User guide for *SeeBand*: A highly efficient, interactive tool for analyzing electronic transport data

This document provides a brief overview of the graphical user interface (GUI) of *SeeBand*, with snapshots illustrating key features and functionalities.

Figure 1 shows the initial window that appears when launching *SeeBand*. In this window, users can import experimental data curves from text files formatted in two columns. The import buttons are highlighted in red. The buttons marked in green are associated with an interpolation function, which allows users to interpolate the experimental data onto an equidistant temperature grid. This feature helps avoid the overweighting of temperature intervals that have a higher density of measurement points. All measurement data should be imported in SI units, leading to the following specifications:

- Seebeck coefficient: [V/K]
- Resistivity: [Ωm]
- Hall coefficient: [m^3/C]

At the top of the figure, a magnified view of the toolbar is shown. The eye icon on the left is the logo and serves no functional purpose. The colored squares icon, marked as (1), corresponds to the data import tab depicted in this figure. The icons marked as (2) allow users to switch between the one-parabolic band (1PB) model and the two-parabolic band (2PB) model for data analysis. The three icons on the right, marked as (3), provide access to the different refinement windows: *Seebeck only fit*, $S + \rho$ *fit*, and $S + \rho + R_H$ *fit*. These refinement windows can be opened using either the 1PB or 2PB model, depending on which option is selected on the toolbar (indicated by the switches marked as (2)).

After ensuring the data have been correctly imported and, if necessary, interpolated, the next step is to select the desired model (1PB or 2PB) and choose which transport properties should be used for analysis and refinement. In this example, the experimental data for the full-Heusler compound $Fe_2VAl_{0.9}Si_{0.1}$ have been imported and will be used to demonstrate the workflow of *SeeBand*. As a first introduction to the GUI, Figure 2 shows the interface for the simplest case: using the 1PB model to fit only the Seebeck coefficient. In this scenario, the *SeeBand* window is divided into two panels. The left panel displays the experimental data for the temperature-dependent Seebeck coefficient as grey circles, while the red solid line represents the calculated $S(T)$ based on the parameters specified in the input fields on the right.

For the single parabolic band model, the only factors influencing $S(T)$ are the position of the Fermi level (E_F) and the sign of the band mass (m_1), which determines whether it is a valence band or a conduction band, thereby dictating the sign of $S(T)$. The absolute value of m_1 does not impact the result. The right panel illustrates the assumed electronic structure derived from the selected parameters.

It is evident that the experimental data cannot be fully described by the 1PB model across the entire temperature range. However, *SeeBand* allows users to extract relevant information by constraining the fit range. This can be done by accessing the advanced options through the button marked in blue, which opens the pop-up window shown on the far right. This window enables users to define limits for the fitting parameters and specify the temperature interval to be considered in the fit.

To obtain a meaningful result from the fit of $S(T)$, the temperature range in this example was constrained to $5 - 240\,\mathrm{K}$. Within this adjusted interval, the experimental data can be adequately fitted, yielding a positive band mass m_1, which corresponds to electron-dominated transport under this convention, and a Fermi level $E_F = 641\,\mathrm{K} (\approx 0.059\,\mathrm{eV})$ doped into the conduction band. The fit result of the Seebeck coefficient, obtained by pressing the *Fit from manipulate* button, is shown in Figure 3 as the dashed green line.

The resulting curves can be exported to a text file using the *Data to file* button, marked as (1) in the image. This export includes the experimental data (measured values), the user-generated curve (reflecting the initial parameters set via the GUI), and the fit curve (showing the refined match between the model and experimental data). Additionally, the fit parameters derived from this analysis can be saved using the *Fit parameters to file* button, marked as (2).

Moreover, other physical properties, such as the temperature dependence of the chemical potential $\mu(T)$ or the electronic thermal conductivity, can be derived from the assumed electronic structure. These additional properties can be accessed via the *Additional graphs* button, marked as (3). This feature will be explored in more detail when discussing the 2PB model for simultaneous fitting of $S(T)$, $\rho(T)$, and R_H in the following. Building on the previous

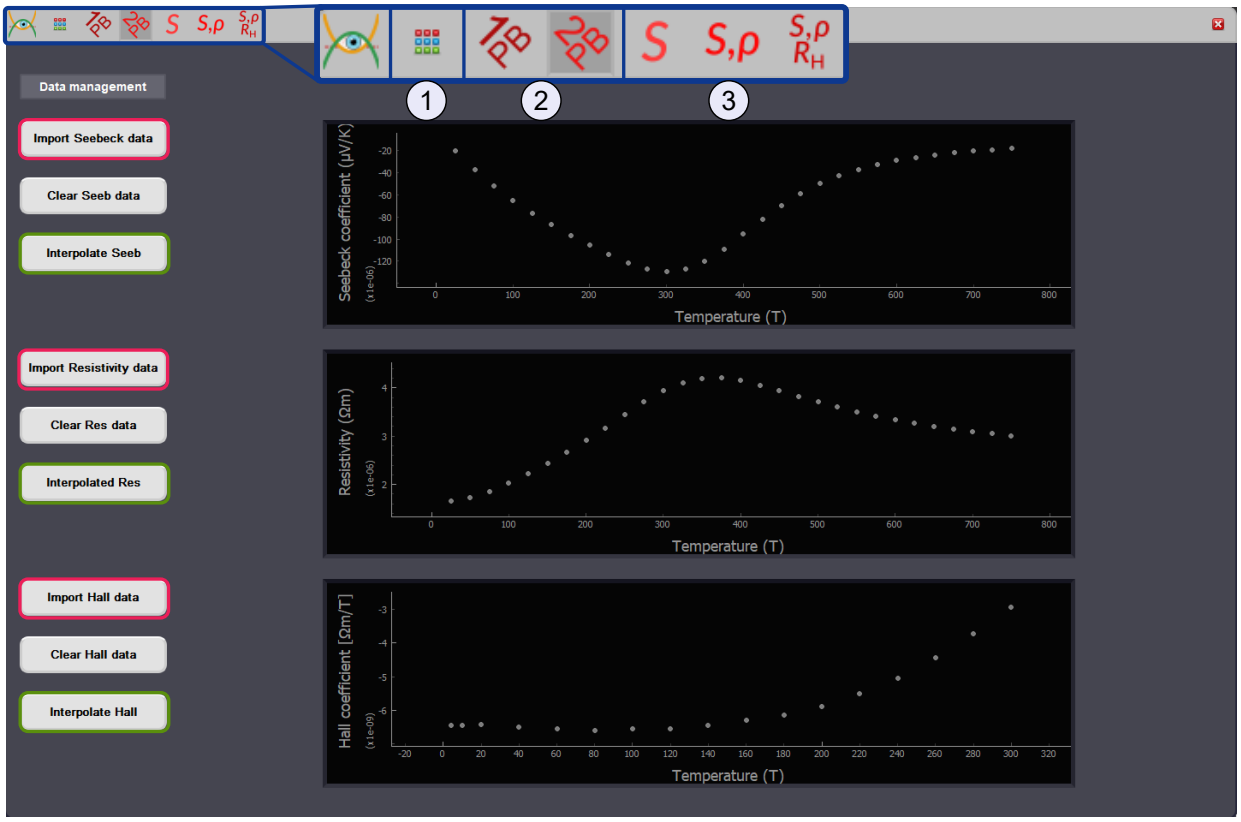

Fig. 1 Start screen of *SeeBand*. This window allows users to import experimental data and visually validate the plotted results. The red-marked buttons open file dialogs for importing data. The green-marked buttons enable interpolation of the imported data onto an equidistant temperature grid, ensuring even weighting across the dataset. The toolbar at the top is magnified, with icons for importing data (1), selecting between the one-parabolic-band and two-parabolic-band models (2), and accessing the fitting windows for *Only Seebeck fit*, $S + \rho$ *fit*, and $S + \rho + R_H$ *fit* (3).

analysis, we now turn to the simultaneous fitting of multiple transport properties, applying the two-parabolic band model. The *SeeBand* window for fitting $S(T)$, $\rho(T)$, and R_H is shown in Figure 4, with the experimental datasets for $Fe_2VAl_{0.9}Si_{0.1}$ imported. This window features four panels displaying $S(T)$, $\rho(T)$, and R_H, as well as a sketch of the effective electronic structure near E_F. The red solid lines represent the calculated transport properties based on initial manual adjustments using the input fields and sliders on the left.

For this fitting procedure all six parameters discussed in the main text are relevant. The (1) degeneracy of the bands is set via the input fields $\mathbf{N}_1$ and $\mathbf{N}_2$, respectively. The remaining band parameters, which are included in the fitting procedure can be set via sliders and input fields as follows: (2) band mass ratio: $\boldsymbol{m_2/m_1}$, (3) band gap: $\boldsymbol{E}_\mathrm{g}$, (4) Fermi level relative to valence band edge: $\boldsymbol{E}_\mathrm{F} = \eta(0)$, (5) scattering time: $\boldsymbol{\tau}_{\mathrm{ph},1}$ for acoustic-phonon scattering and scattering time ratio: $\boldsymbol{\tau}_{\mathrm{ph},2}/\boldsymbol{\tau}_{\mathrm{ph},1}$, and (6) band mass of band one $\boldsymbol{m_1} = m_1$ in units of the electron mass m_e. The dominant scattering parameter can chosen via the combo box on the top, marked as (7). Here, the user can choose between acoustic-phonon scattering, alloy-disorder scattering and a combination of the two. To combine the two scattering mechanisms with similar energy-dependence the Matthiessen rule is applied:

$$\frac{1}{\tau_\mathrm{tot}} = \sum_i \frac{1}{\tau_i} \,. \tag{1}$$

Using the neural network, a good first guess is made for the parameters governing the transport properties of $Fe_2VAl_{0.9}Si_{0.1}$. For a successful fit utilizing the 2PB model, a precise initial guess for the Seebeck curve is crucial. The fit of $S(T)$ is the most delicate one, as the refined parameters define the assumed electronic structure.

Figure 5 depicts the updated user window, after the *Fit from manipulate* button was pressed. The least-squares fits, obtained from fitting the experimental curves and the updated parameters are depicted in green. While $S(T)$ is fitted very nicely, the fit for the resistivity deviates slightly from the experimental data at low temperatures. This is mainly due to the fact that for acoustic-phonon scattering $\rho(T = 0\,\mathrm{K}) = 0$ is a precondition, which clearly is not fulfilled in the experimental data. To accurately describe the resistivity of $Fe_2VAl_{0.9}Si_{0.1}$ at low temperatures, the combined scattering times of acoustic-phonon scattering and alloy-disorder scattering have to be considered.

The Hall coefficient is described decently well within

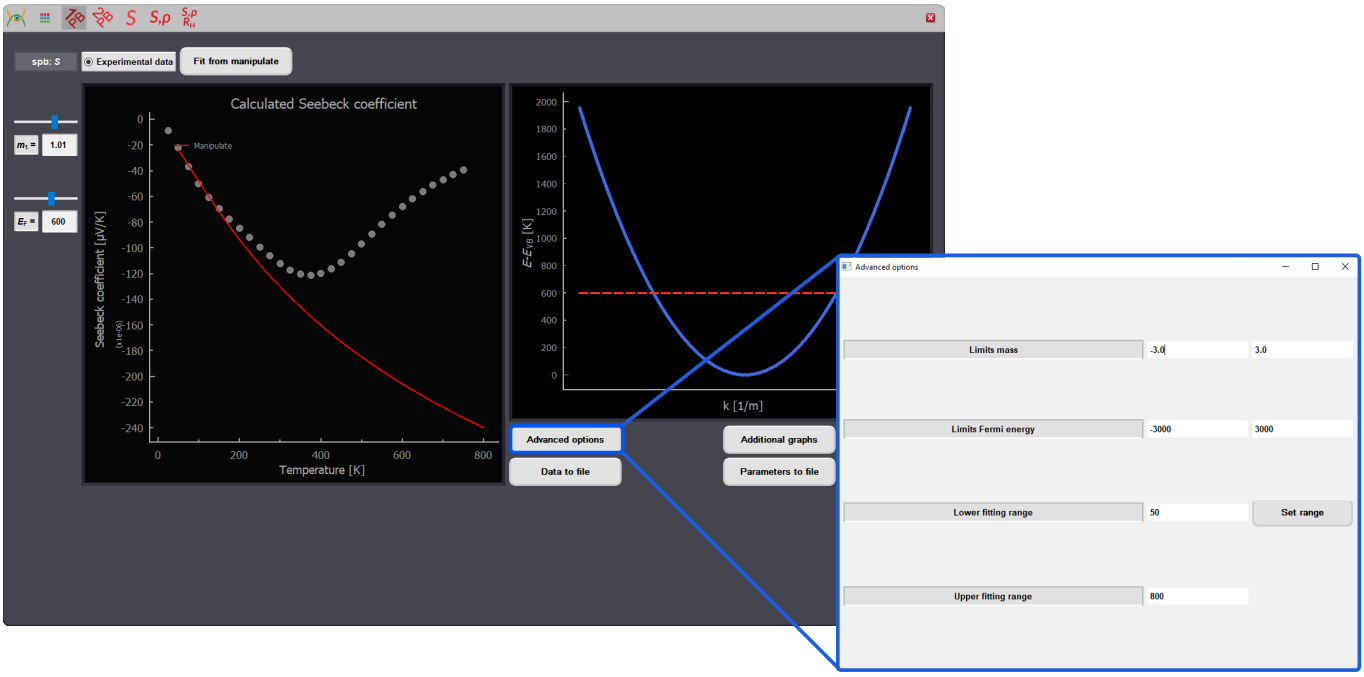

Fig. 2 ***Only Seebeck fit*** **window using the 1PB model.** The *SeeBand* window for analyzing and refining the Seebeck coefficient using the 1PB model is shown. The left panel displays the experimental data for $Fe_2VAl_{0.9}Si_{0.1}$ as grey circles, alongside the calculated data, represented by a red solid line, using the parameters set with the sliders or input fields on the left. For a single parabolic band, the Seebeck coefficient depends only on the position of the Fermi level, as explained in the main text. The sign of the effective mass determines the sign of $S(T)$, while its absolute value does not affect $S(T)$. The right panel in Figure 2 illustrates the assumed band structure used in the fit, represented by a single conduction band with the Fermi level positioned 600 K into the band. As shown, the data cannot be accurately described over the entire temperature range when assuming one-band transport. To restrict the temperature range considered in the fit, the advanced options window can be accessed, as depicted in the pop-out window on the far right. This window allows users to set limits on the fitting parameters and define the temperature range, a feature particularly important for the 1PB model since multiple bands often become relevant at higher temperatures due to the broadening of the Fermi-Dirac distribution. Notably, this feature can also be used to fix certain parameters, by adjusting the limits to a very narrow interval.

the model. For the refinement of $R_H(T)$ only the value of m_1 is adjusted, setting the overall value of R_H. Therefore, the fit of R_H validates the results obtained from fitting $S(T)$ and $\rho(T)$. After successfully fitting the imported data, the *Adjust to fit* button can be pressed, to align the adjustable parameters with the refined values. After that, specific parameters can be changed utilizing the sliders or the input fields. This can be very useful to assess the impact of different parameter changes to the transport properties of the considered material, showcased e.g. in Chapter 6 of Ref.[?] .

The panels on the bottom of Figure 5 reveal additional information, which can be accessed by pressing the *Additional graphs* button. The panel on the left depicts the temperature-dependent chemical potential $\mu(T)$ derived from the parameters. Importantly, even for this approximated electronic structure, with a relatively small gap, $\mu(T)$ exhibits significant changes with increasing T and is shifted out of the conduction band and closer to the valence band. This behavior significantly impacts the calculated transport coefficients.

The panel on the right depicts the individual contributions of the two bands to the Seebeck coefficient $S(T)$. The valence and conduction bands are represented as the red and blue solid lines, respectively, while the grey line depicts the total $S(T)$. Notably, the individual $S(T)$ curves are already weighted with the conductivity of the respective band, to determine their actual contribution:

$$S_{cont,i} = \frac{S_i \sigma_i}{\sigma_1 + \sigma_2} \,. \tag{2}$$

The middle panel shows the electronic contribution to the thermal conductivity. For the determination of λ_e, typically the simple Wiedemann-Franz law ($\kappa_e = L\sigma T$) is employed, either by using the Lorenz number for metals $L = 2.44 \cdot 10^{-8}\,\mathrm{V^2K^{-2}}$ or using more educated guesses like the one given in Ref.[?] . In the framework of the 2PB model, the Lorenz number can be directly calculated from the band parameters. Moreover, also the bipolar contribution λ_{bp} is considered within this model, stemming from the electron-hole coupling[?] , by applying **??** to directly calculate λ_e. Although often neglected in the analysis of λ_e when dissecting λ_{tot}, this additional term can increase λ_e significantly, especially at high temperatures. As the bipolar term λ_{bp} is not directly accessible via experimental methods, the estimation of λ_{bp} from the 2PB fit constitutes a favorable approach to model λ_e more accurately.

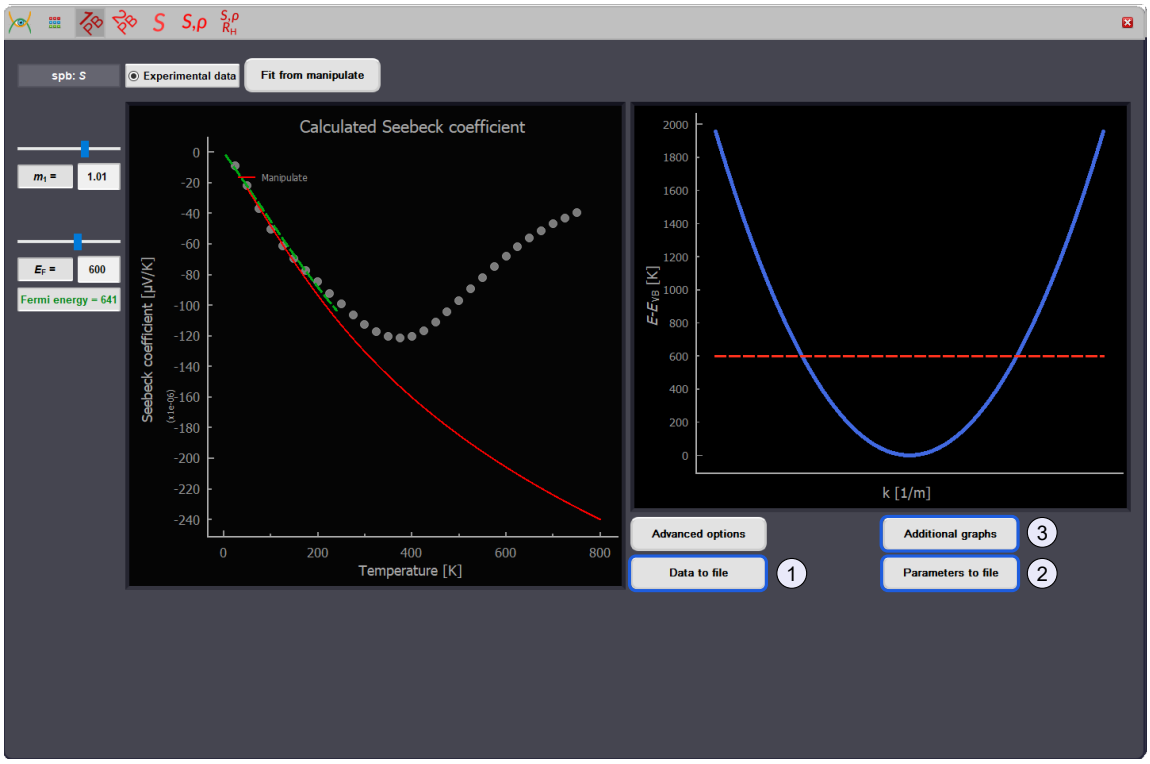

Fig. 3 ***Only Seebeck fit*** **window displaying the 1PB model fit** Here, the *SeeBand* window for the analysis and refinement of the Seebeck coefficient in the 1PB model is depicted. The left panel shows the experimental data of $Fe_2VAl_{0.9}Si_{0.1}$ as grey circles, together with the calculated data, applying the parameters set with the sliders or the input fields on the left, as red solid line. The least-squares fit within the 1PB model for the temperature range from 5-240 K is depicted as the green dashed line. The fitting parameters are depicted on the left as green text below the input fields. For the limited temperature interval the experimental curve can be well described applying one parabolic band. The experimental data, together with the resulting fit curve and the curve from the user input parameters can be printed to a text file using the *Data to file* button, marked as (1). A comprehensive list of the parameters can be printed to a text file using the similar-named button, marked as (2). Moreover, additional transport properties can be calculated from the assumed electronic structure, which can be accessed using the *Additional graphs* button marked as (3).

The presented analysis of the sample serves as a guide for how the fitting process works and how *SeeBand* can be utilized to analyze the temperature-dependent transport properties of materials.

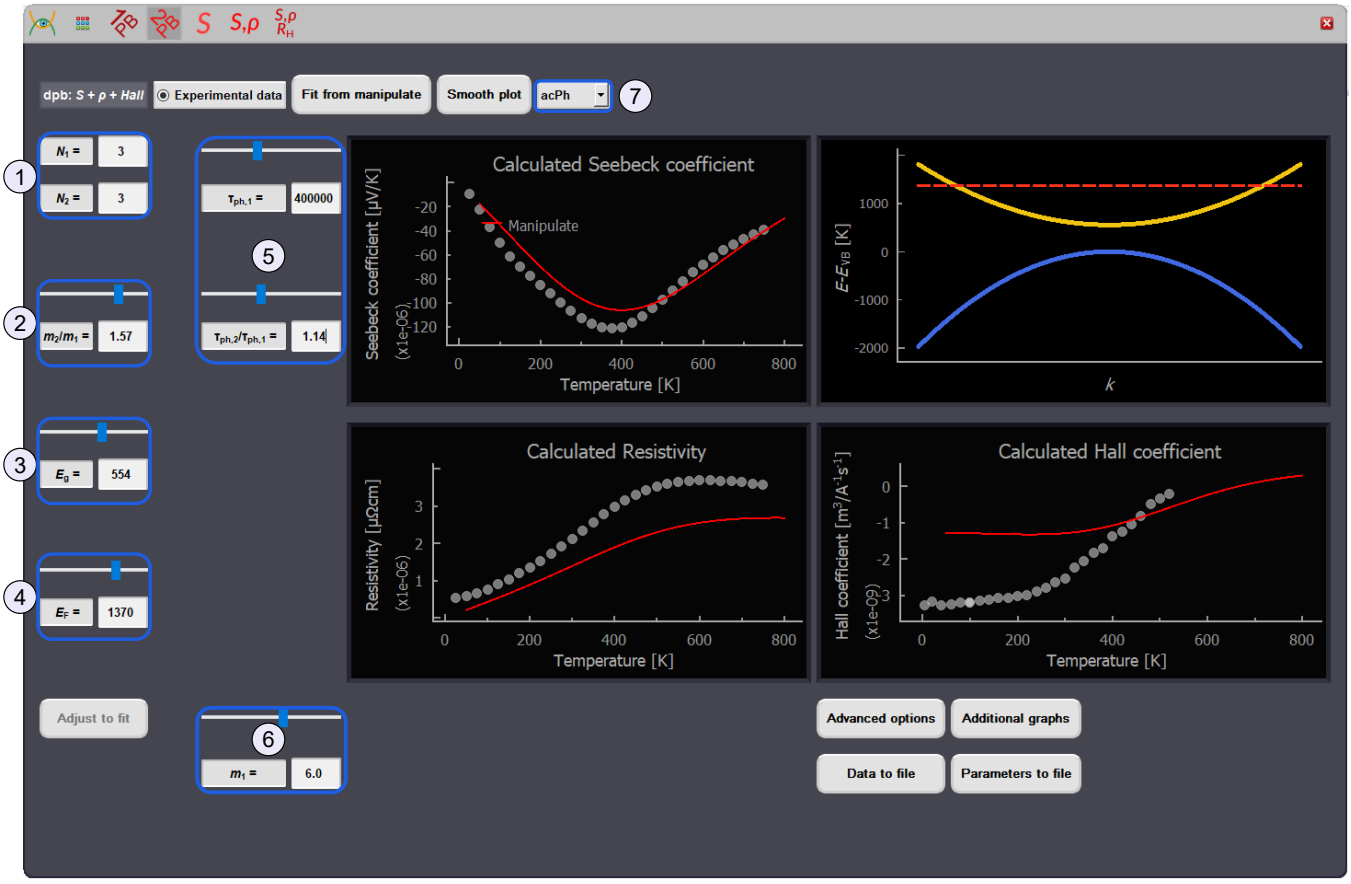

Fig. 4 *SeeBand* window for the 2PB fit of $S(T)$, $\rho(T)$, and $R_{\mathrm{H}}(T)$ The experimental data for the three transport properties $S(T)$, $\rho(T)$ and $R_{\mathrm{H}}(T)$ are depicted as grey circles in the respective panels. The red solid line represents the calculated transport properties from the manually adjusted band parameters using the input tools on the left. The top right panel depicts the effective band structure close to the Fermi level E_{F} determined by the manually set parameters. The different parameters, which can be adjusted by the user, are highlighted by blue rectangles and enumerated: Number (1) denotes the band degeneracies of the two parabolic bands, which are not refined during the fit. The other parameters are (2) the band mass ratio $\boldsymbol{m_2/m_1}$, (3) the band gap $\boldsymbol{E}_{\mathrm{g}}$, (4) the Fermi level relative to the valence band edge $\boldsymbol{E}_{\mathrm{F}}$, (5) scattering parameters $\boldsymbol{\tau_{ph,1}}$ and $\tau_{ph,2}/\tau_{ph,1} \equiv \epsilon_\tau$ and (6) the absolute value of the effective mass of the first band m_1 in units of the electron mass m_e. The dominant scattering mechanism can be set via the combo box on the top, denoted as number (7). Evidently, the initial guess is already relatively close to the experimental data, indicating that they can be described within the two-parabolic band model.

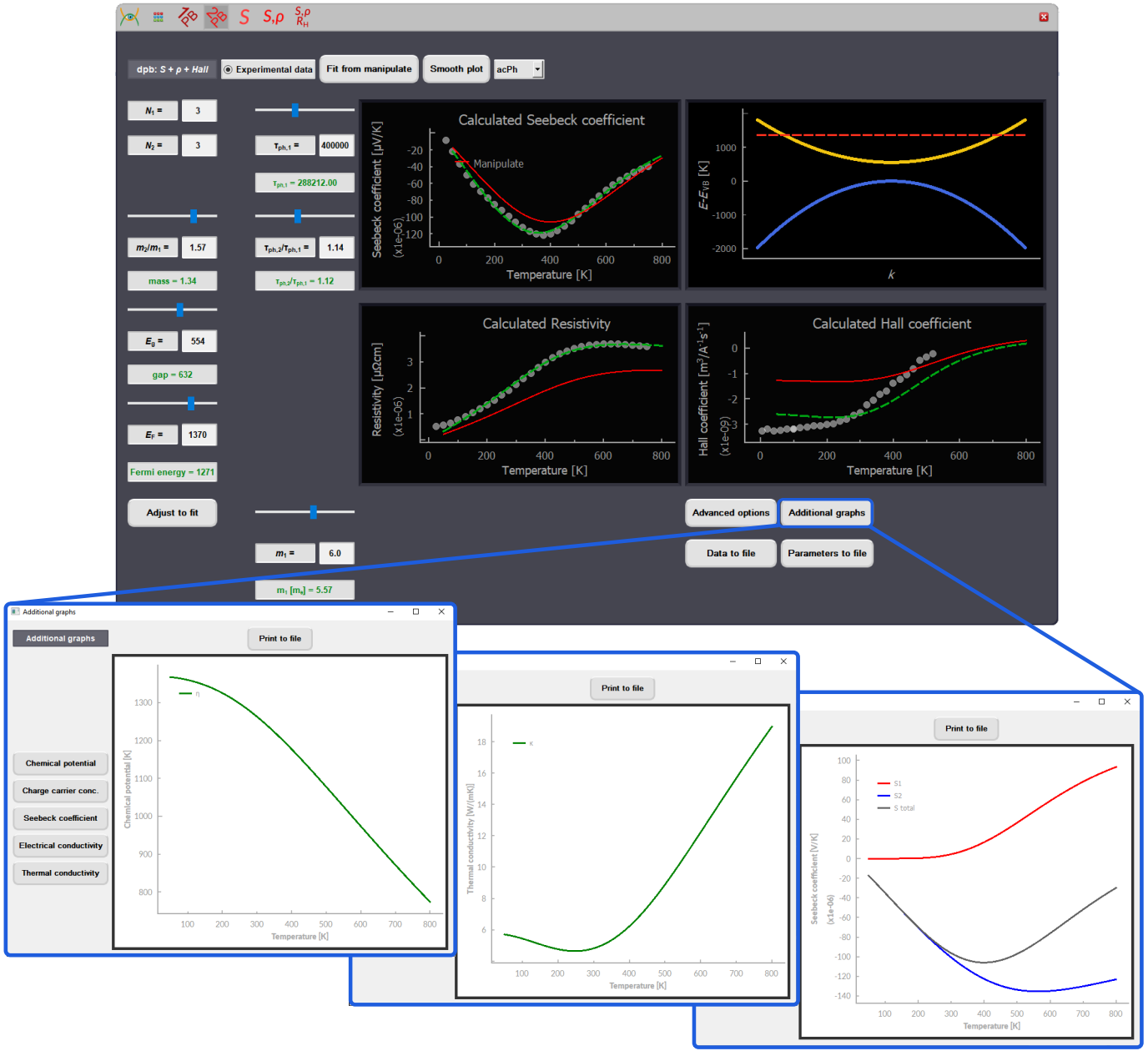

Fig. 5 S, ρ, R_{H}-fit in the 2PB model Here, the *SeeBand* window for the analysis and refinement of the Seebeck coefficient $S(T)$, resistivity $\rho(T)$ and Hall coefficient R_{H} is depicted. The panels show the data of $Fe_2VAl_{0.9}Si_{0.1}$ as grey circles, together with the curves from the manual guess as red solid lines, and the resulting fit curves as dashed green lines, together with the approximated electronic structure in the top right. Using the extracted parameters, additional physical properties can be calculated from the refined electronic structure. The panels on the bottom depict the temperature dependence of the chemical potential $\mu(T)$, the electronic thermal conductivity λ_e as well as the individual $S(T)$ contributions of the individual bands, as detailed in the text. Notably, the chemical potential exhibits a strong temperature dependence even for the small gap assumed for this dataset.