High-Entropy Alloys Predicting Software HEAPS V1.0

The software is available for use in two manners: as a software or as a MATLAB code. HEAPS as software runs in 32/64 bits Windows systems and requires 2 GB of disk space for its installation. The installation files may be found in www.rpm.usm.cl.

The software possesses two different calculation modes. Firstly, the Single Calculation mode, in which the physical and semi-empirical parameters, as well as the evaluation of several criteria, of single alloy composition, at a particular temperature of evaluation, are computed. Secondly, the Exploration mode allows to calculate the physical and semi-empirical parameters, as well as the different criteria, includes in HEAPS, of multiple alloys. Although there is not an exact routine to perform a computation in HEAPS, the present document addresses the recommended pathways to properly use both calculation modes using the software interface. Additionally, it also addresses the pathways to use HEAPS by means of the MATLAB codes, as well as some additional features that are not incorporated in the software version of HEAPS.

i) Software version: Single Calculation mode

Figure 1 depicts the default settings of the HEAPS interface, just after running the executable file. The first action could be select the constituent elements (by clicking in the respective element button). After selecting an element, the button will show a darker gray color, and the element will be listed in the Selected constituent elements section, as depicted in Figure 2. If a clicked element button is clicked again, the element will be erased from the Selected constituent elements section.

After selecting the constituent elements, the following aspect is to select the composition of the alloy. The software incorporates three composition scales: molar ratio, weight percent, and atomic percent. Figure 3 depicts the dropdown bar that addresses this aspect. The user may take in account that in the case that the weight percent or atomic percent composition scales are selected, the composition of the first component will be disabled and set in order that the sum of all the components would be equal to 100. Next to each element there is an edit field in which the user may enter the composition of each element. By default, in the molar ratio scale composition the value of the composition of the elements is 1, and in the other cases, is equal to 10 (except for the first component that will be set to sum 100).

Then, the user must enter the temperature of evaluation, in the Kelvin scale. The default value is equal to 1000. Figure 4 depicts the entering of the temperature of evaluation.

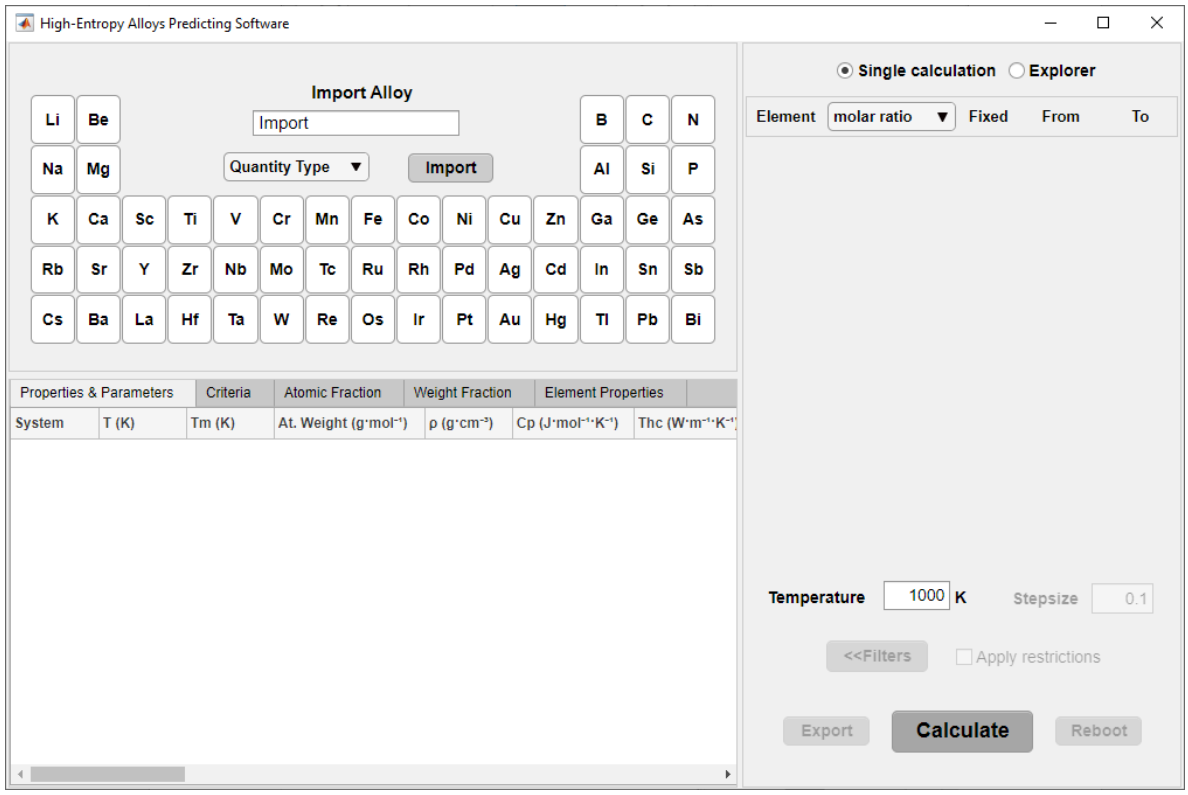


Figure 1: Default settings of HEAPS interface.

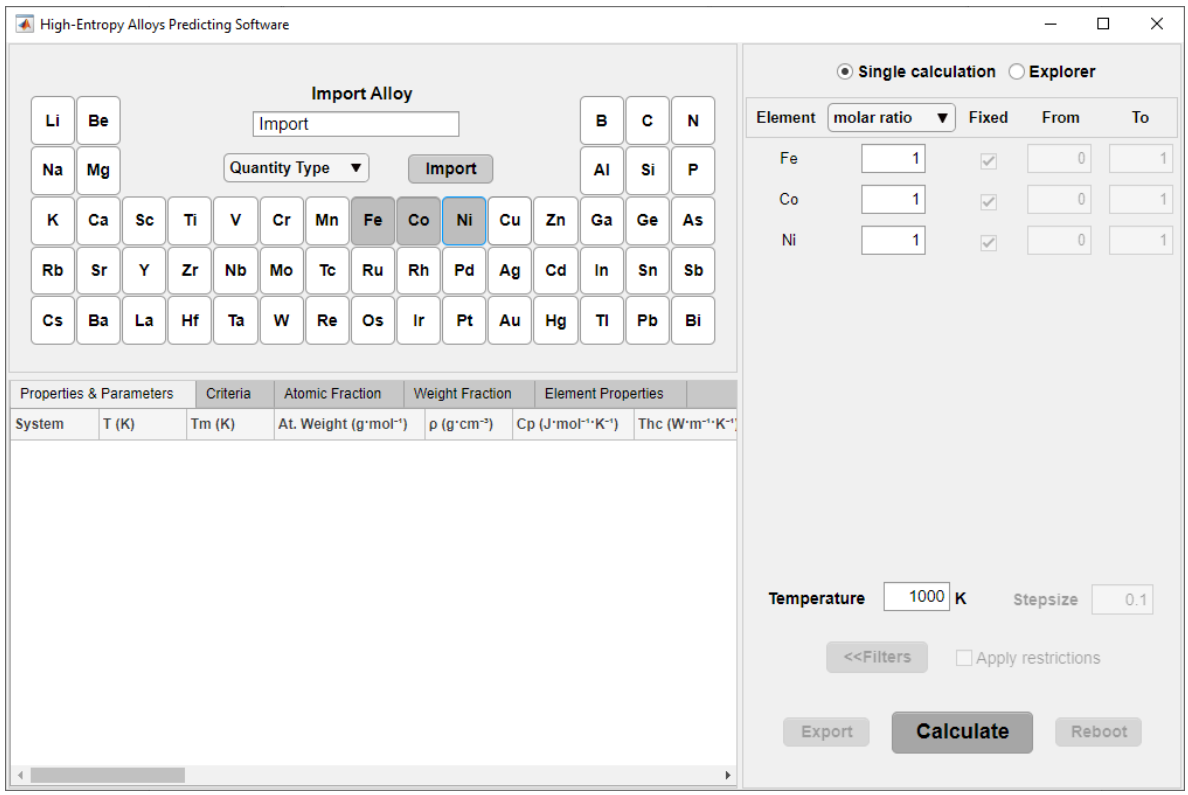


Figure 2: Selection of constituent elements.

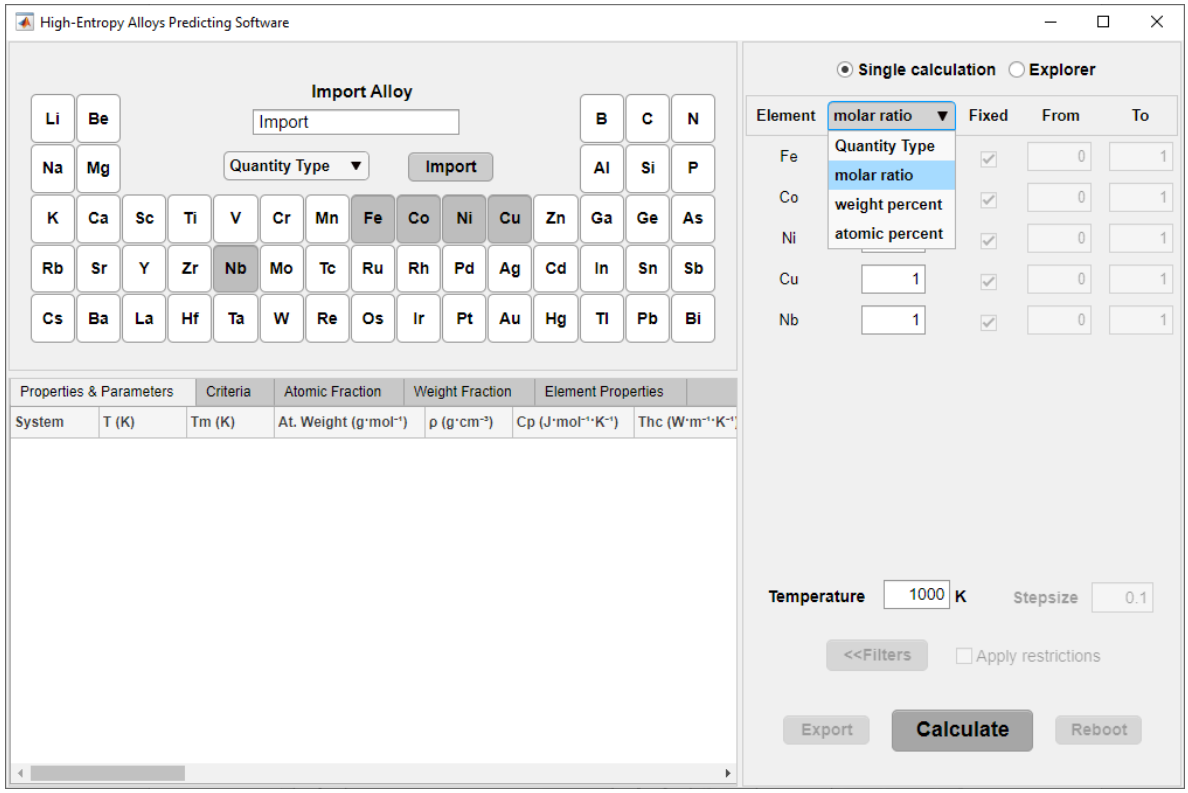


Figure 3: Selection of composition scale

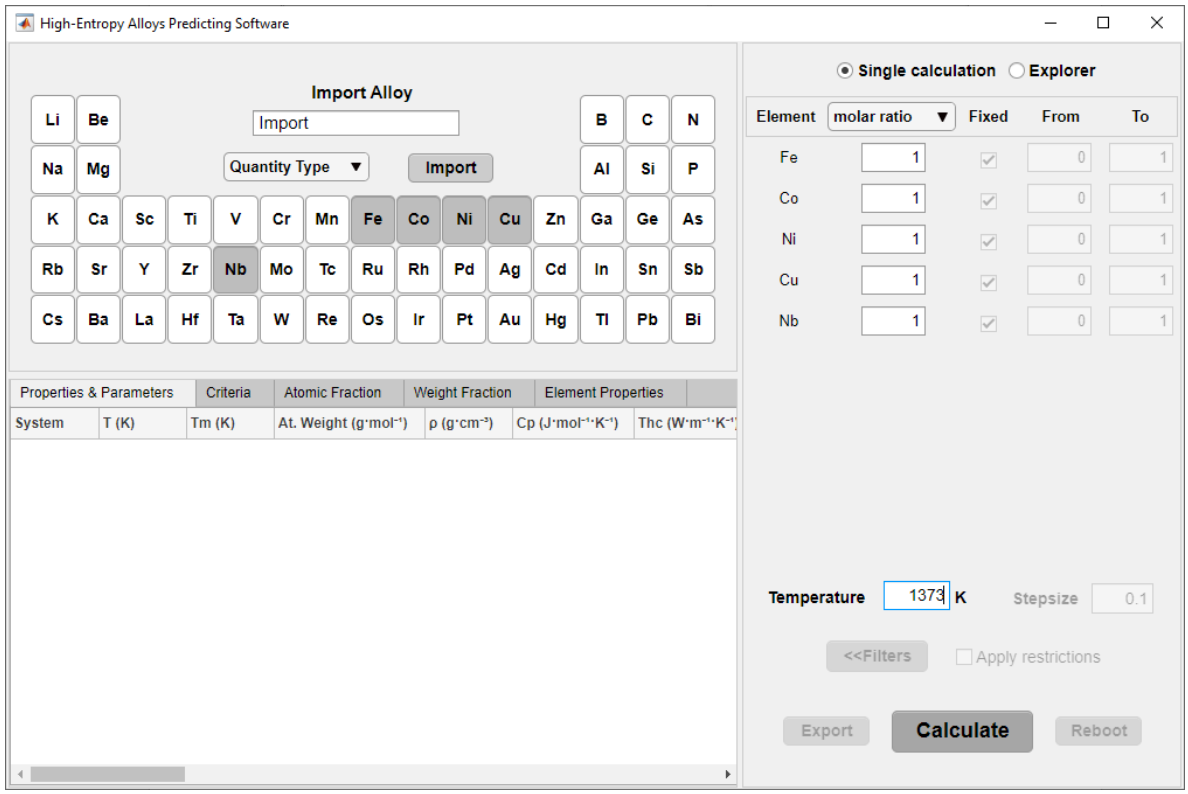


Figure 4: Selection of temperature of evaluation

Then, after clicking the Calculate button, the computation will be performed, and the results will be depicted in the Results Table at the bottom-left corner, as shown in Figure 5. By default, the values of the computed parameters are shown in the interface; however, there are five tabs depicting information about the alloys or the constituent elements. Figure 6 depicts the tab of elemental properties of constituent elements.

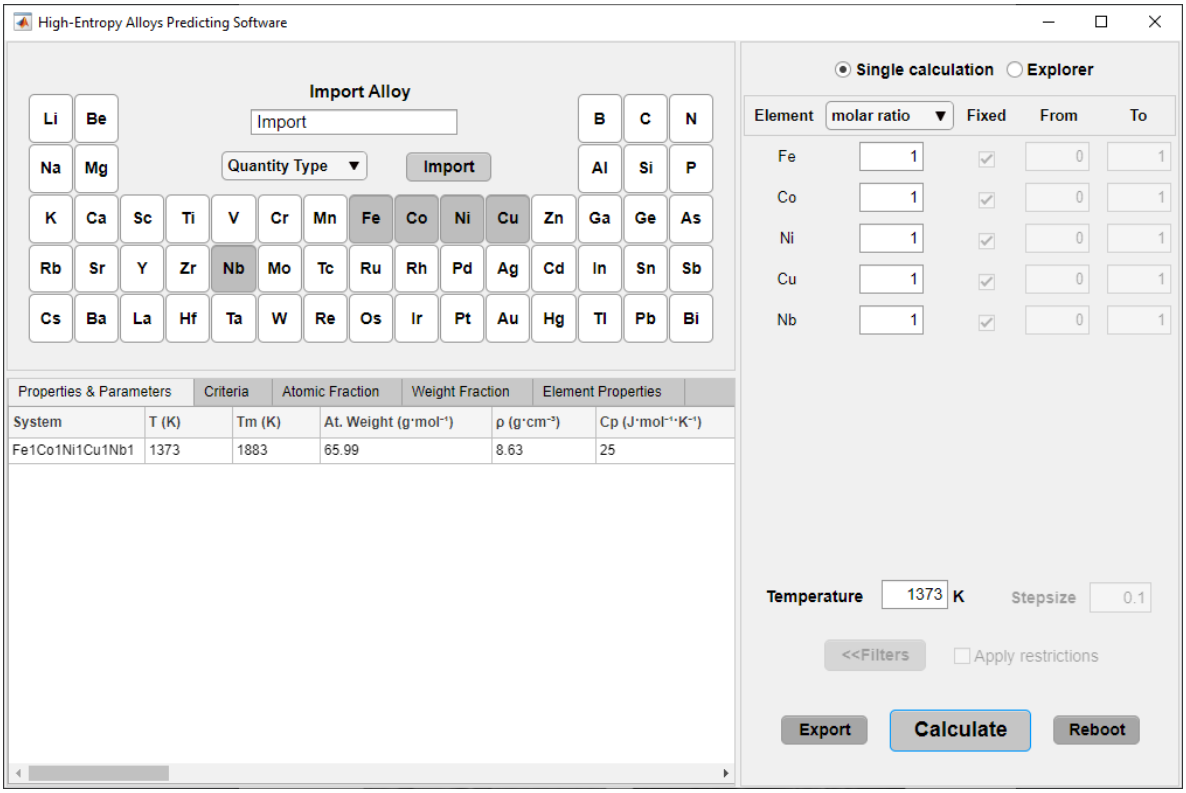


Figure 5: Table of results depicting computed parameters.

After performing the calculation, the user has the option to export those results into an XLS file. This action is performed by clicking the Export button, located at the left of the Calculate button (as is highlighted in Figure 7). Then, the directory browser will appear, and the user must select the XLS in which the results will be exported (as depicted in Figure 8). Figure 9 shown the XLS file after exporting the results obtained with HEAPS. As the reader may note, five sheets are generated in the XLS file, each of them depicting the information depicted in the respective tab of the Table of results of the interface.

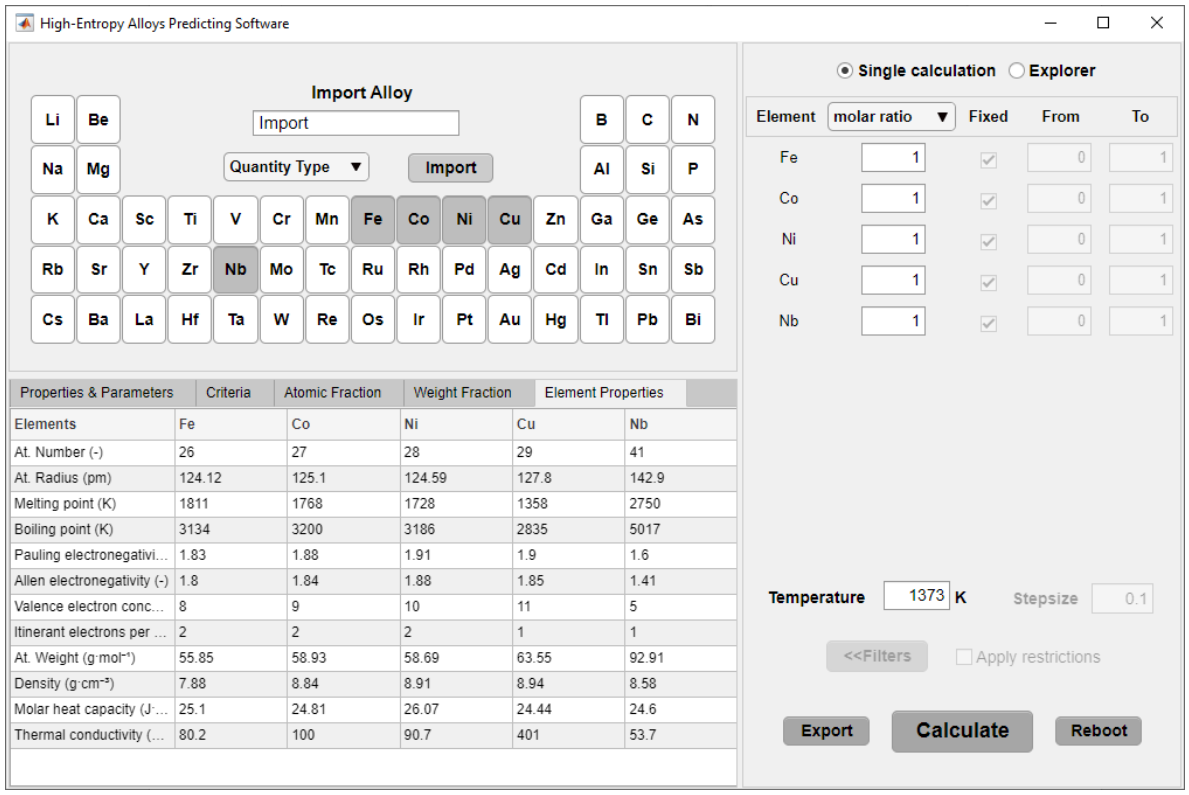


Figure 6: Table of results depicting elemental properties of constituent elements.

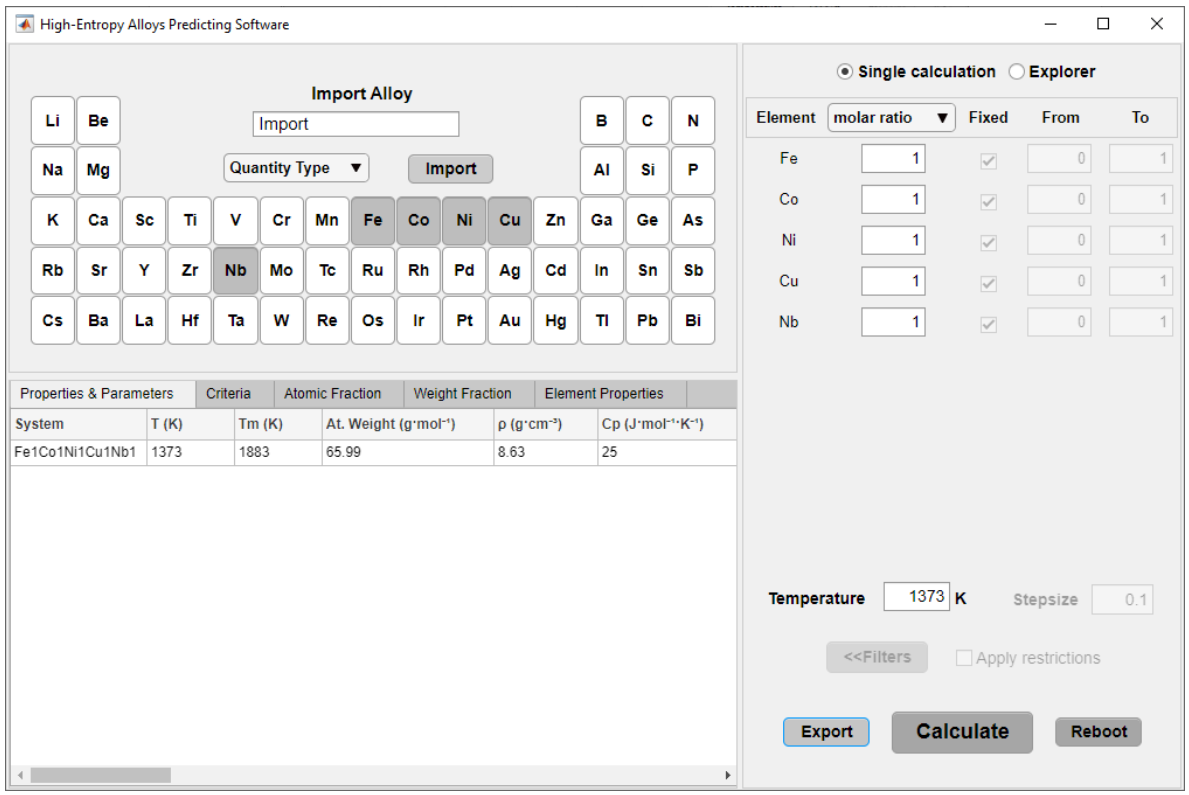


Figure 7: Export button.

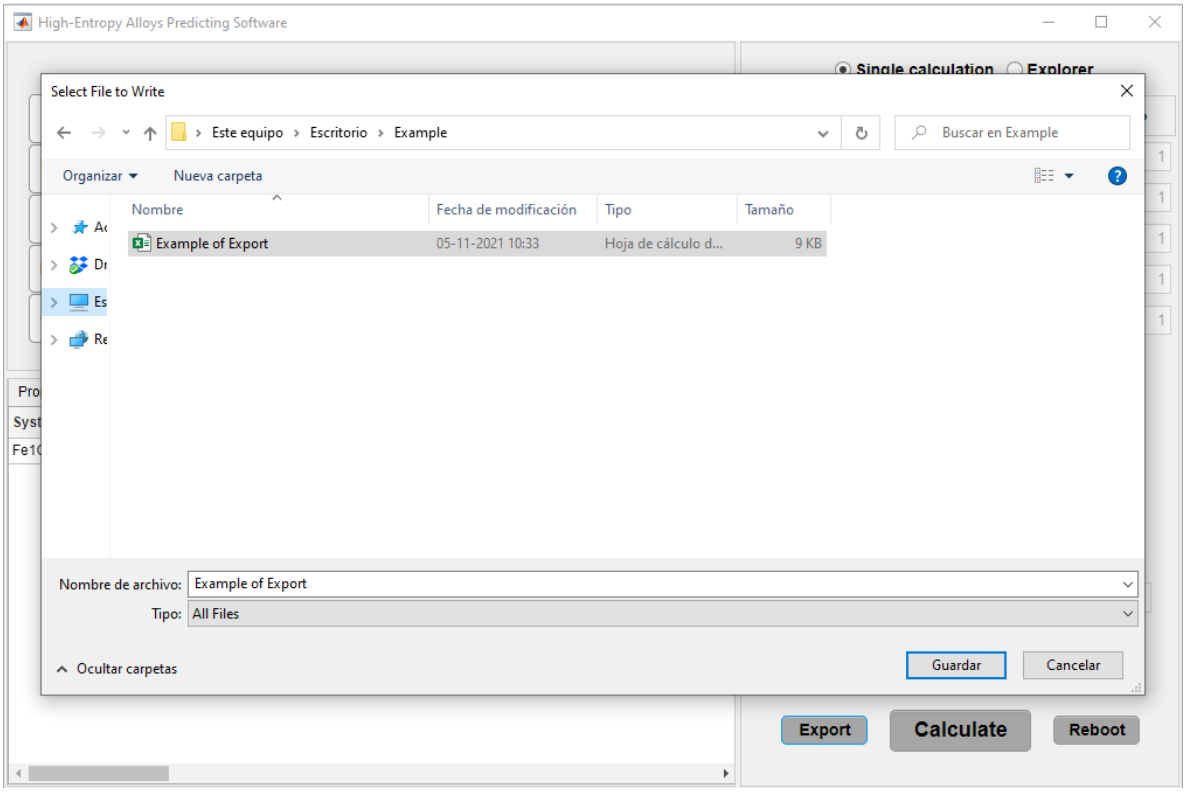


Figure 8: Selection of the XLS file.

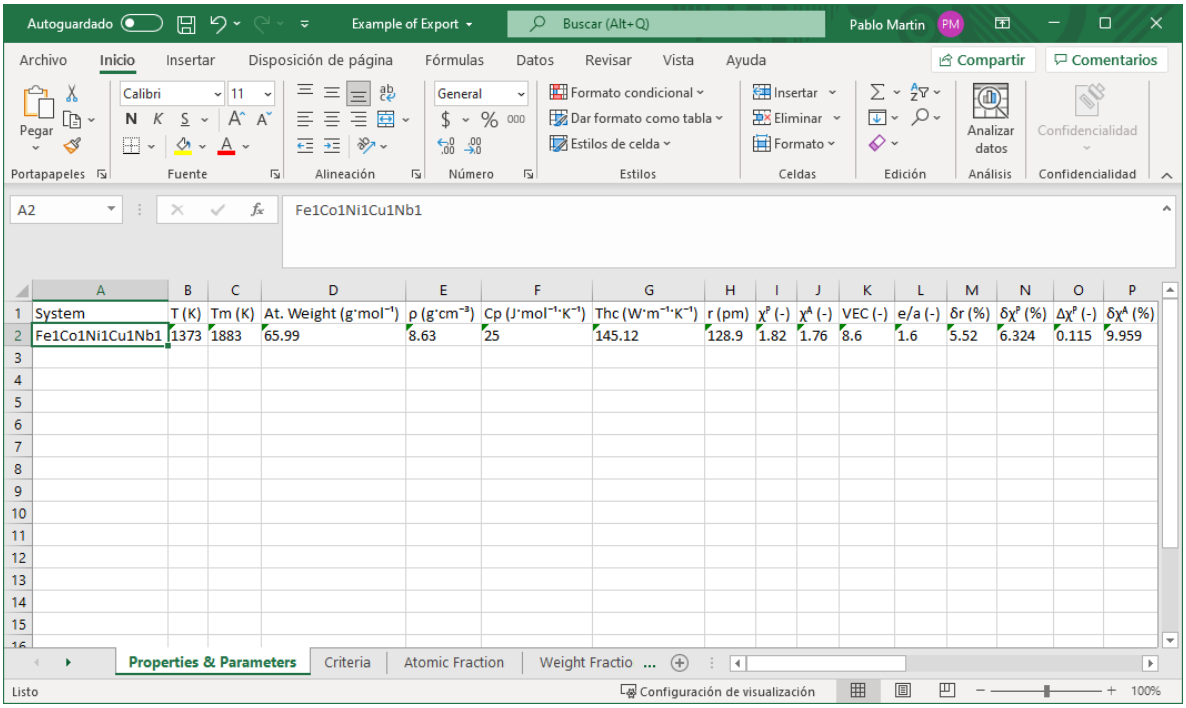


Figure 9: XLS file depicting the computed results.

Another feature included in HEAPS is the possibility to import alloy data in order to calculate their physical and semi-empirical parameters and evaluate the corresponding criteria, without the need

of entering the alloy compositions manually into the software. Figure 10 depicts the format in which the alloy data must be entered in the XLS file: first column with the alloys in the format A1B1C1D1, with A, B, C, and D corresponding to the symbol of the corresponding chemical element, and the number at its right corresponds to their presence in the alloy in a certain composition scale; the second column indicates the temperature of evaluation of the respective alloy. As the reader may notice, the example includes an alloy with no corresponding temperature (A5 and B5, respectively), and an alloy with unknown elements (A7). In the first case, if a temperature of evaluation is missing, the software will perform the computations using the temperature of evaluation set in the GUI. In the second case, the alloy is not considered in the computation.

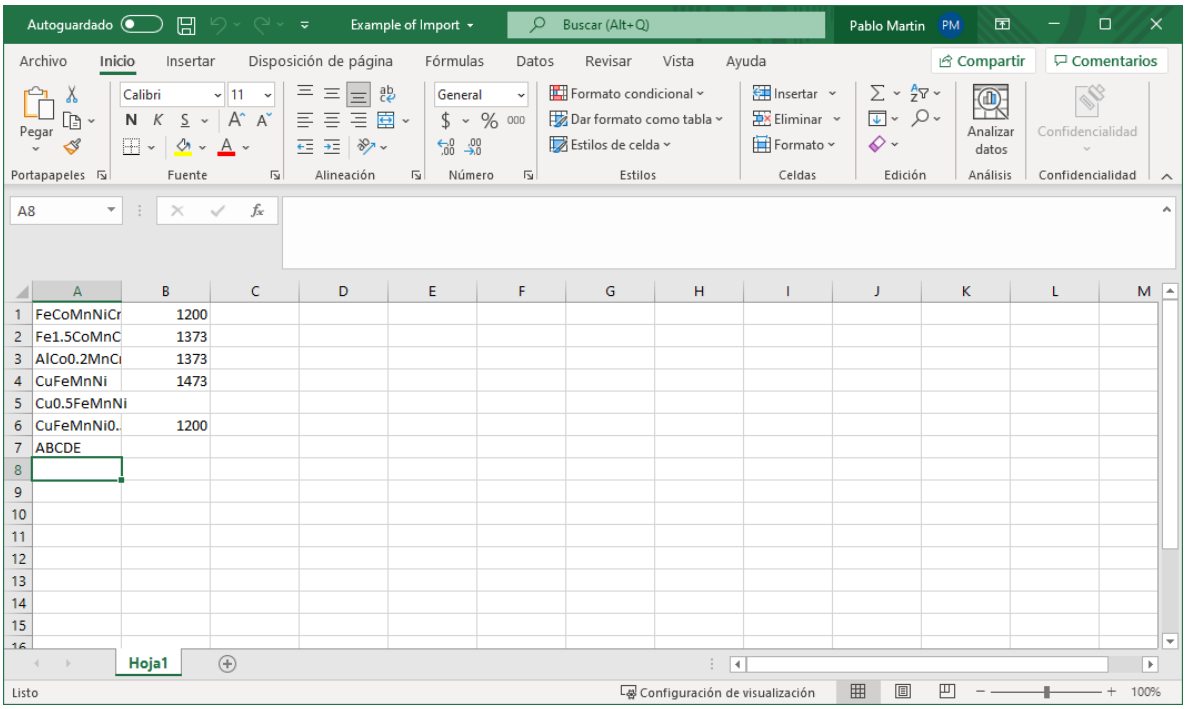


Figure 10: Format of the data in the XLS file for importing to HEAPS.

The first action to import alloy data, is define the composition scale in the dropdown bar as shows Figure 11. Hence, the alloy data in the XLS file should be entered in a unique composition scale. After that, the user must click the Import button, and the directory file window will pop up (as Figure 12 shows). Then, the user must select the XLS file containing the data, and the software will perform the computation. The results will be depicted in the Table of Results, as Figure 13 depicts, but they will be also stored in the origin XLS file, as Figure 14 depicts.

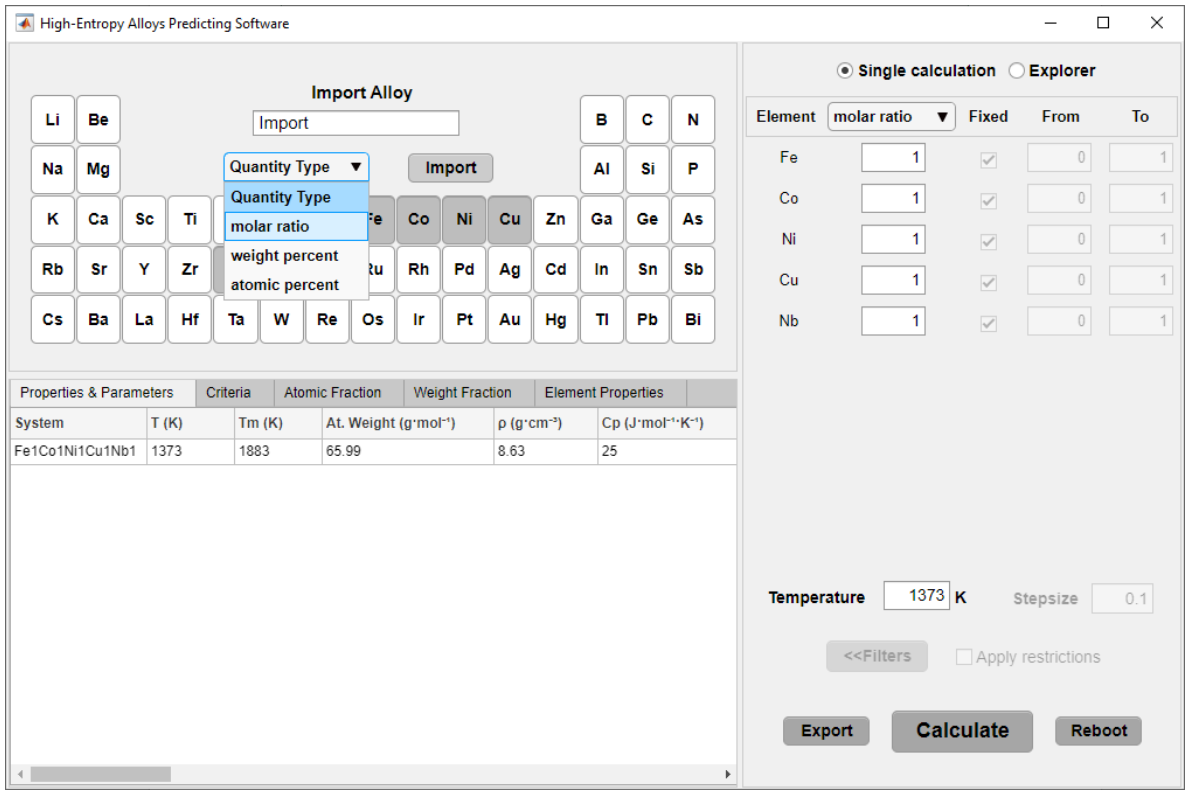


Figure 11: Selection of the composition scale to use the Import feature.

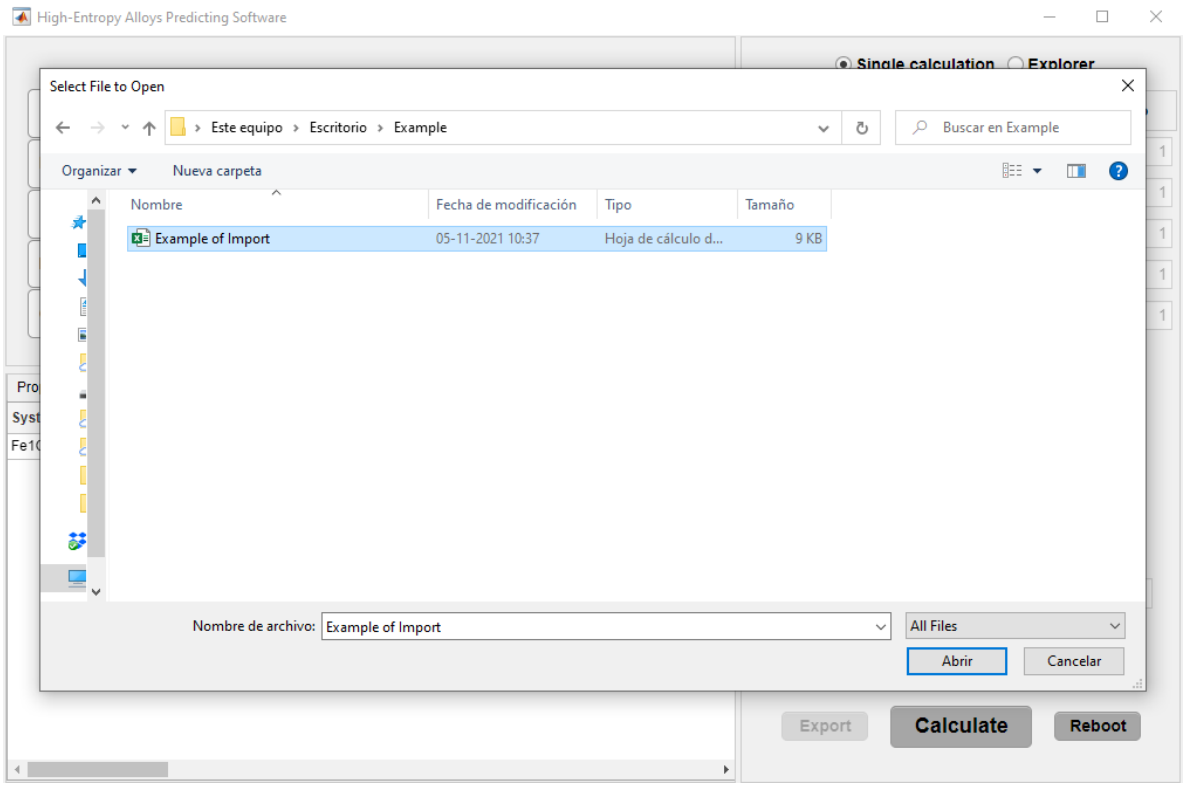


Figure 12: Selection of the XLS file containing the alloy data to be imported to HEAPS.

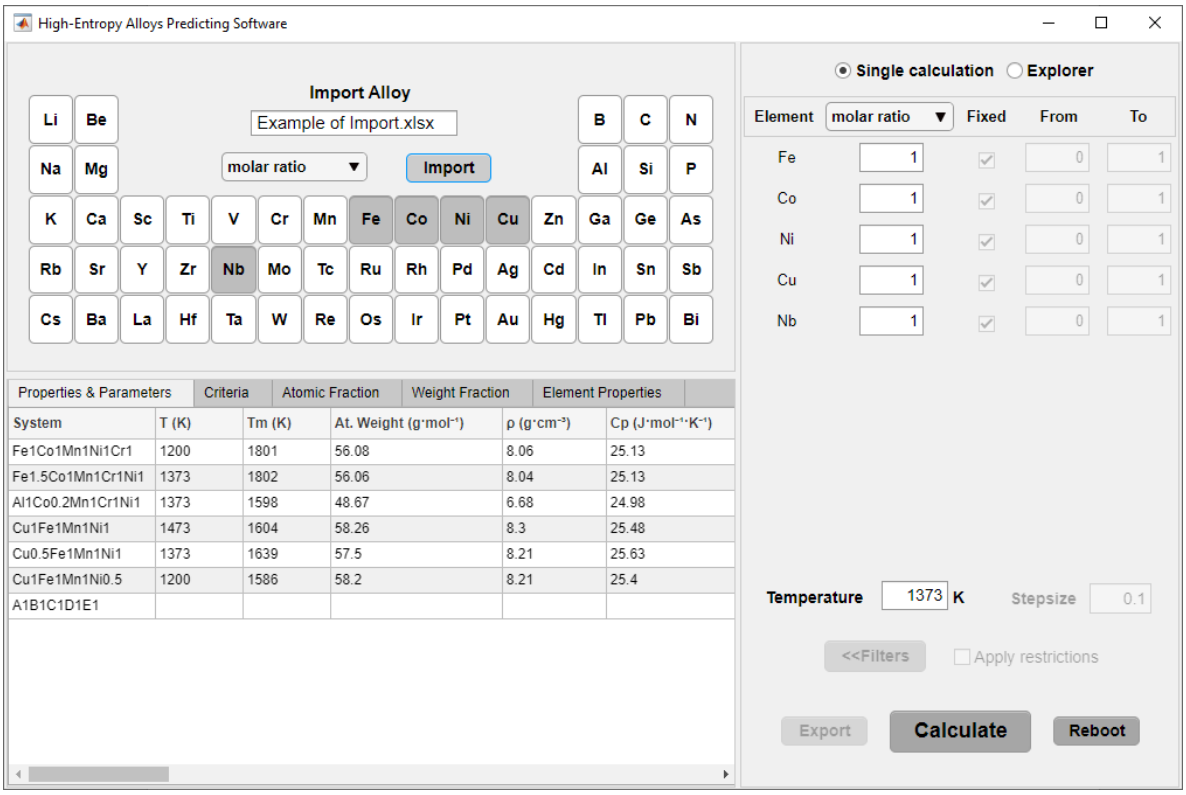
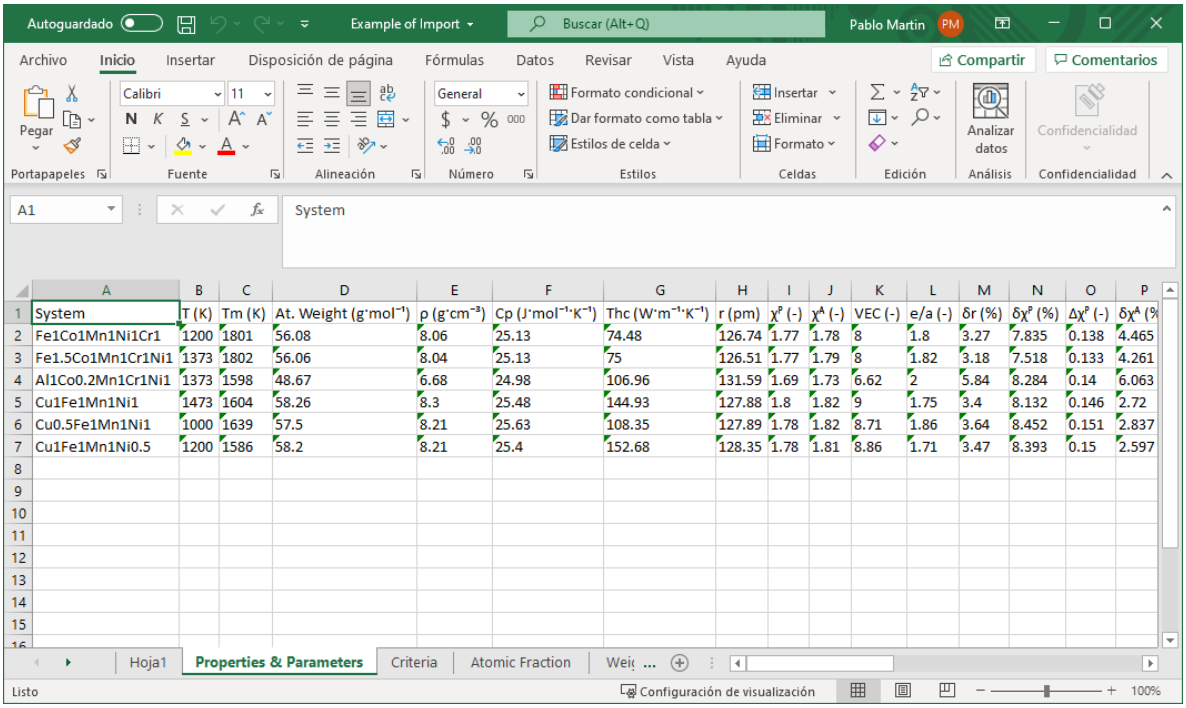


Figure 13: Table of results depicting the results of the imported alloy data.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	System	T (K)	Tm (K)	At. Weight (g·mol⁻¹)	ρ (g·cm⁻³)	Cp (J·mol⁻¹·K⁻¹)	Thc (W·m⁻¹·K⁻¹)	r (pm)	χ^P (-)	χ^A (-)	VEC (-)	e/a (-)	δr (%)	$\delta\chi^P$ (%)	$\Delta\chi^P$ (-)	$\delta\chi^A$ (%
2	Fe1Co1Mn1Ni1Cr1	1200	1801	56.08	8.06	25.13	74.48	126.74	1.77	1.78	8	1.8	3.27	7.835	0.138	4.465
3	Fe1.5Co1Mn1Cr1Ni1	1373	1802	56.06	8.04	25.13	75	126.51	1.77	1.79	8	1.82	3.18	7.518	0.133	4.261
4	Al1Co0.2Mn1Cr1Ni1	1373	1598	48.67	6.68	24.98	106.96	131.59	1.69	1.73	6.62	2	5.84	8.284	0.14	6.063
5	Cu1Fe1Mn1Ni1	1473	1604	58.26	8.3	25.48	144.93	127.88	1.8	1.82	9	1.75	3.4	8.132	0.146	2.72
6	Cu0.5Fe1Mn1Ni1	1000	1639	57.5	8.21	25.63	108.35	127.89	1.78	1.82	8.71	1.86	3.64	8.452	0.151	2.837
7	Cu1Fe1Mn1Ni0.5	1200	1586	58.2	8.21	25.4	152.68	128.35	1.78	1.81	8.86	1.71	3.47	8.393	0.15	2.597
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Figure 14: Origin XLS file after the computation of imported alloy data.

ii) Software version: Explorer mode

Figure 15 depicts the default interface when the Explorer calculation mode is selected. The main difference that the user may notice is that the Stepsize edit field and the Apply Restrictions checkbox are enabled.

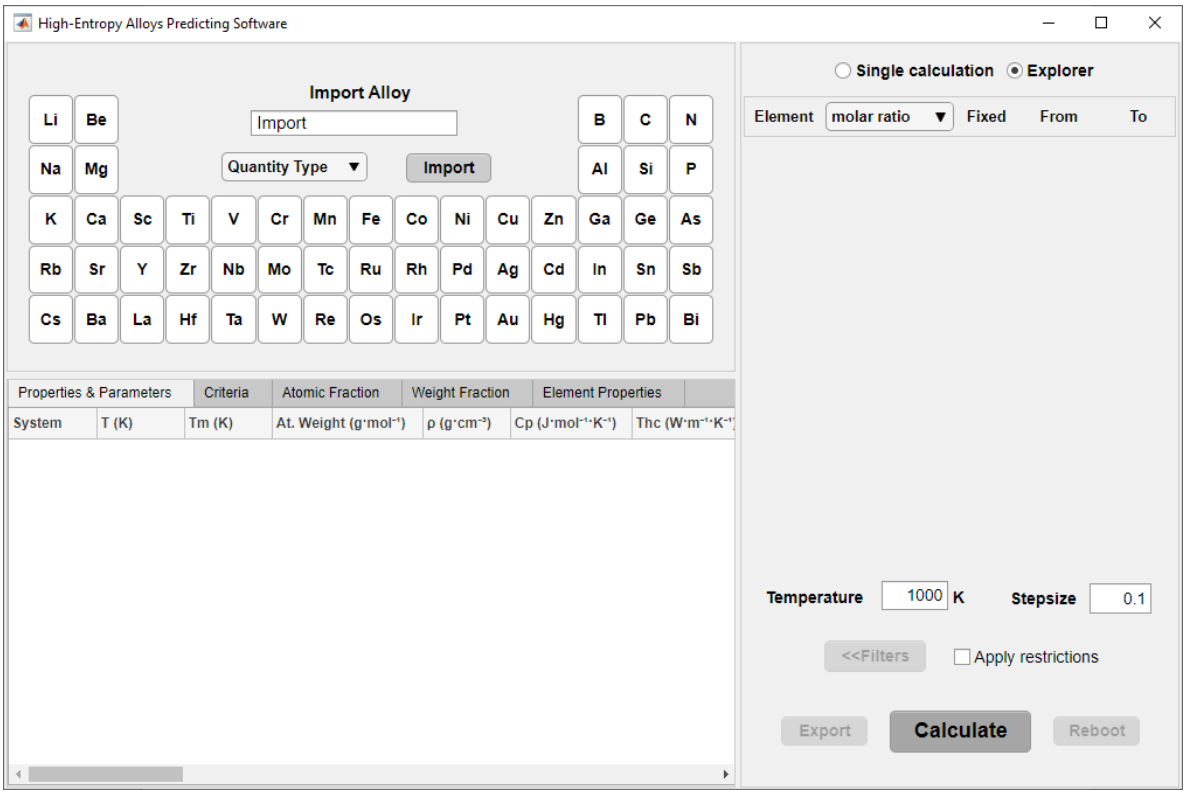

Figure 15: Default settings of the interface after selecting the Explorer mode.

Just as in the previous case, the user must select the constituent elements by clicking the respective button, and the elements will be listed as the Figure 16 shows. Then, and after selecting the composition scale, the user must define the composition rules. This is performed by unchecking the respective Fixed checkboxes, as Figure 17 depicts. Hence, the respective From and To edit fields will be enabled. These edit fields will define the lower and upper limit in which the respective element will vary during the computation, with a step size also defined by the user in the Step size edit field. The user can also define these lower and upper limit values, as Figure 17 shows. Lastly, the user can click the Calculate button, and a pop-up window will indicate the number of alloys that will be computed (according to the composition rules defined by the user, in this example, 144 alloys will be evaluated) and the progress of the calculation (as Figure 18 shows). Just as in the Single calculation mode, the results will be immediately depicted in the Table of Results, as Figure 19 indicates.

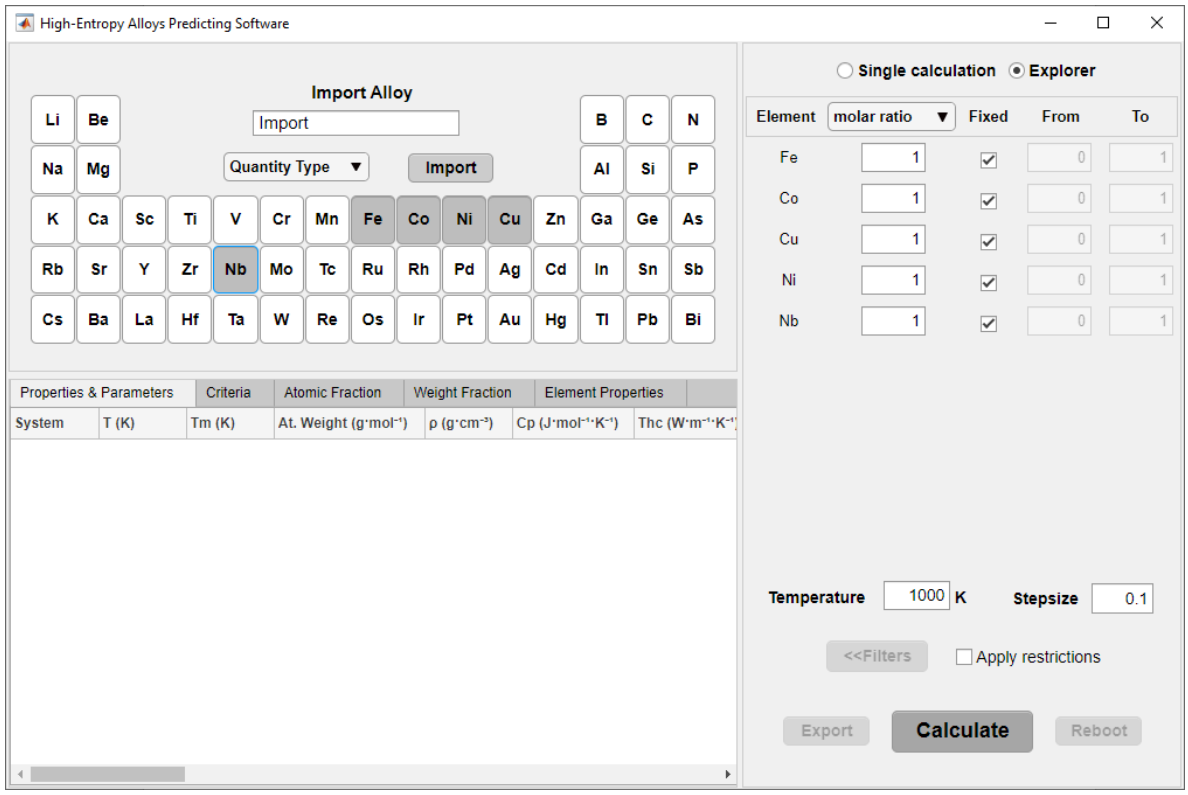

Figure 16: Selection of constituent elements in the Explorer mode.

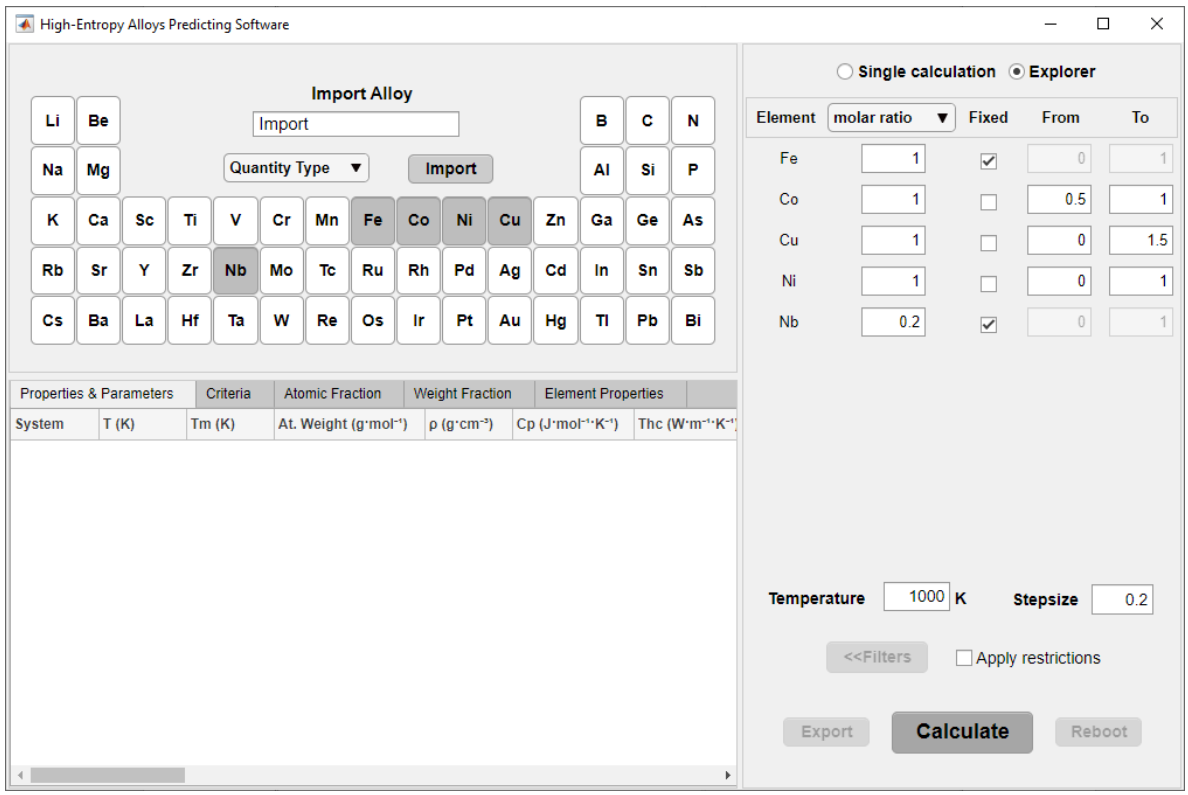

Figure 17: Selection of the composition rules.

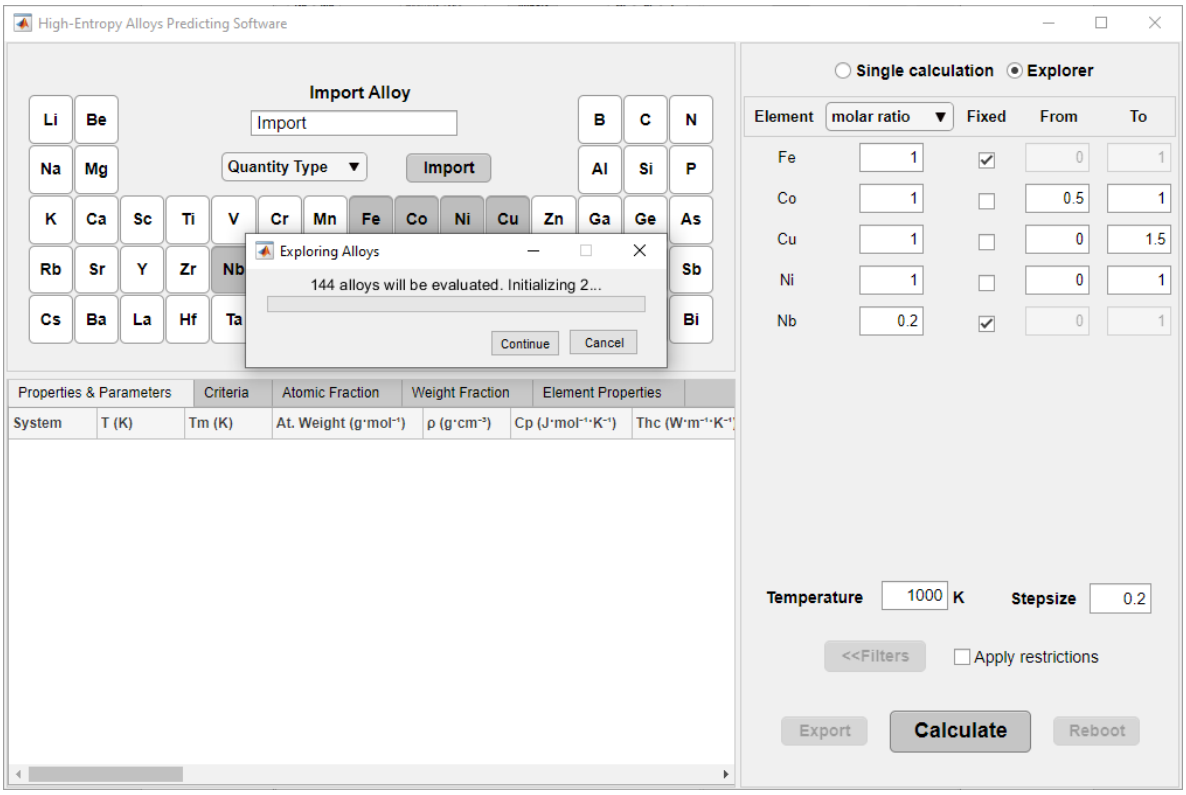

Figure 18: Computation of user-defined alloys using the Explorer mode.

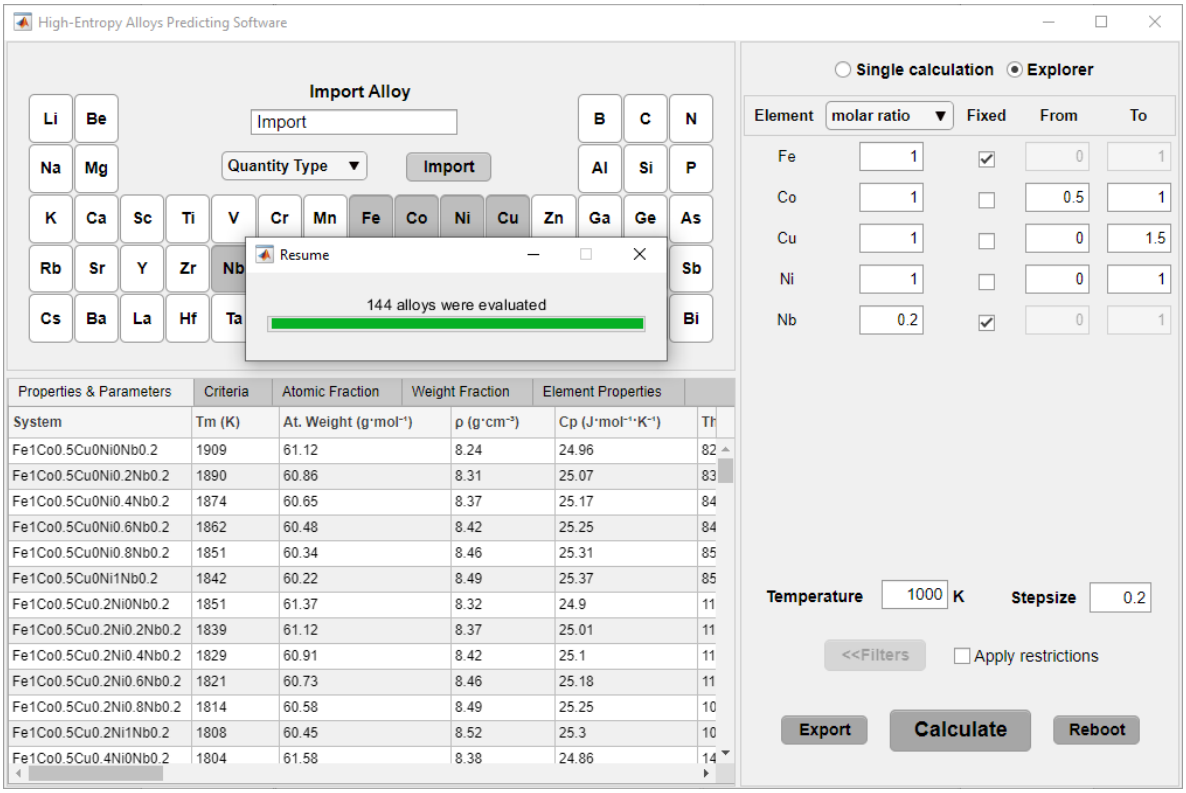

Figure 19: Table of results and pop-up window depicting the results of the computation in the Explorer mode.

The user may need to explore a larger amount of alloys, or alloys with particular characteristics. One of the most relevant features of HEAPS is the possibility to screen and design high-entropy alloys restricting the alloy composition by means of physical and semiempirical parameters as well as different criteria. To access to this feature (exclusive of the Explorer mode), the user must check the Apply restriction checkbox, and click the <<<Filters button. The Filters Panel will pop up at the left side of the interface, as Figure 20 depicts.

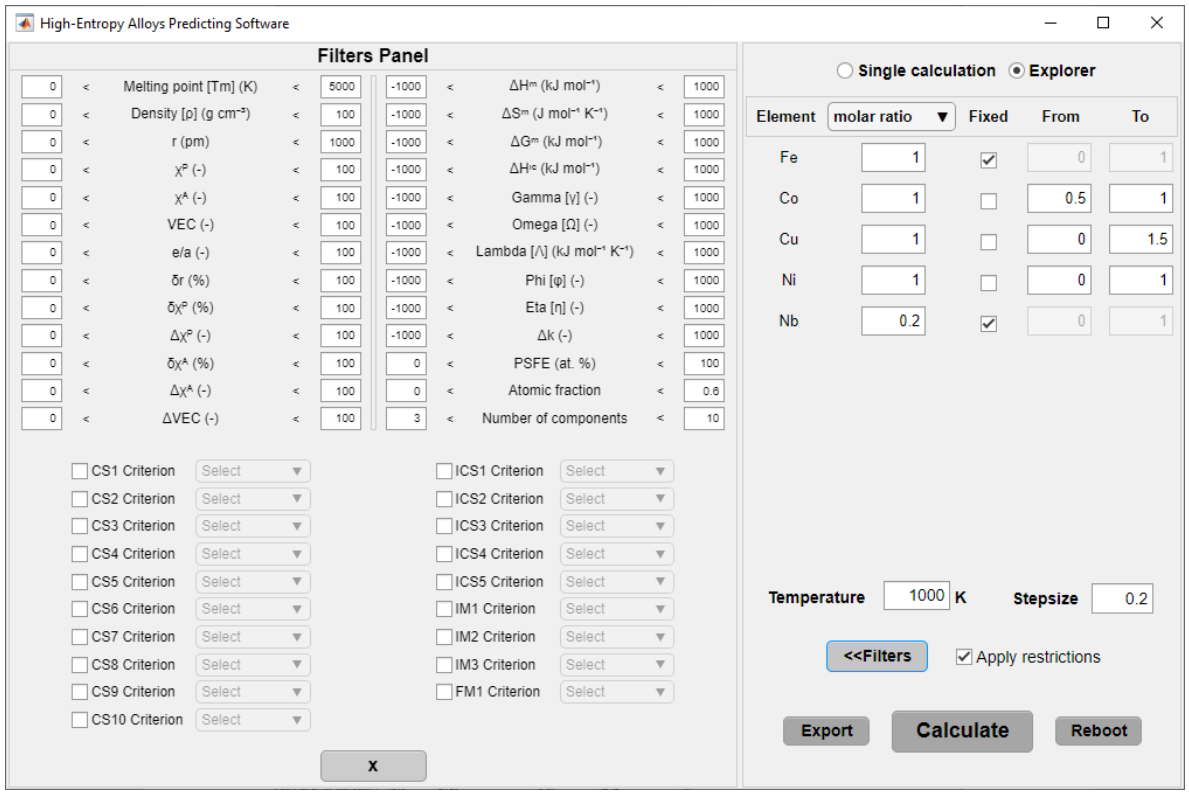

Figure 20: Default Settings of the Filters Panel.

To explore the use of different criteria regarding the microstructure and properties prediction of high-entropy alloys, the software includes 19 different criteria (further information about the criteria can be found situating the mouse pointer over the respective criterion). To use a criterion, the user must check the respective checkbox (as Figure 21 depicts), and the click on the respective dropdown bar, and select the desired prediction goal (as Figure 22 depicts). Then, the user can choose up to 19 different prediction goals; however, the user may bear in mind that only similar prediction goals must be selected (for example, selecting SS in a criterion is not compatible with selecting IM in other one).

Additionally, the user can restrict the alloys by establishing lower and upper limit values of the different physical and semiempirical parameters included in HEAPS, by simply editing the respective edit field, as Figure 23 shows. However, the user must bear in mind that if the prediction goal of a certain criterion is selected, the parameters (used by the criterion to predict a particular aspect) will be disabled and previously entered values in these parameters will not be considered. For example, in Figure 23, the edit fields of the δr, ΔH^m and Ω parameters are disabled, because they are addressed by the CS1, CS2, and CS3 criteria.

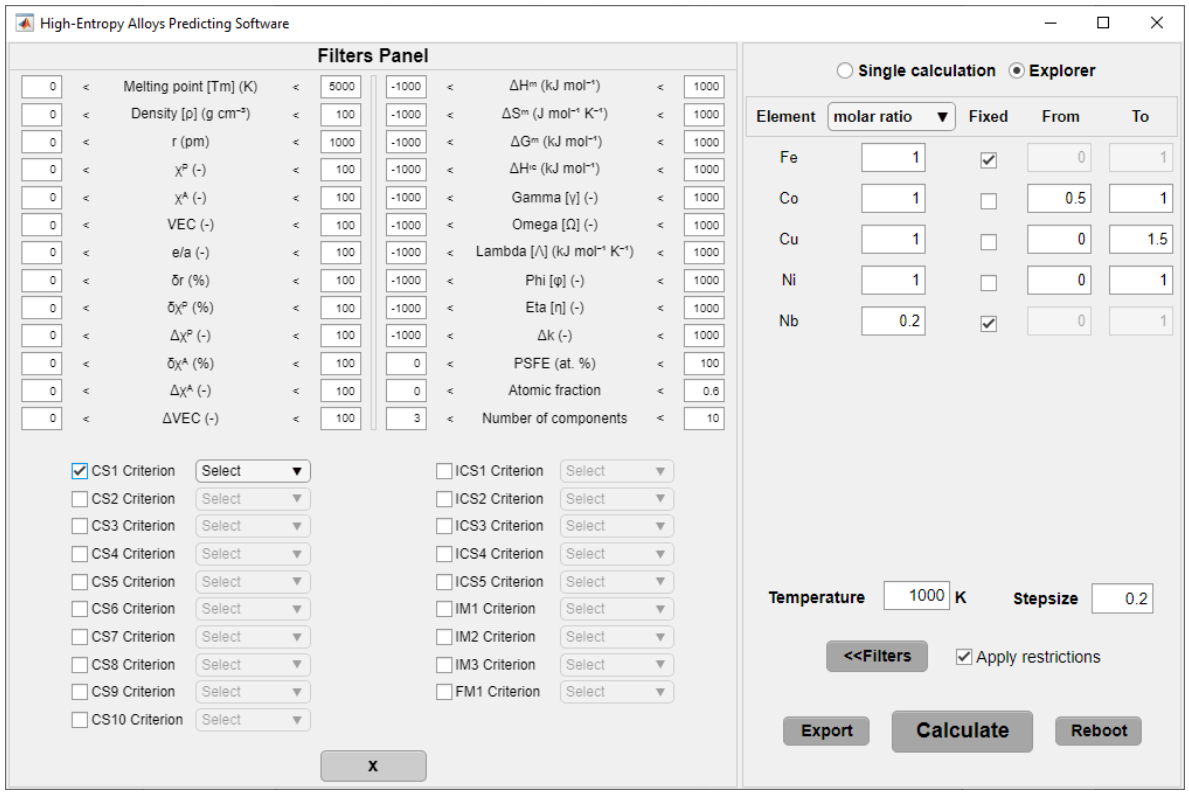

Figure 21: Enabling the CS1 Criterion.

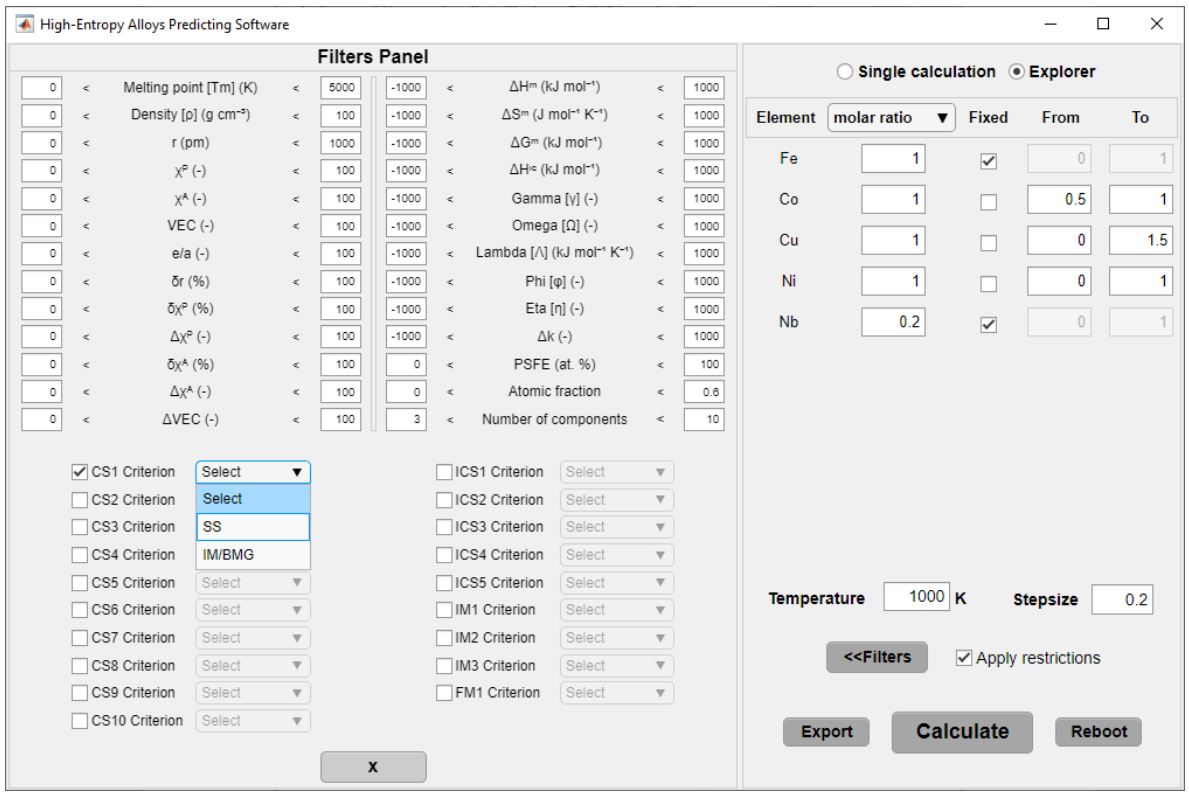

Figure 22: Selecting a prediction goal of the CS1 Criterion.

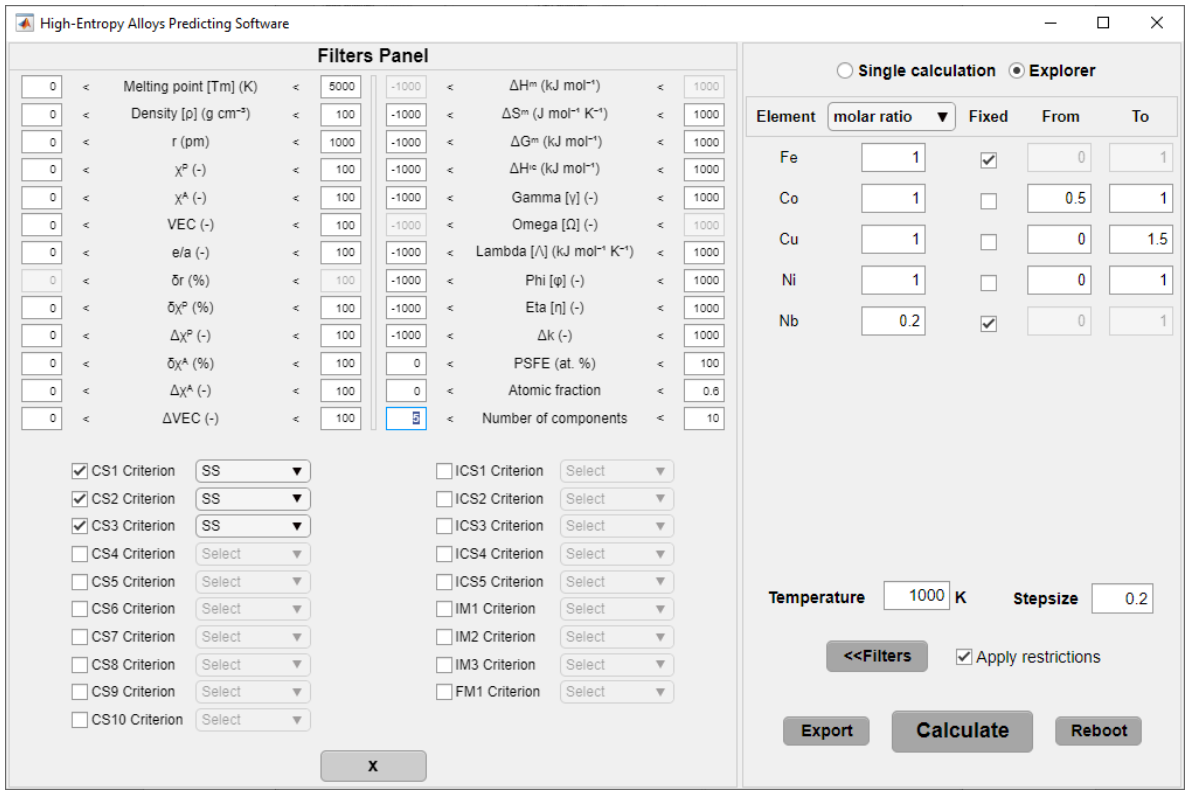

Figure 23: Editing the Number of components edit fields.

After selecting the desired criteria and parameters value, the user must click the Calculate button. Again, a pop-up window indicating the number of alloys that will be computed will appear, also showing the progress. After the computation is completed, the number of computed alloys, as well as the number of alloys that fulfilled the user requirements will be indicated in the pop-up window, and these will be depicted in the Table of Results, as Figure 24 depicts. The user must consider that the settings selected in the Filters panel will be considered only if the Apply restrictions checkbox remains checked.

If the user wants to erase the depicted data in the Table of Results, in the Single calculation mode as well as in the Explorer mode, the user must click the Reboot button (located at the right-down corner of the interface). Then, the interface will look like Figure 25 shows.

The Import and Export functions of HEAPS will function just as in the Single calculation mode.

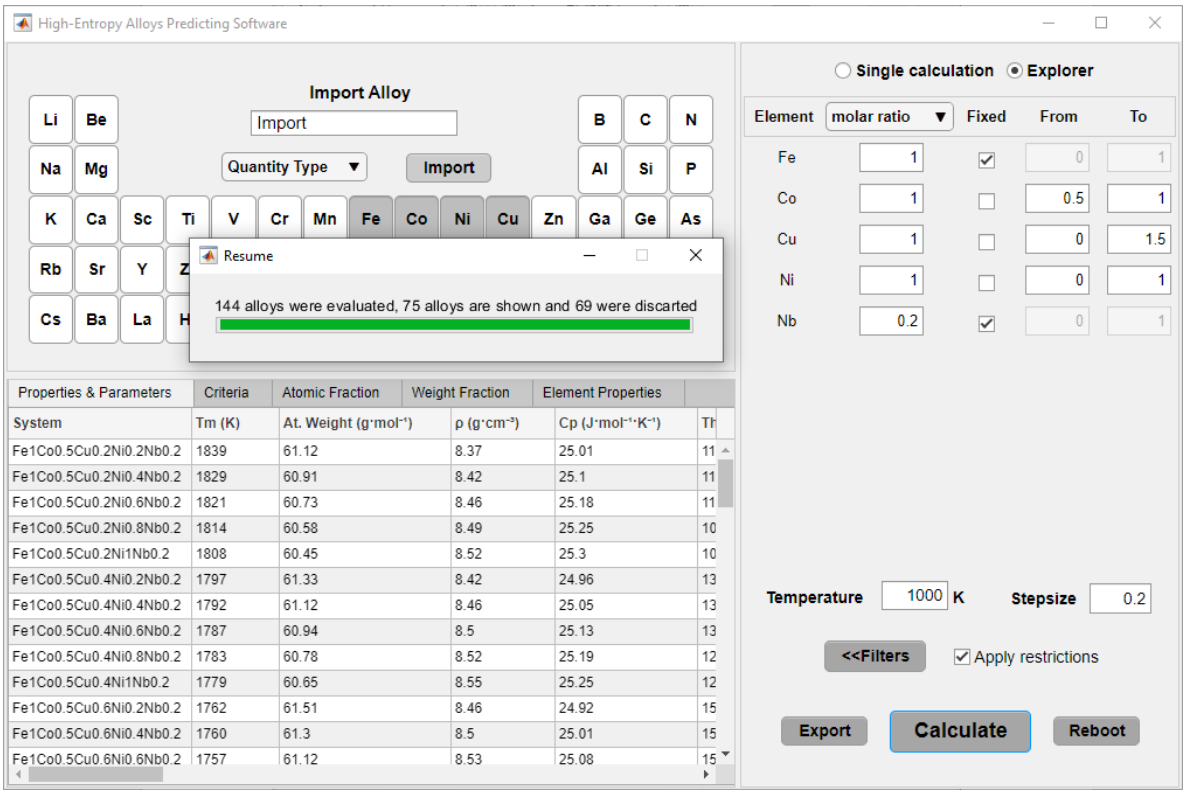

Figure 24: Table of results and pop-up window depicting the results of the computation, after using the Apply restrictions option.

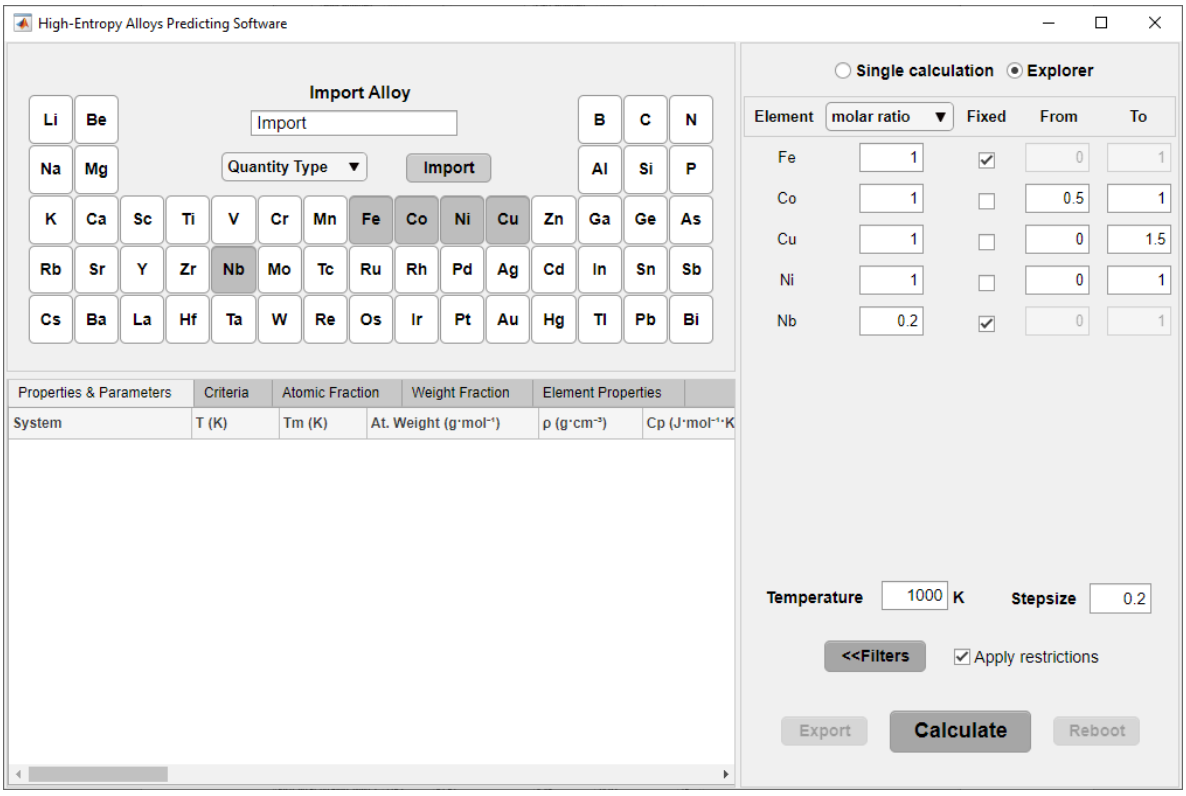

Figure 25: Interface after clicking the Reboot button.