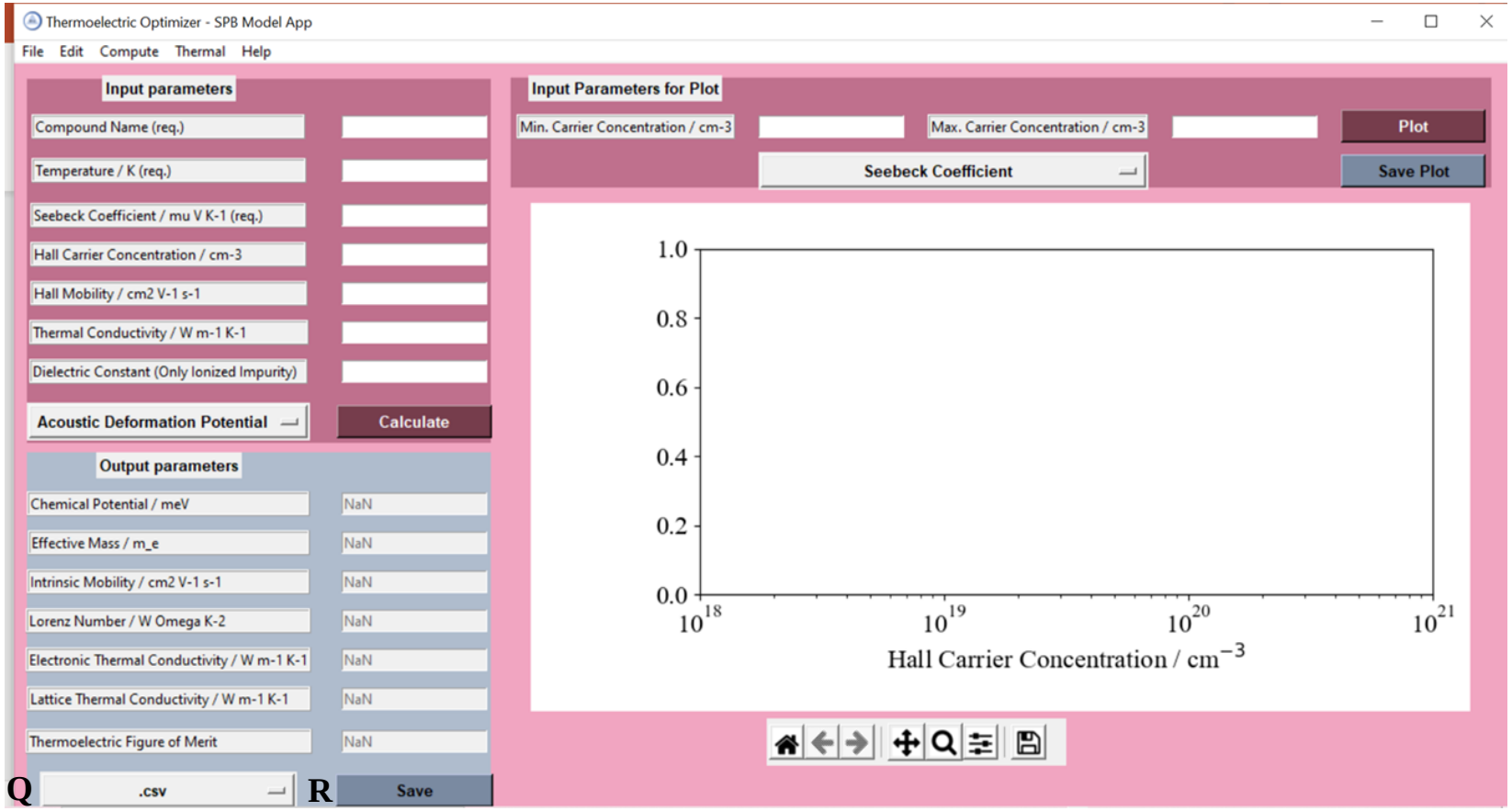
N : Electronic Thermal Conductivity in $W\ m^{-1}\ K^{-1}$ (Computed from the Seebeck coefficient, Carrier Concentration, and Mobility)

O : Lattice Thermal Conductivity in $W\ m^{-1}\ K^{-1}$ (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



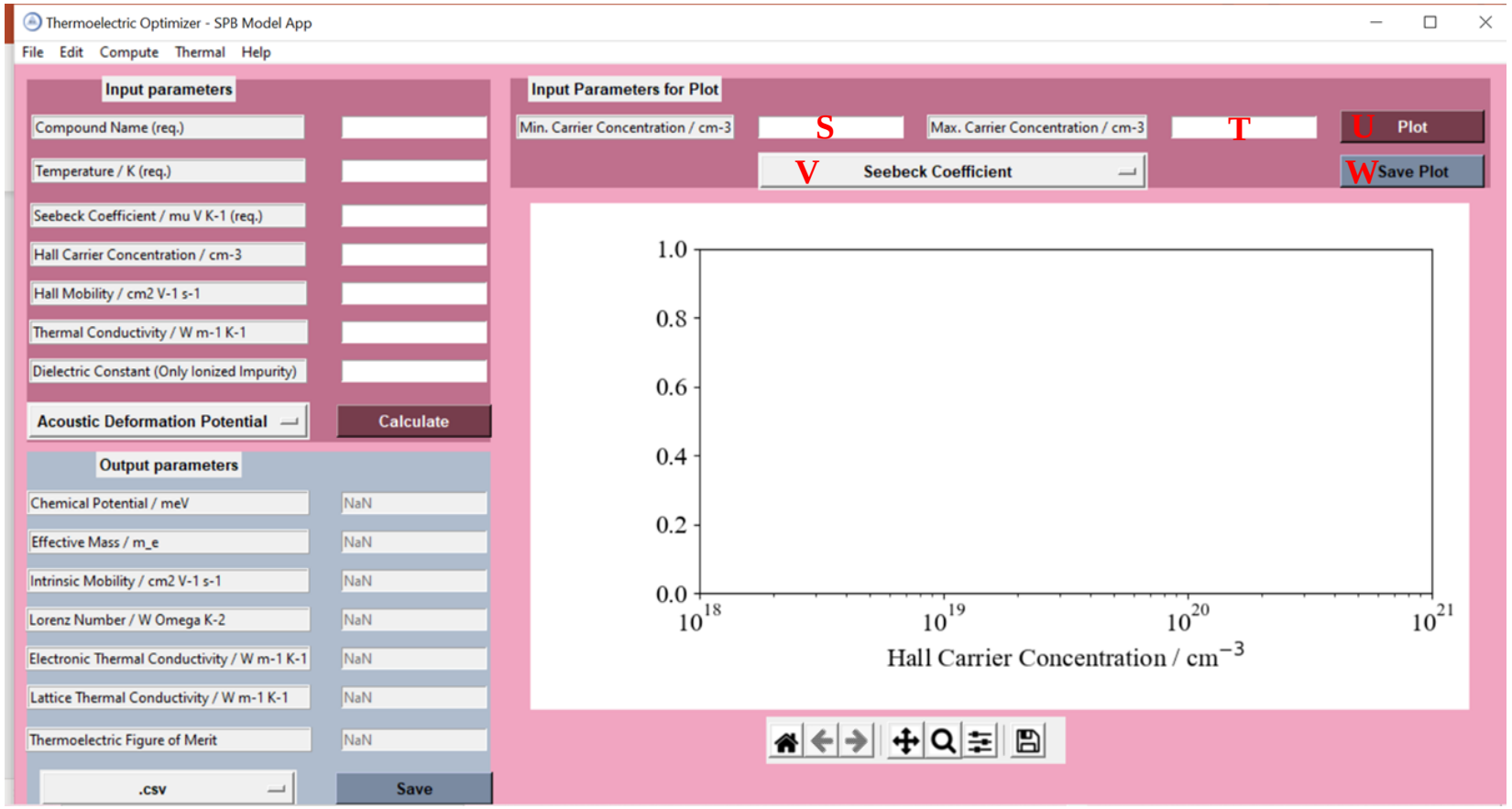
Q : Extension of File to save the above properties

- **.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 accidently 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 1E12 and below 1E24 cm^{-3})

T : Maximum Carrier Concentration in cm^{-3} (required; only positive values) (Carrier Concentration should be above 1E12 and below 1E24 cm^{-3} and should be higher than minimum Carrier Concentration)

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

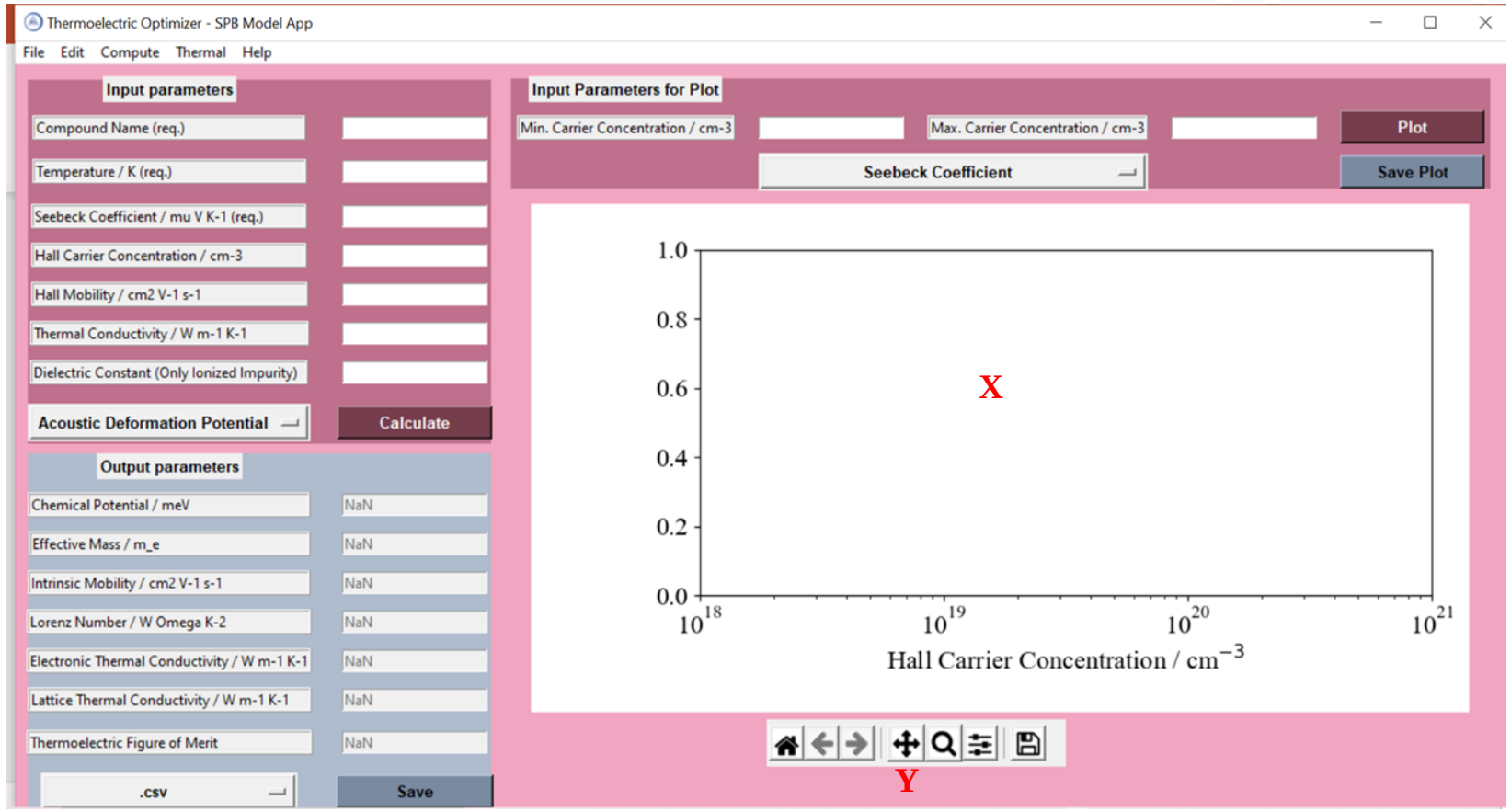
V : Plot Data on y-axis *

- **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)**

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

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

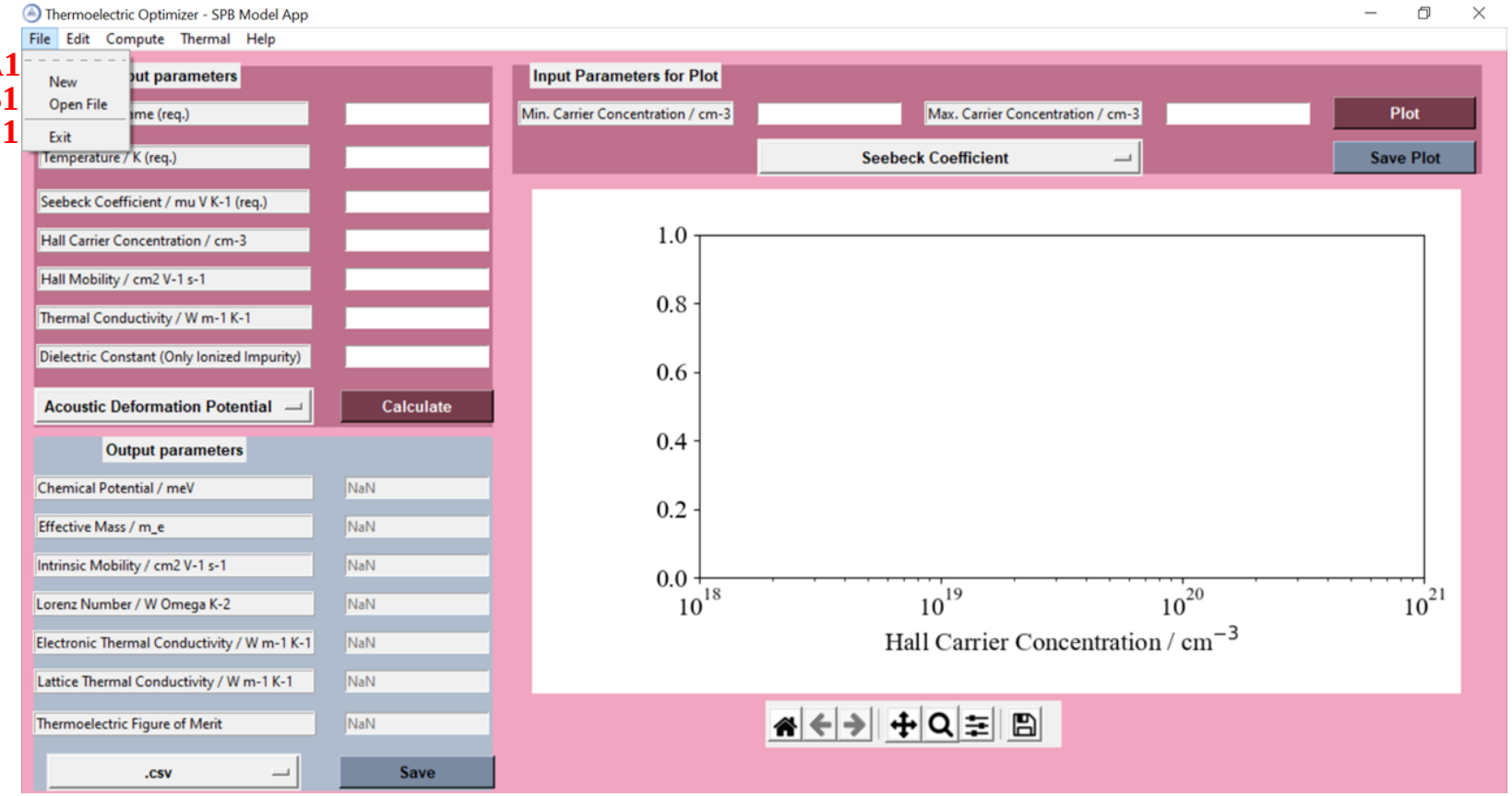
Start Window



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

Compound Name

Temperature in K

Seebeck Coefficient in μV K^{-1} → needs to be positive

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

Mobility in cm^2 V^{-1} s^{-1}

Thermal Conductivity in W m^{-1} K^{-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 V K -1	Carrier Concentration / cm-3	Mobility / cm2 V-1 s-1	Thermal Conductivity / W m-1 K-1	Dielectric Constant		
2	A1	300	140	3.00E+19	80	3.4	200		
3	A1	400	180	3.60E+19	60	2.7	200		
4	A1	600	220	3.90E+19	34	2.1	200		
5	B1	450	35	3.00E+21	10	12	10		
6	C1	303	98	1.00E+20	112	5	80		
7	C1	403	145	2.00E+20	97	4.6	80		
8	C1	503	200	2.20E+20	87	4.3	80		
9									
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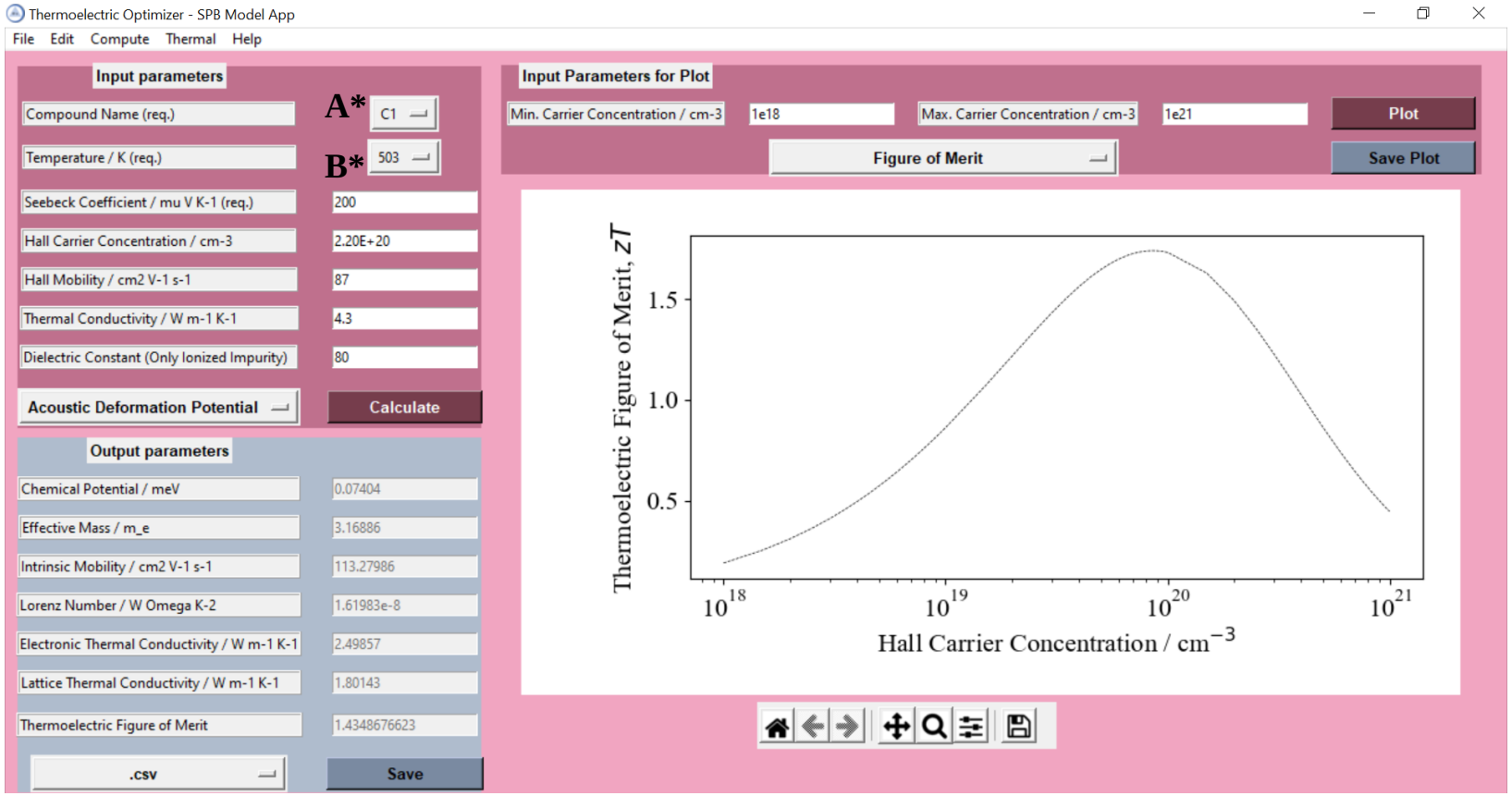
21									

Example

Uploaded Data

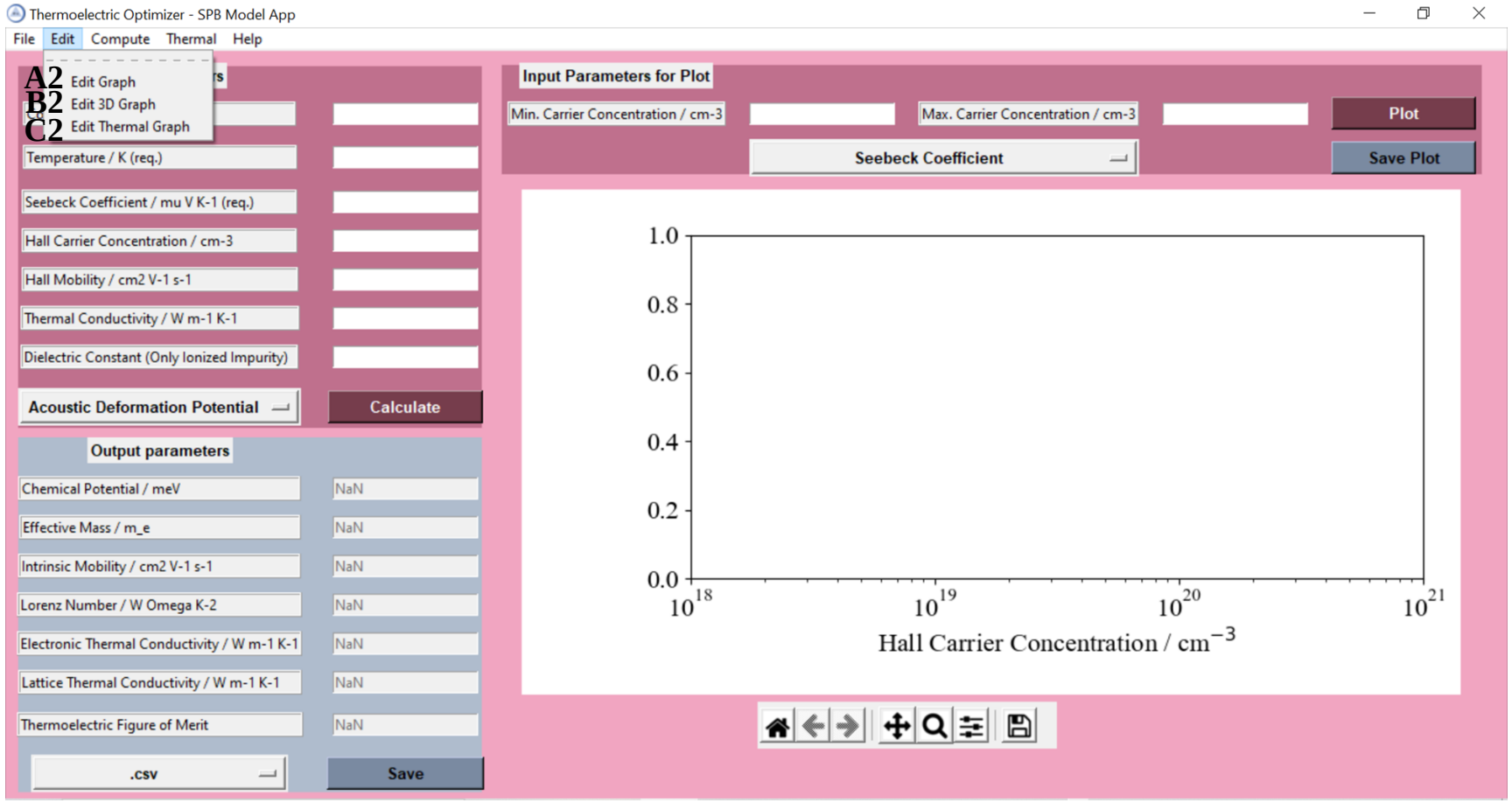


A* : List of Compound names
B* : List of Temperatures for the Corresponding Compound

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**

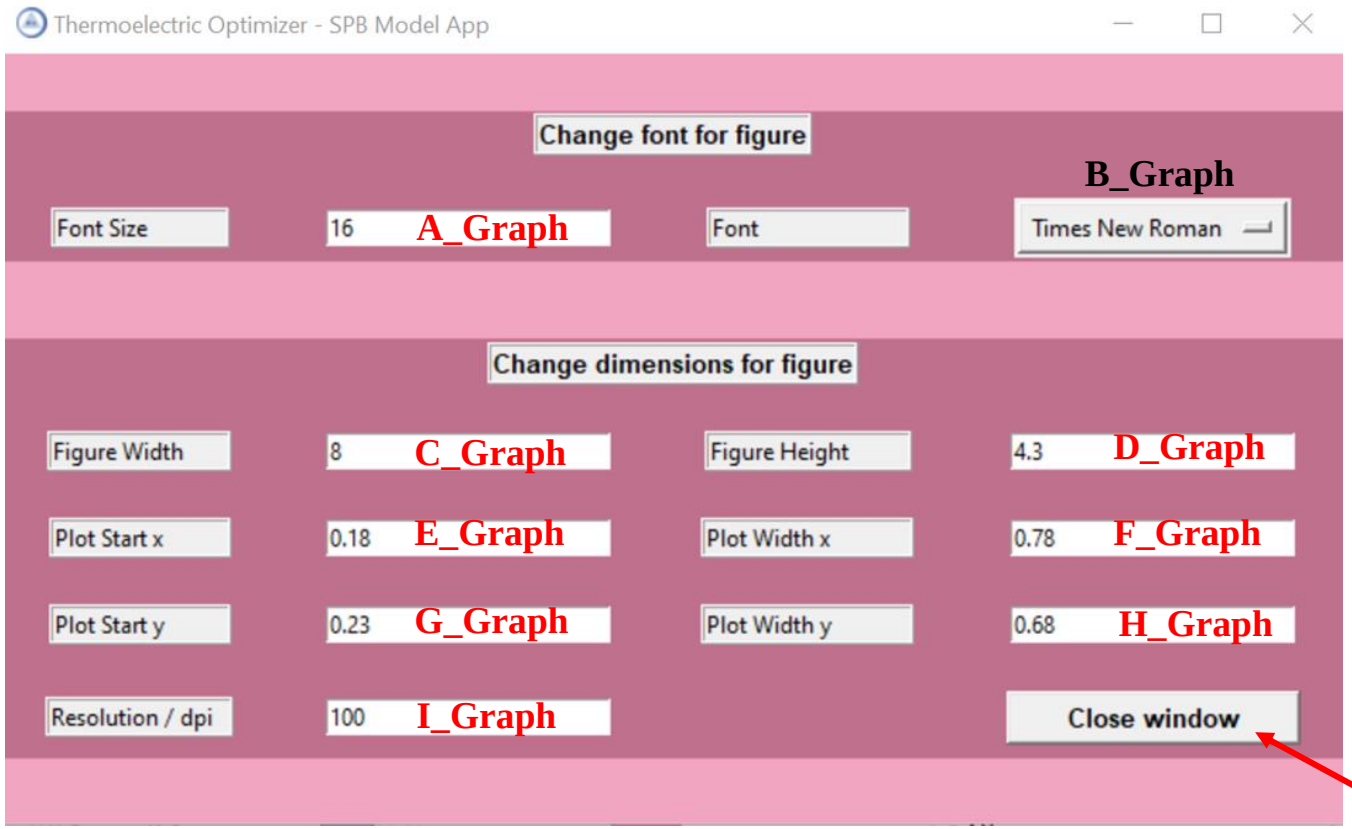
B2 : Edit 3D Graph

- **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



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

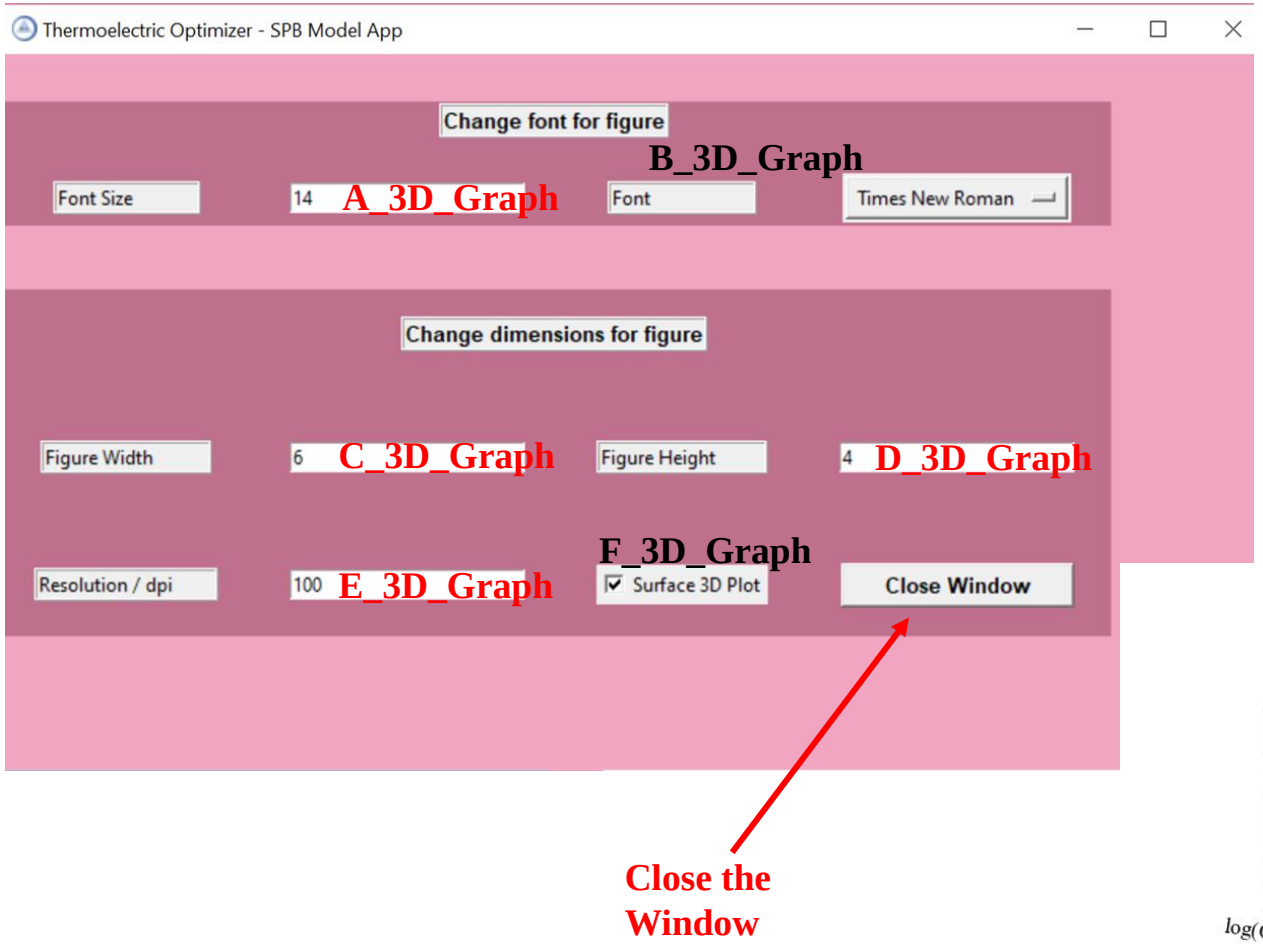
G_Graph : y-point where the plot starts in the figure
H_Graph : Height of the plot

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

Close the window (produce an empty graph)

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

Edit Graph 3D



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

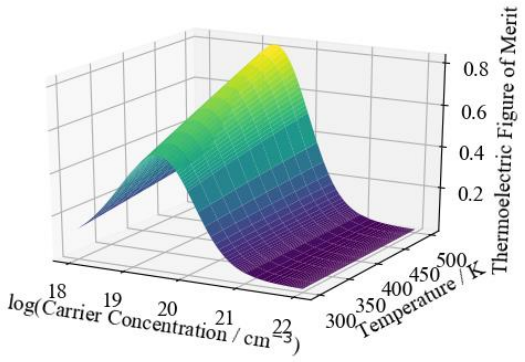
A_3D_Graph : Font Size
B_3D_Graph : Font (Choose selected fonts) *

C_3D_Graph : Width of the 3D figure
D_3D_Graph : Height of the 3D figure

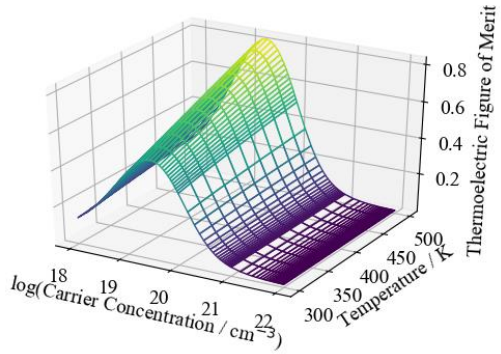
E_3D_Graph : resolution of the graph (change figure size)

F_3D_Graph : Change between a surface or wired 3D Figure

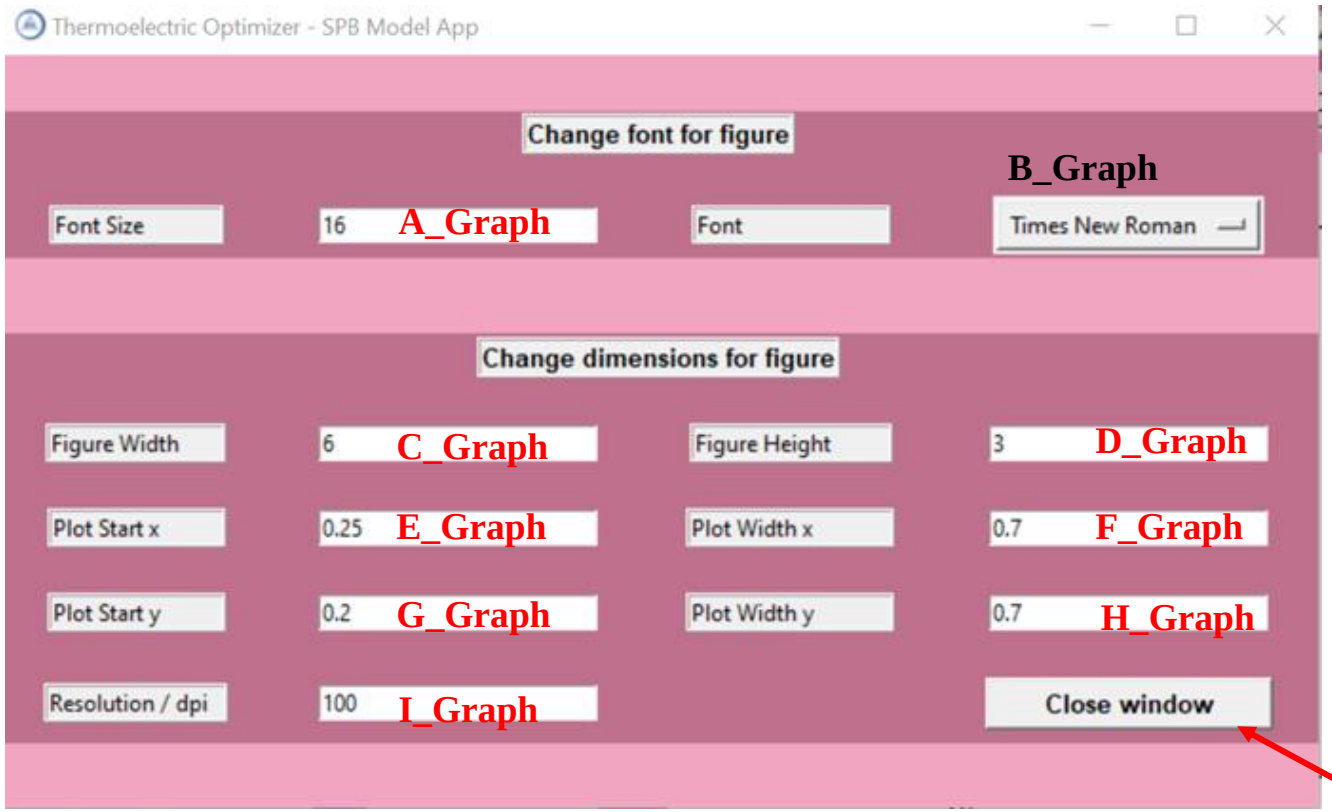
Surface:



Wired:



Edit Thermal Graph



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

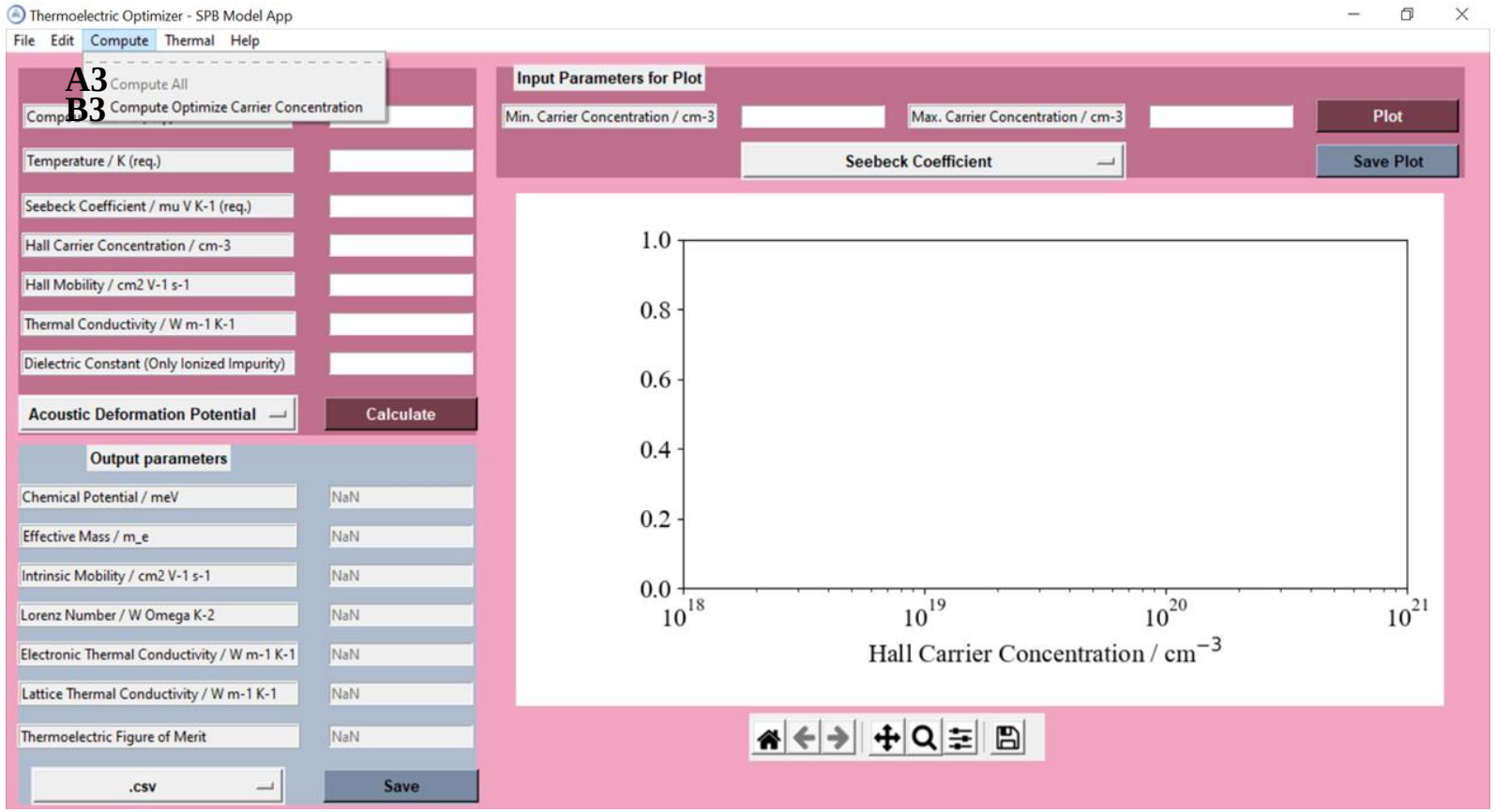
G_Graph : y-point where the plot starts in the figure
H_Graph : Height of the plot

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

Close the window (produce an empty graph)

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

Compute Menu



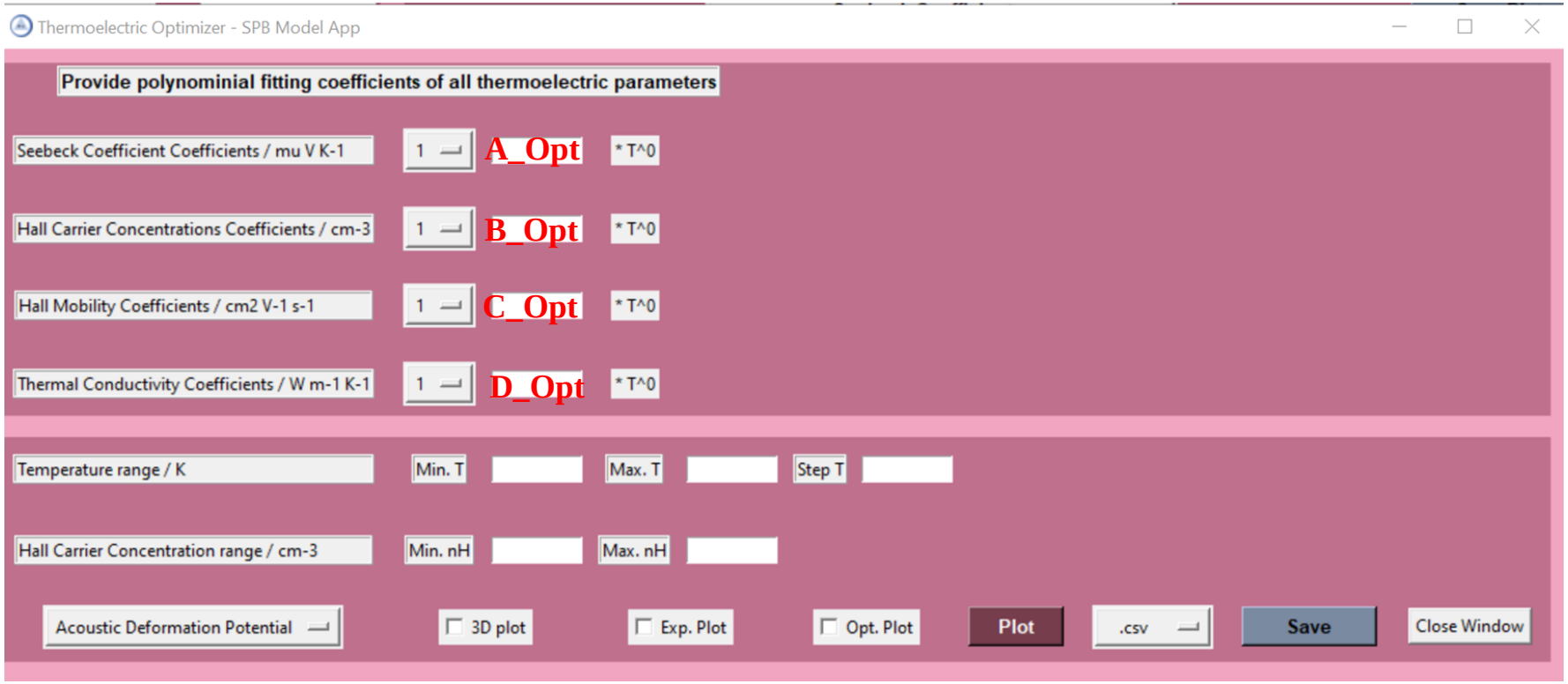
A3 : Compute All (enabled when a file was open)

- **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 Thermo-electric Figure of Merit**

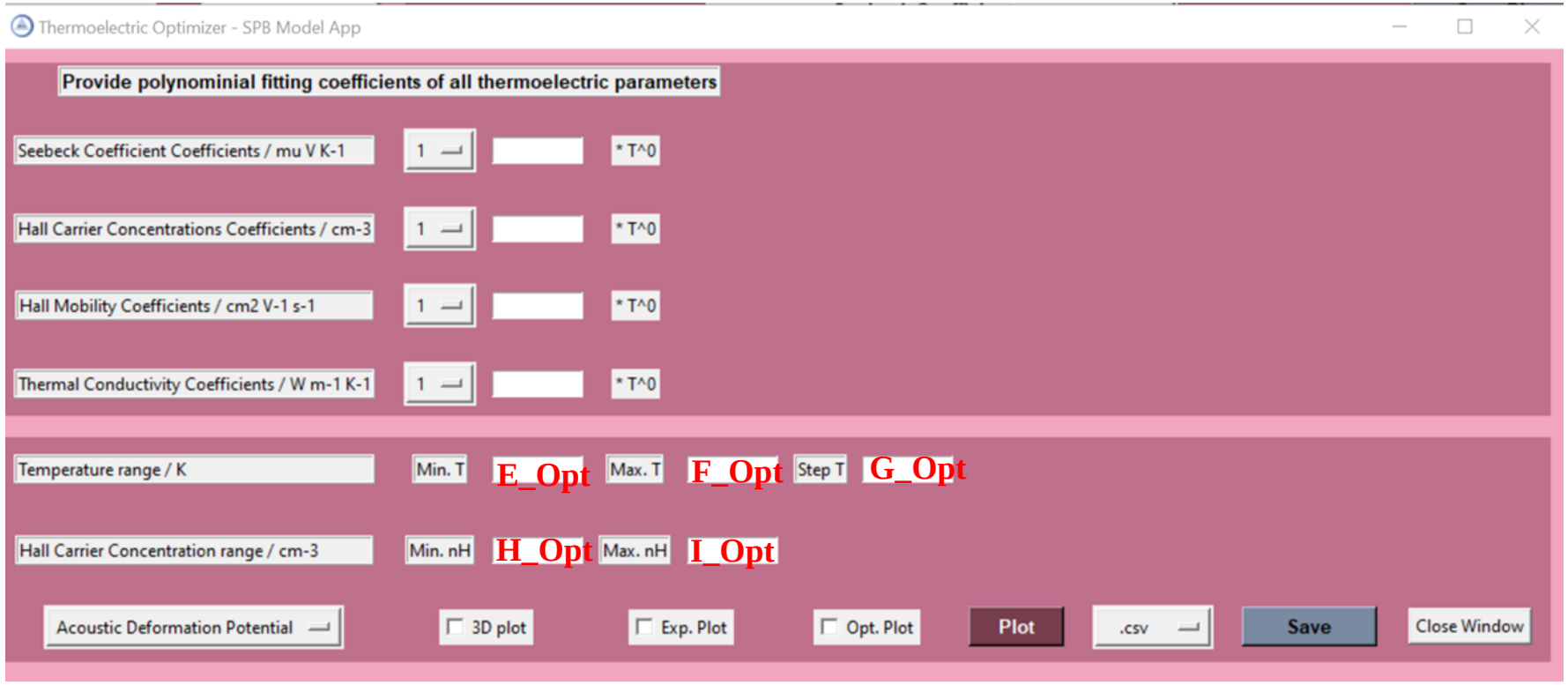
Compute Optimized Carrier Concentration



A_Opt: Temperature-dependent Seebeck Coefficient in µV K^{-1} described by polynomial to the fifth order
For example: $S = 100 * T^0 + 0.8 * T^1 + -1E-5 * T^2$ → Change List to 3 and write 100, 0.8, and -1E-5 in the three fields

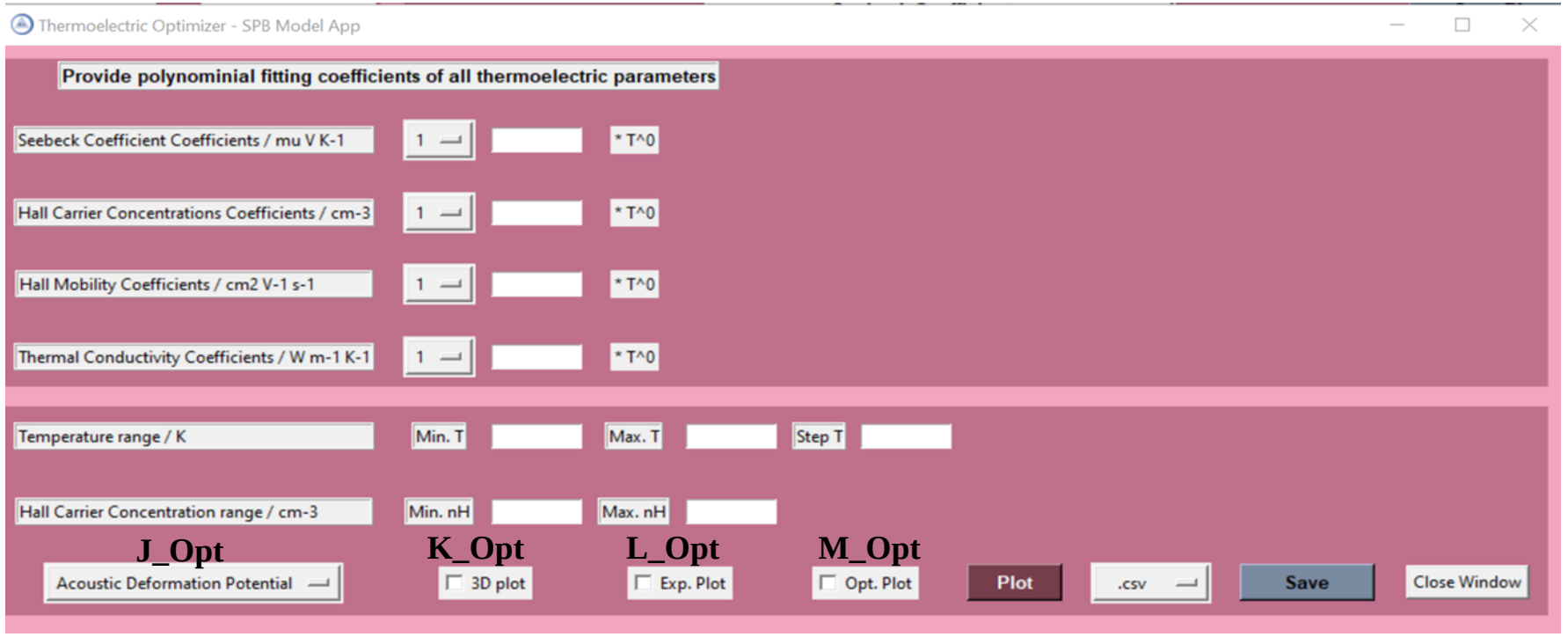
B_Opt: Temperature-dependent Carrier Concentration cm^{-3} described by polynomial to the fifth order
C_Opt: Temperature-dependent Mobility in $cm^2 V^{-1} s^{-1}$ described by polynomial to the fifth order
D_Opt: Temperature-dependent Thermal Conductivity in $W m^{-1} K^{-1}$ described by polynomial to the fifth order

Compute Optimized Carrier Concentration



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 W m^{-1} K^{-1} described by polynomial to the fifth order

Compute Optimized Carrier Concentration



J_Opt: Choose the scattering mechanism (5)

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

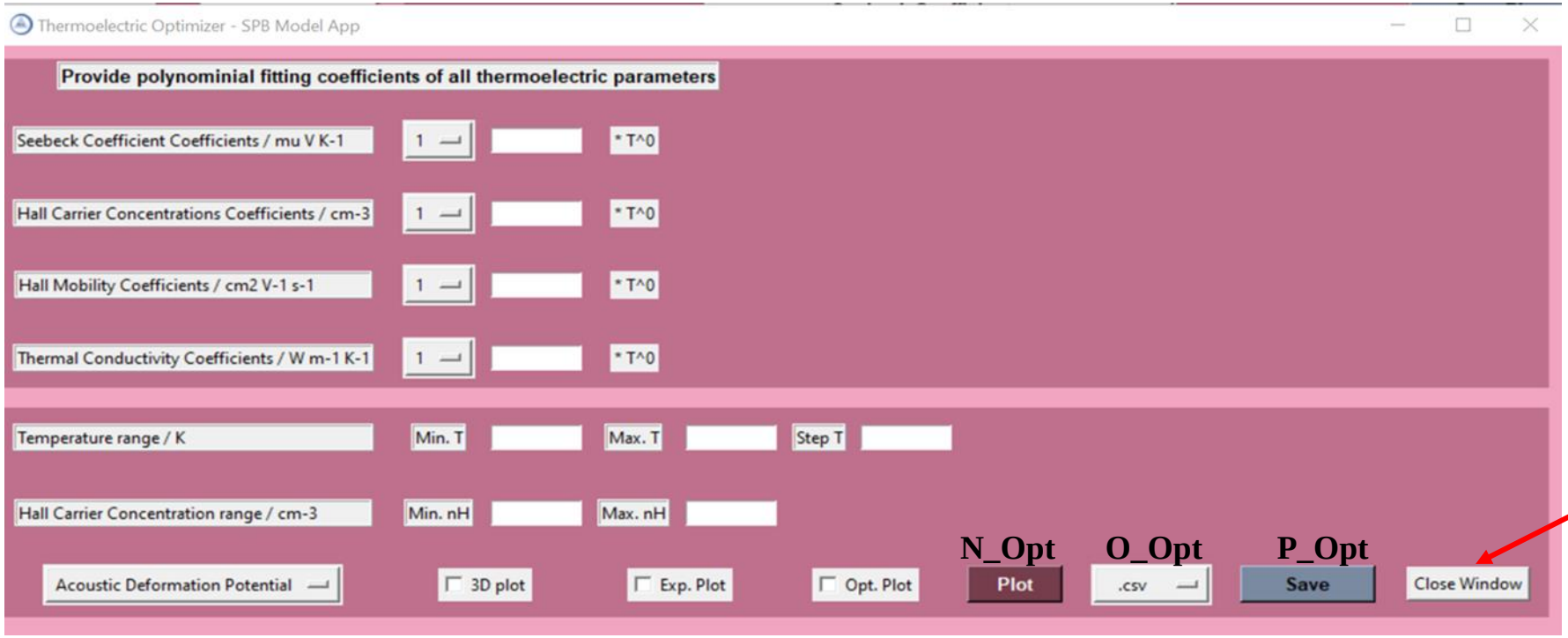
K_Opt: Create a 3D plot (Temperature, Carrier Concentration and Thermoelectric Figure of Merit

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 Figrue of Merit are compared to the optimized values)

Compute Optimized Carrier Concentration



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

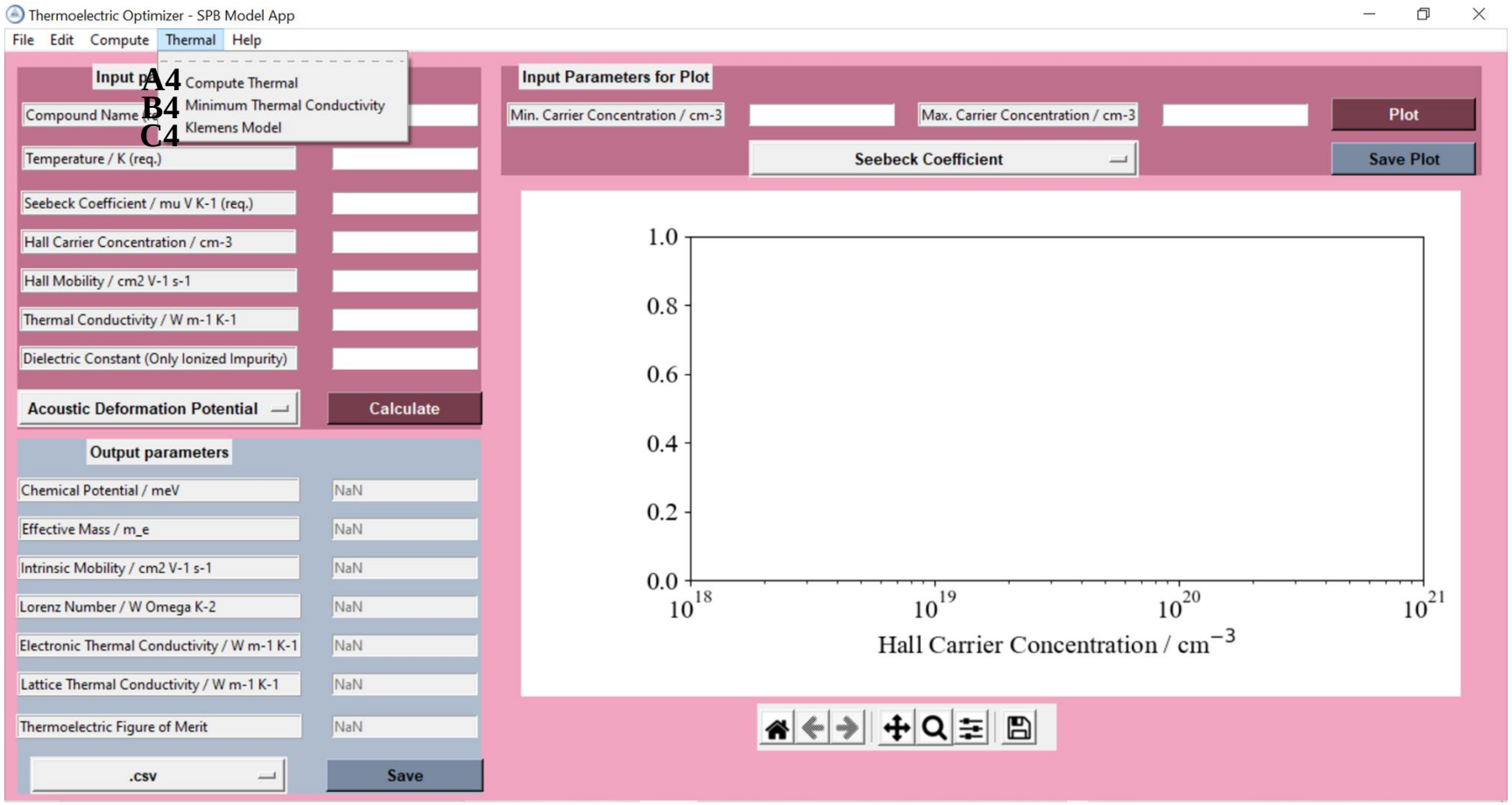
O_Opt : Choose the format to save the computed data (experimental versus optimized data)

- **.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**

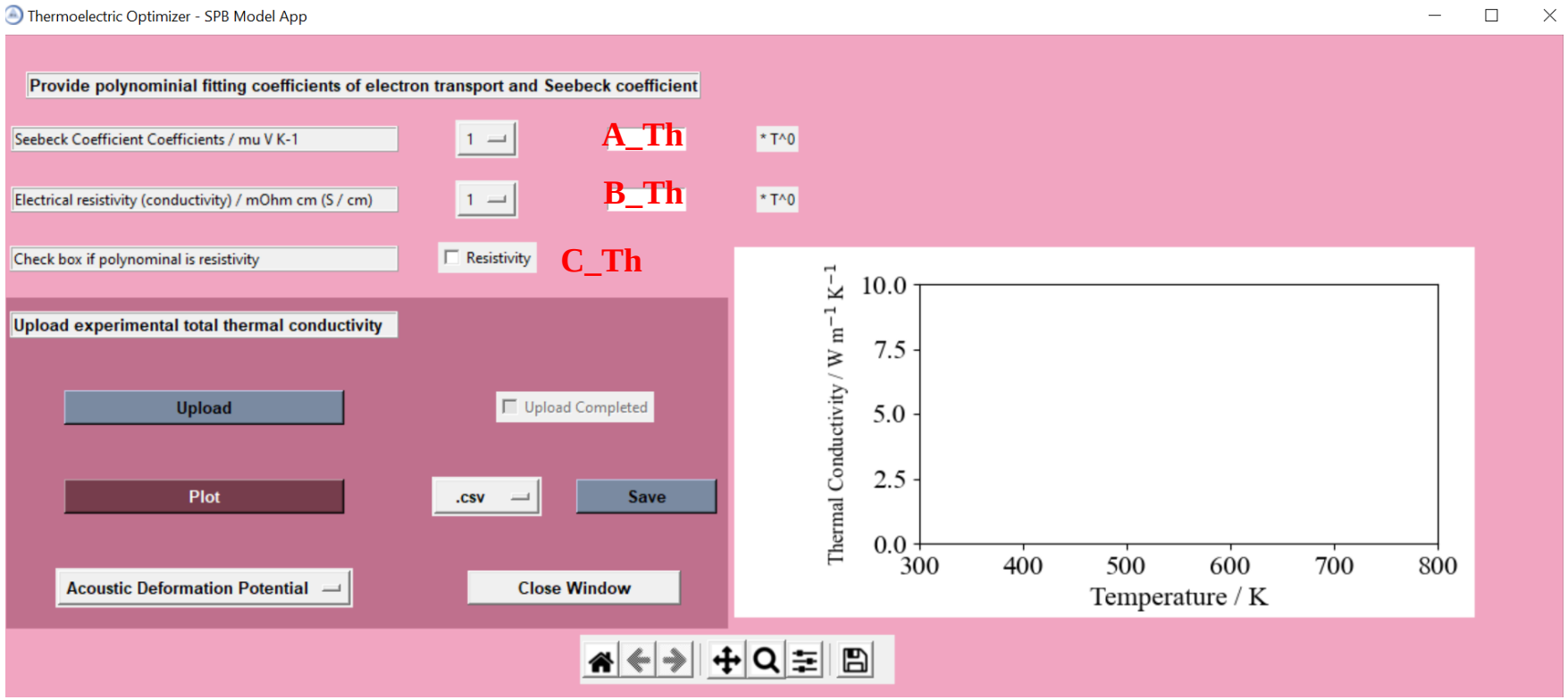
B4 : Minimum Thermal Conductivity

- **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

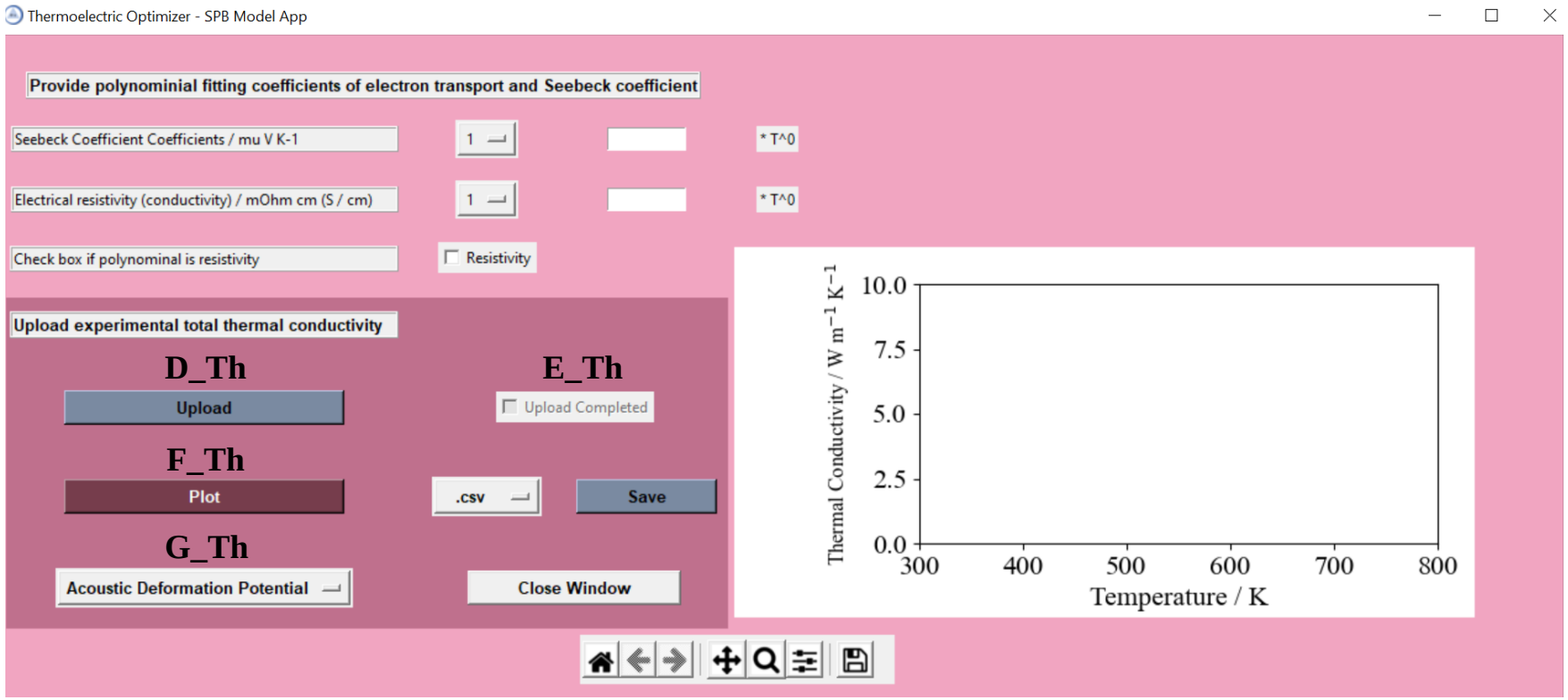


A_Th : Temperature-dependent Seebeck Coefficient in μV K^{-1} described by polynomial to the fifth order
For example: $S = 100 * T^0 + 0.8 * T^1 + -1E\text{-}5 * T^2$ → Change List to 3 and write 100, 0.8, and -1E-5 in the three fields

B_Th : Temperature-dependent electrical resistivity in mΩ 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.

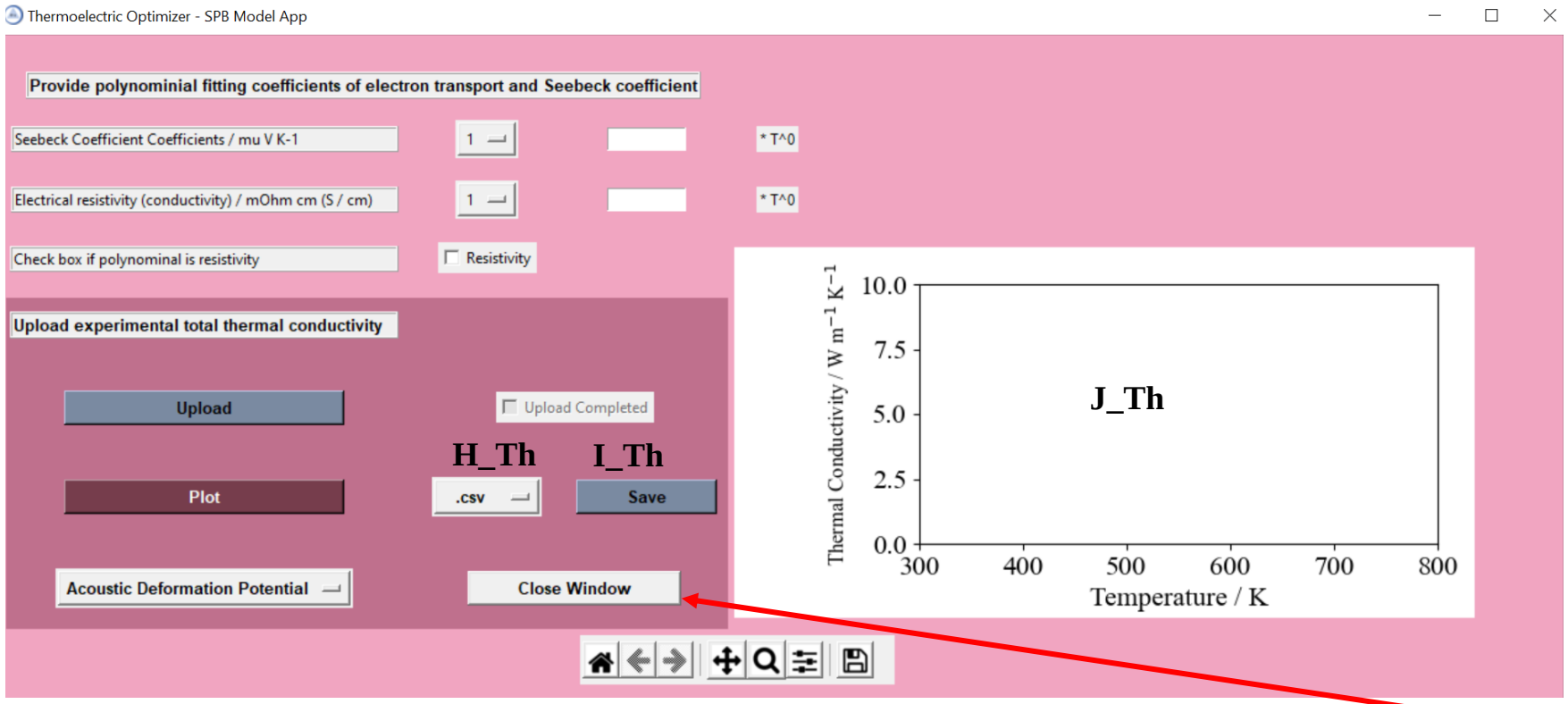
Compute Thermal



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



Close the Window

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.

Upload Thermal File

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

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

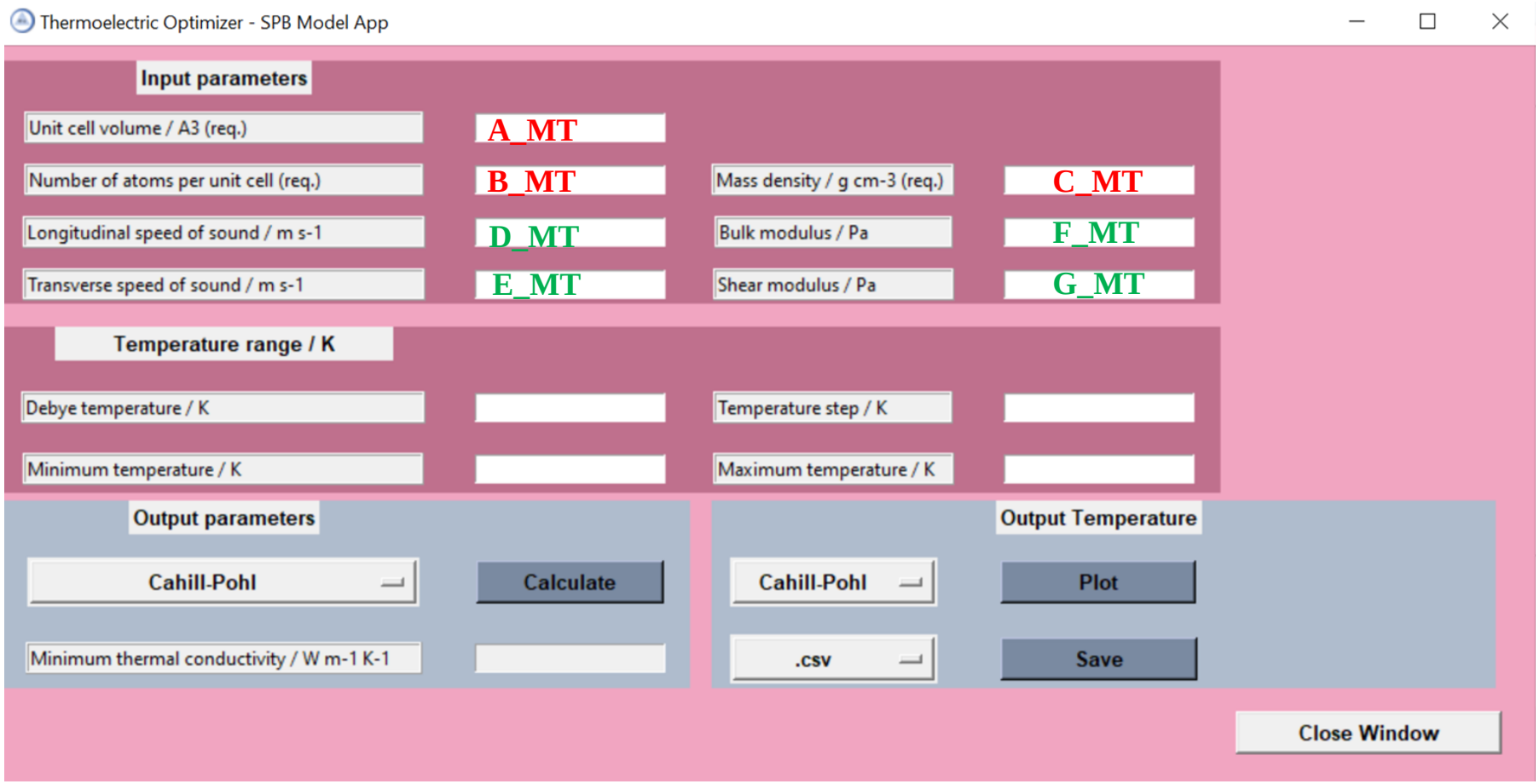
in the first row)

Temperature in K

Total Thermal Conductivity in W m^{-1} 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									

Minimum Thermal Conductivity



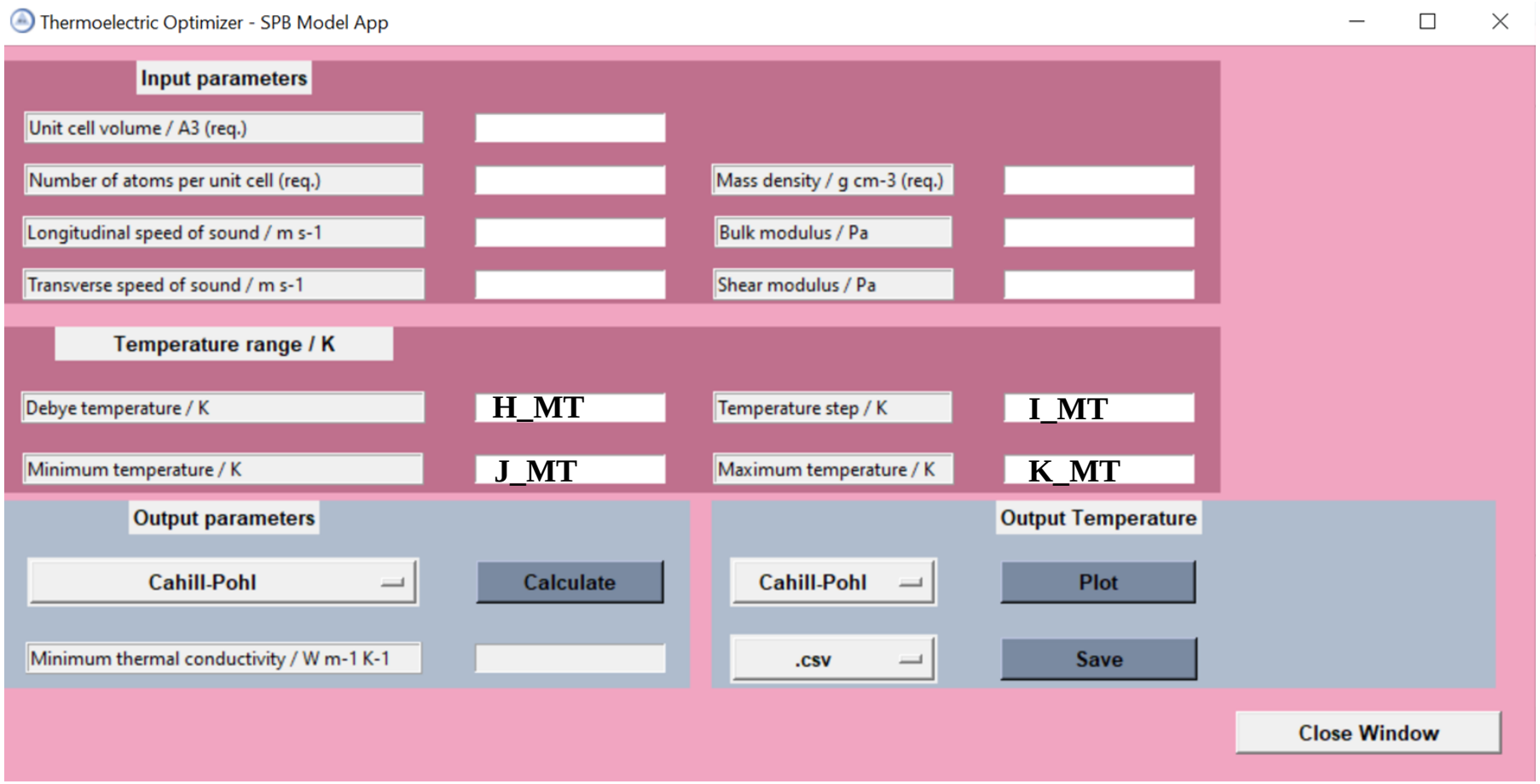
A_MT : Unit Cell Volume in Å^3 (required)
B_MT : Number of atoms per unit cell (required)
C_MT : Mass density in g cm^{-3} (required)

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 <u>need to</u> provide longitudinal and transverse speed of sound <u>OR</u> bulk and shear modulus)

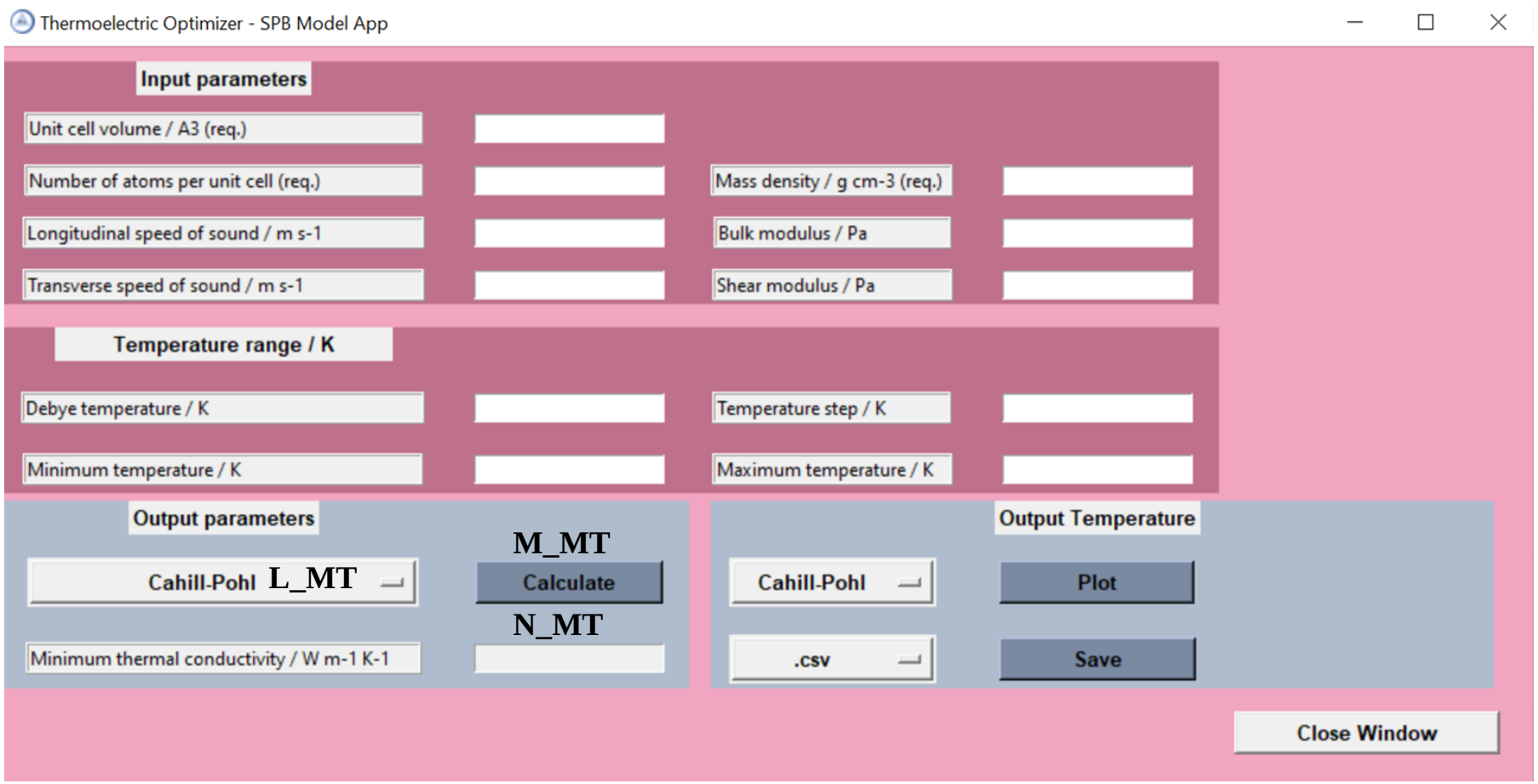
Minimum Thermal Conductivity



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



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

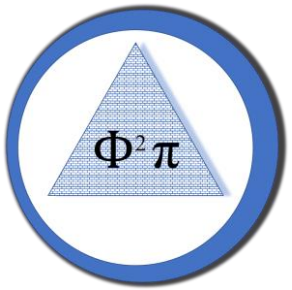
- **Cahill-Pohls**
- **Pohls**
- **Dynamic**
- **Diffusion**
- **Clarke**

(see next slide)

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

N_MT : Minimum temperature in W m^{-1} 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.

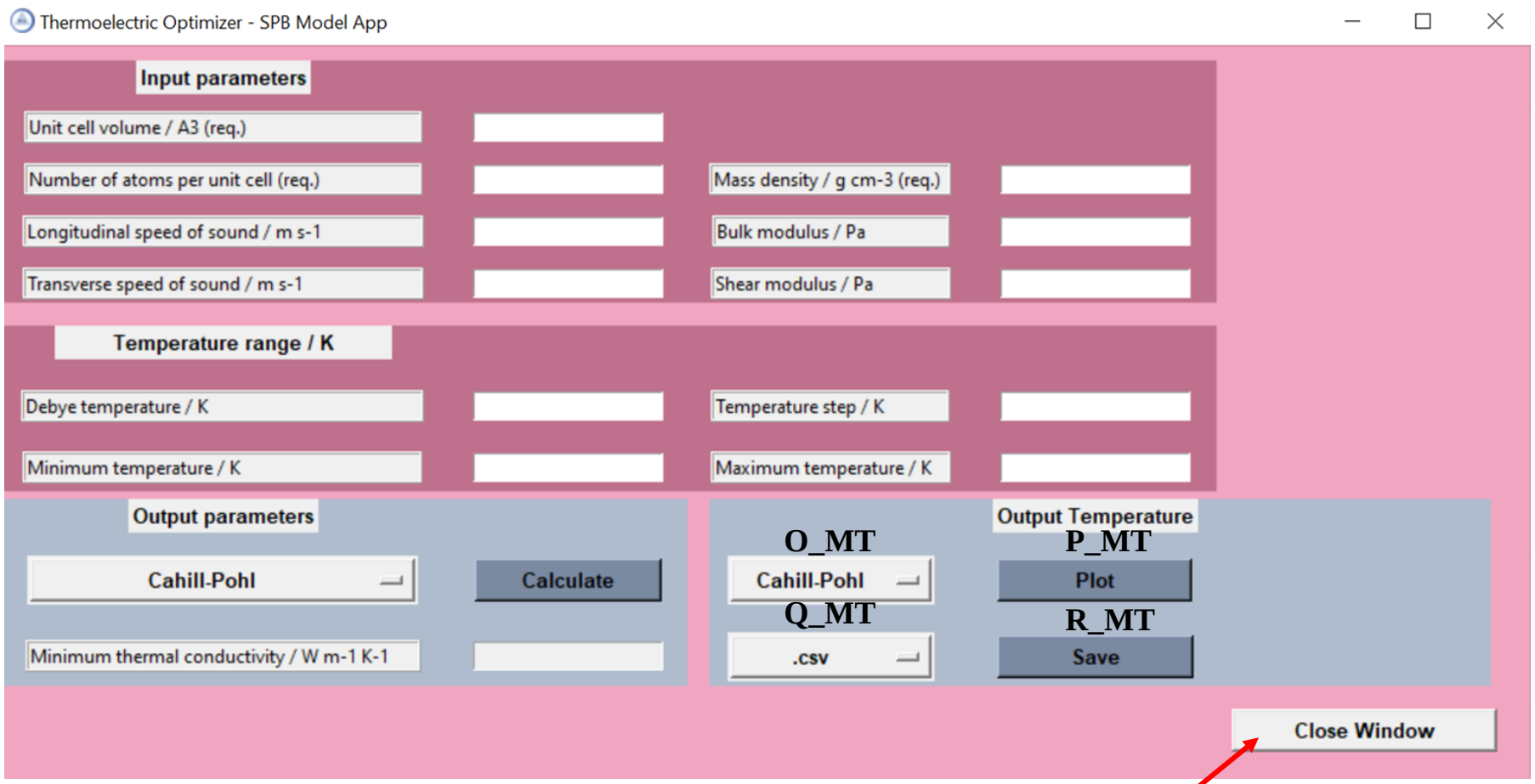
Pohls: J.-H. Pohls, M. B. Johnson, and M. A. White, “Origins of ultralow thermal conductivity in bulk [6,6]-phenyl-C61-butyric acid methyl ester (PCBM),” Physical Chemistry Chemical Physics, 18, 1185–1190, 2016.

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



Close the Window

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**

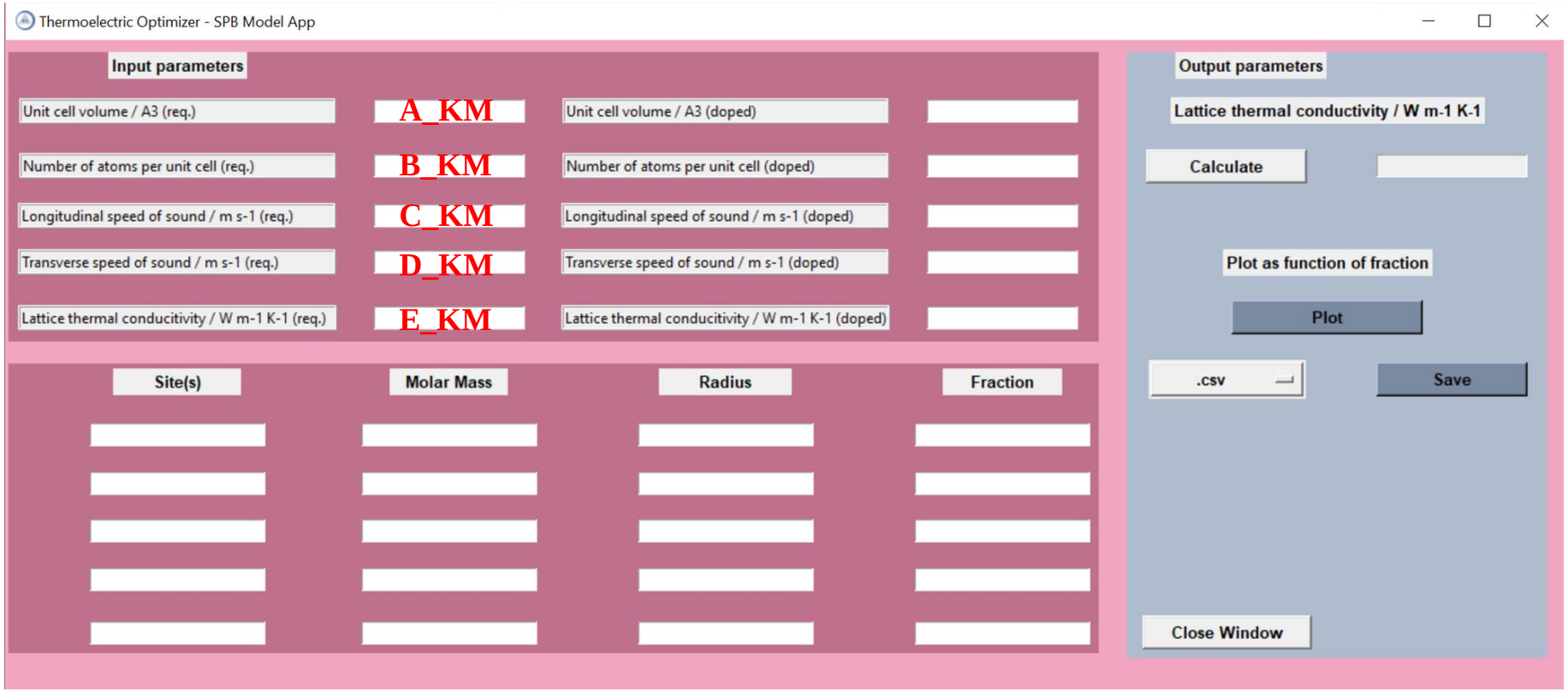
P_MT : Plot the minimum thermal conductivity in W m^{-1} K^{-1} as function of temperature

N_MT : Choose the format to save the computed data

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

R_MT : Save button

Klemens Model



Parameters of the undoped sample

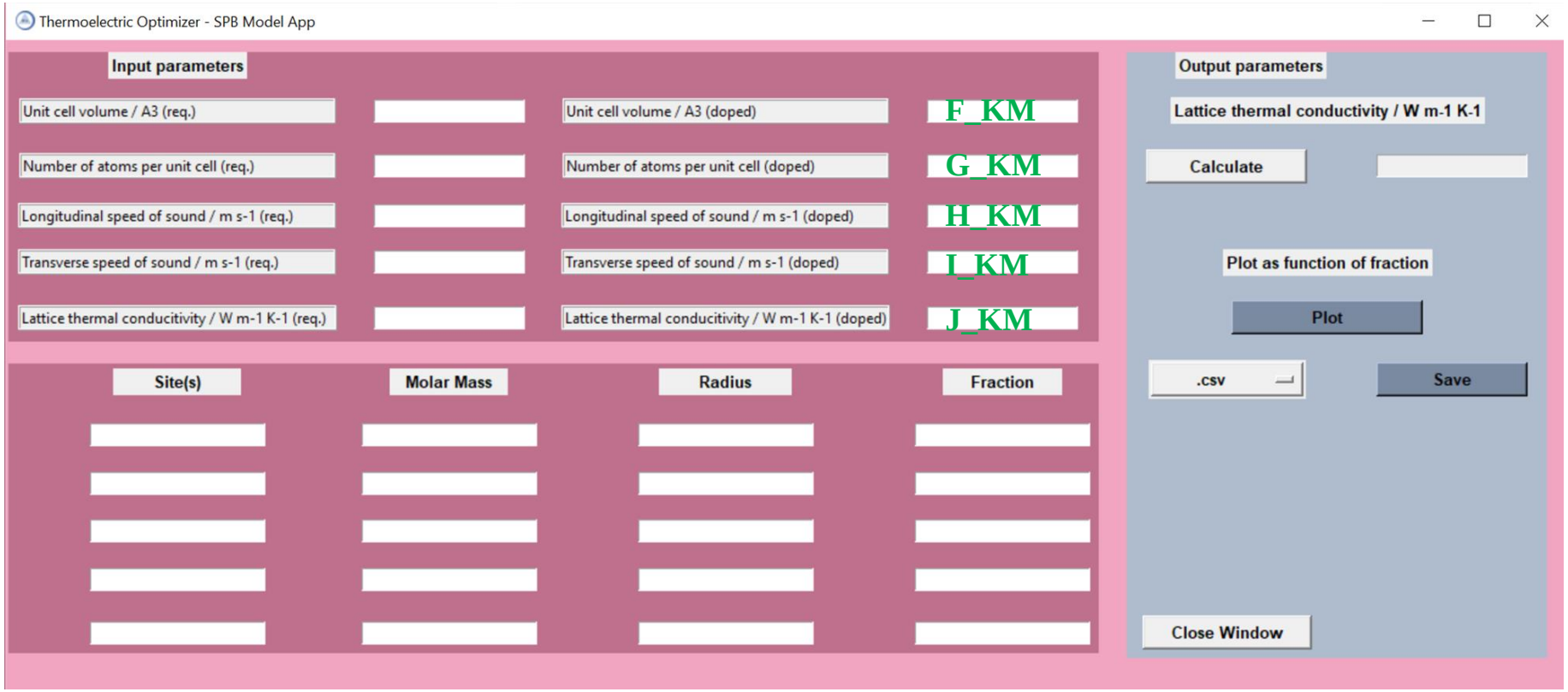
A_KM : Unit Cell Volume in Å^3 (required)
B_KM : Number of atoms per unit cell (required)

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



Parameters of the doped sample (only for the plot)

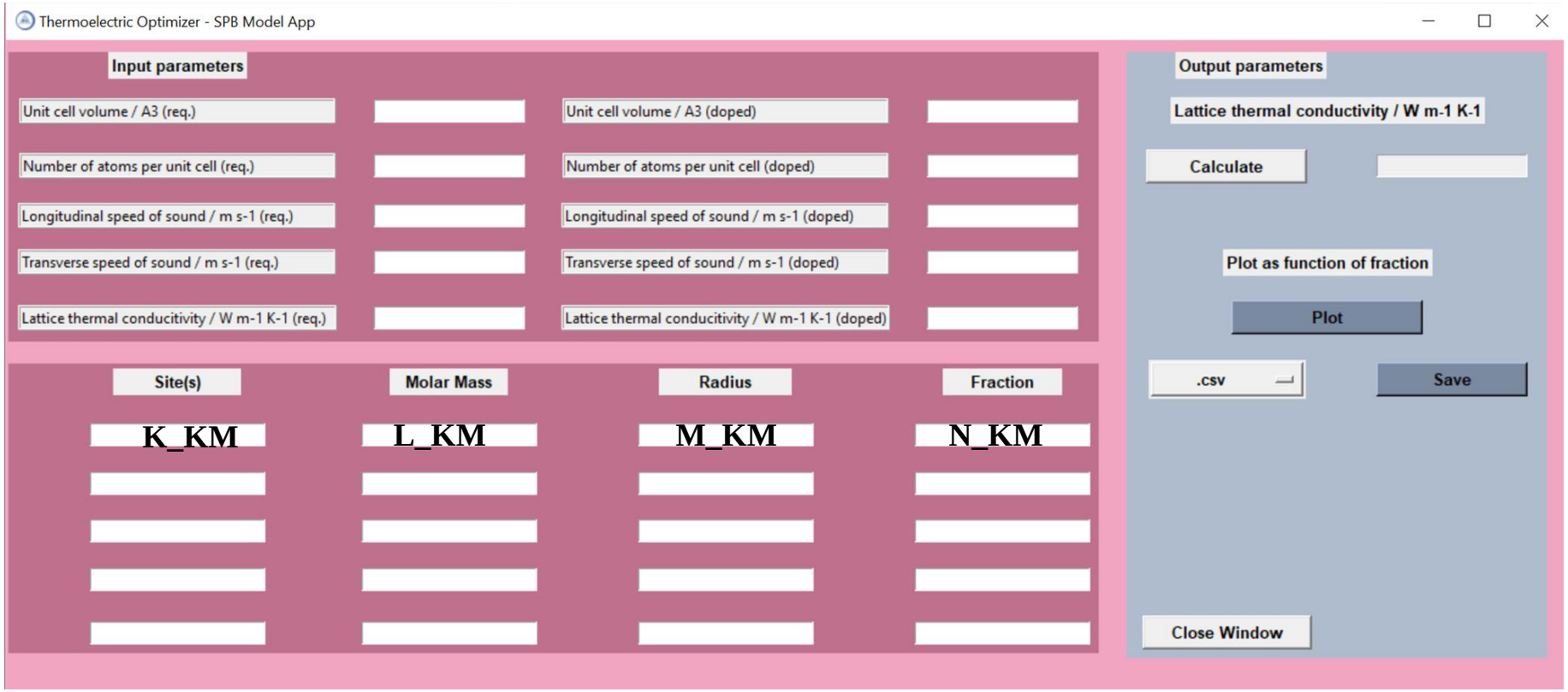
F_KM : Unit Cell Volume in Å^3
G_KM : Number of atoms per unit cell

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



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)

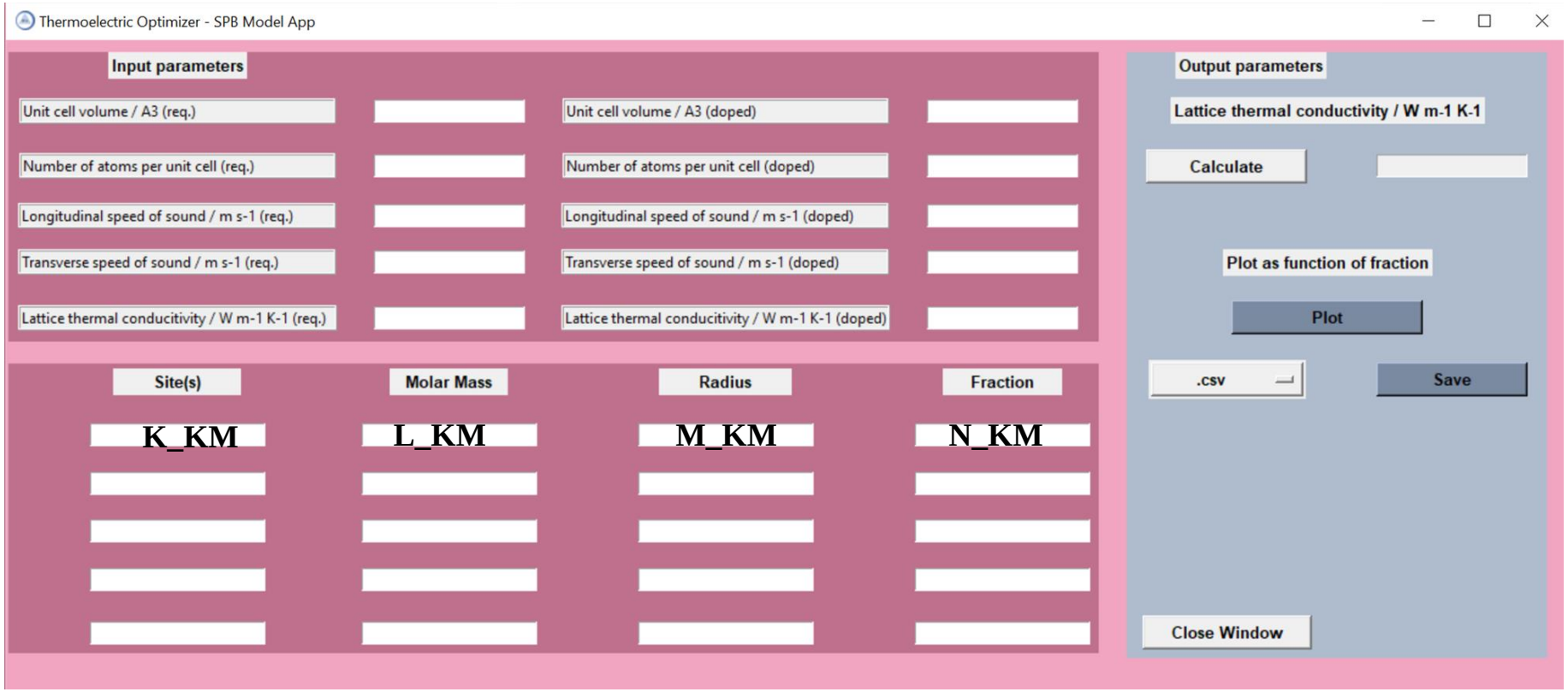
L_KM : Molar Mass (unit does not matter as long as it is consistent)

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



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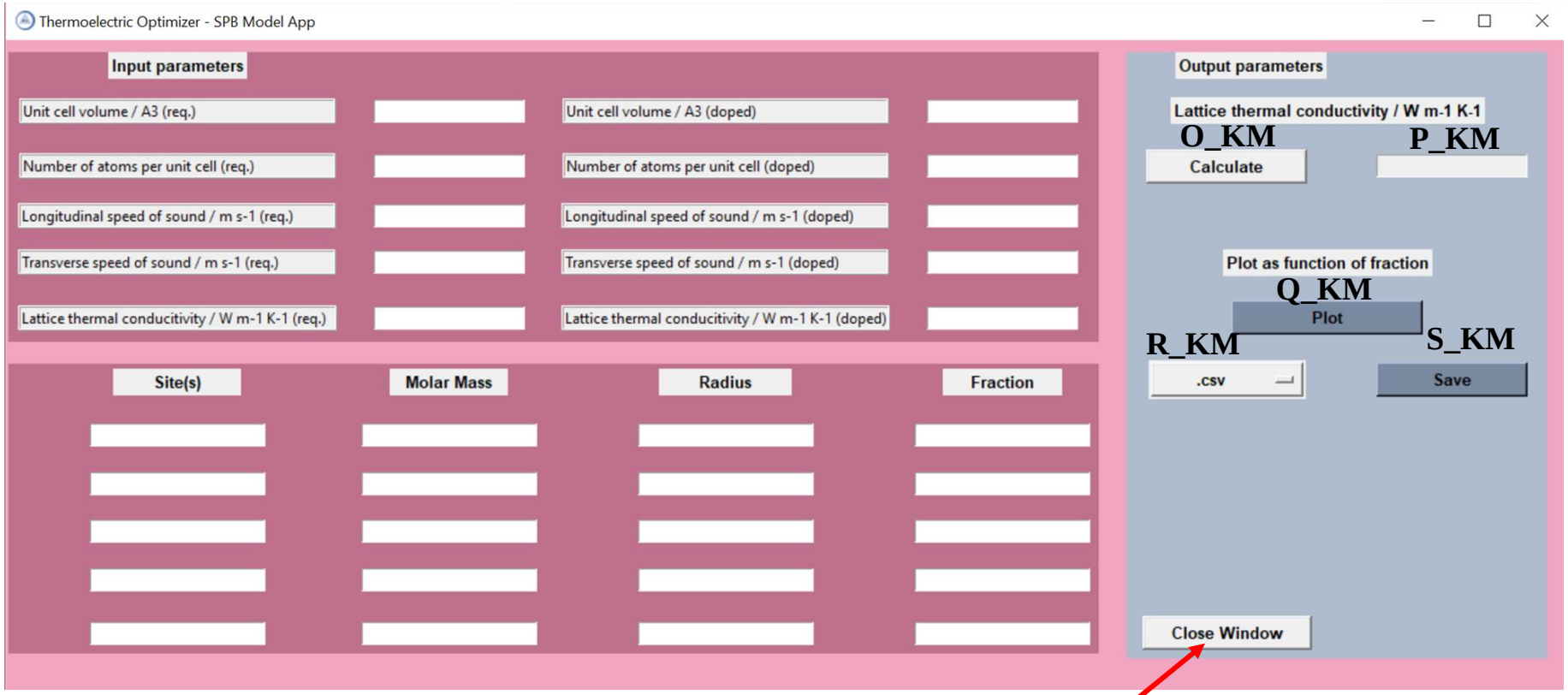
(For the plot, only the first two rows are considered)

Klemens Model



Close the Window

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

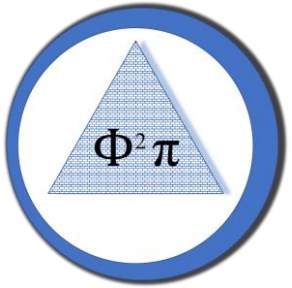
P_KM : Lattice thermal conductivity in W m^{-1} K^{-1} for different doping elements and levels

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 – SPB Model App