1. After running the executable file, a window will pop up as in Fig. 1

Fig.1: Main window of PyPhyEIS

2. Depending on the geometries of your active particles, choose the suitable model:

- #1: 1-dimensional, e.g. plates
- #2: 2-dimensional, e.g. cylinders
- #3: 3-dimensional, e.g. spheres

3.

- Data file for fitting/simulation is loaded by clicking the “Data” button. Impedance file needs to be in text format (.txt), includes 3 columns of frequency, real, imaginary values, and each column is separated by a tab character
- After loading data file, the “Data Path” will show the directory of the working file.

4.

- To start fitting/simulation the impedance, click “Run Fit/Simulation” button

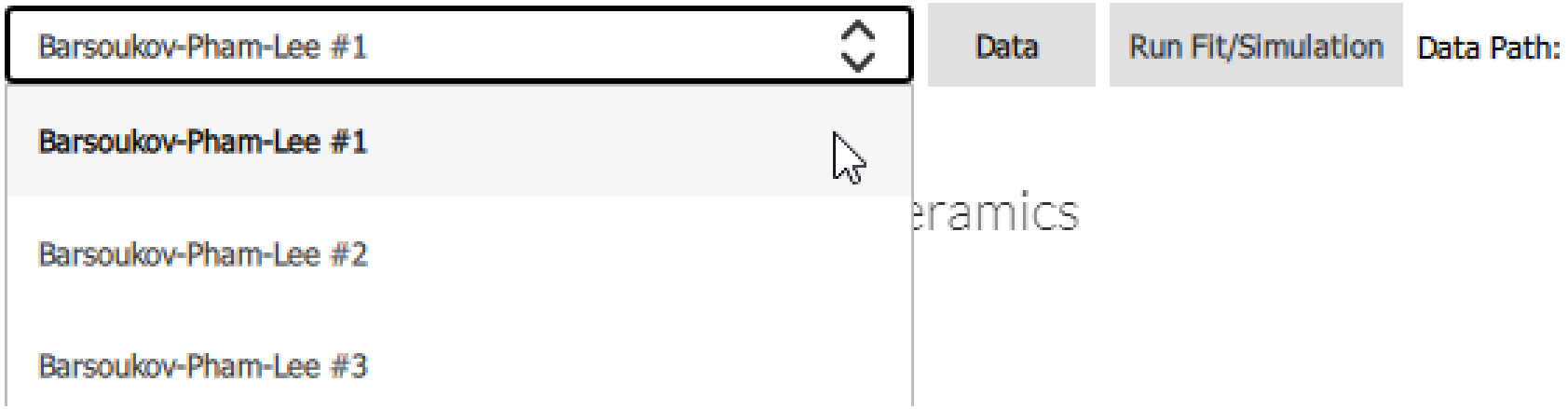
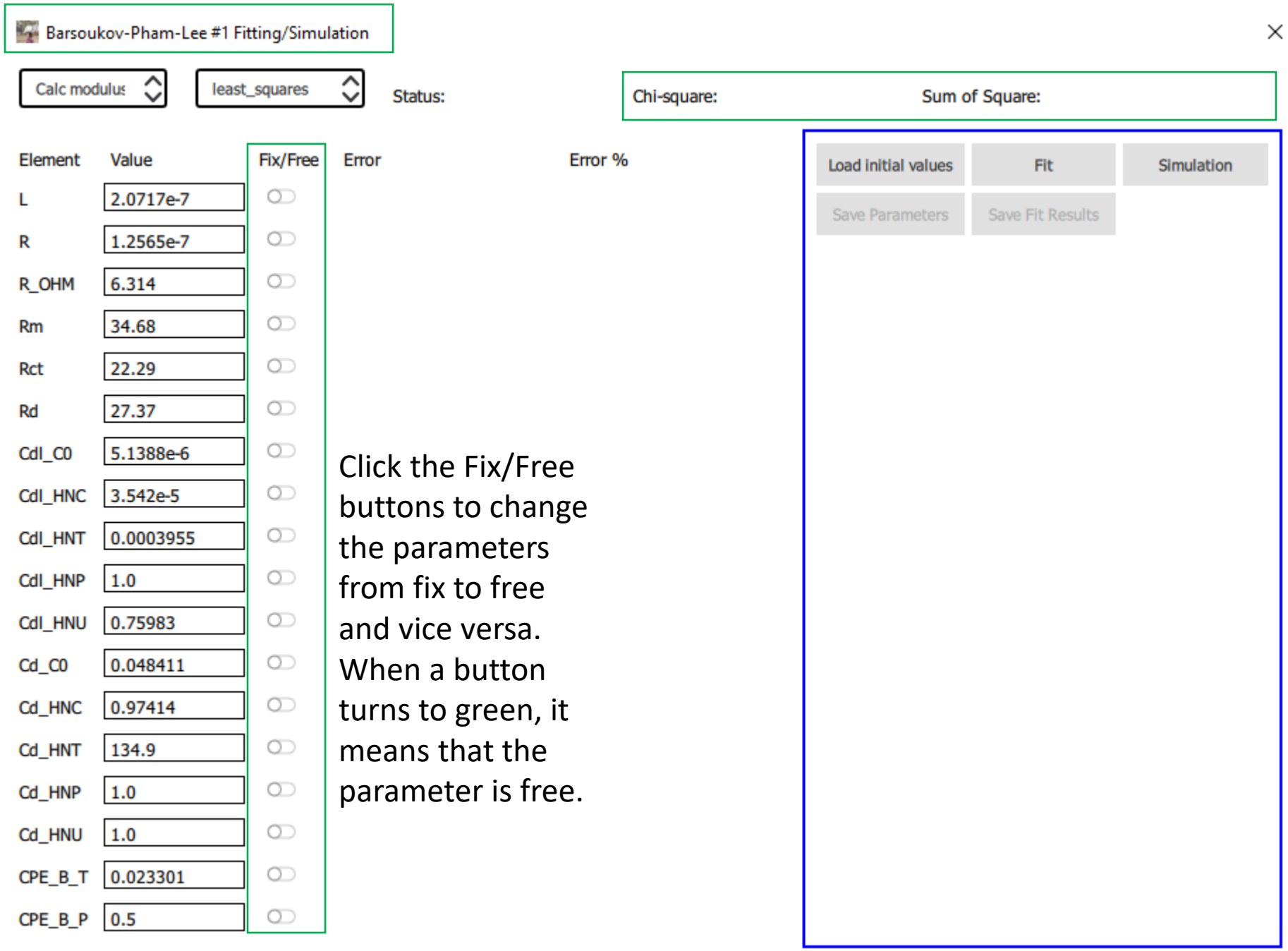


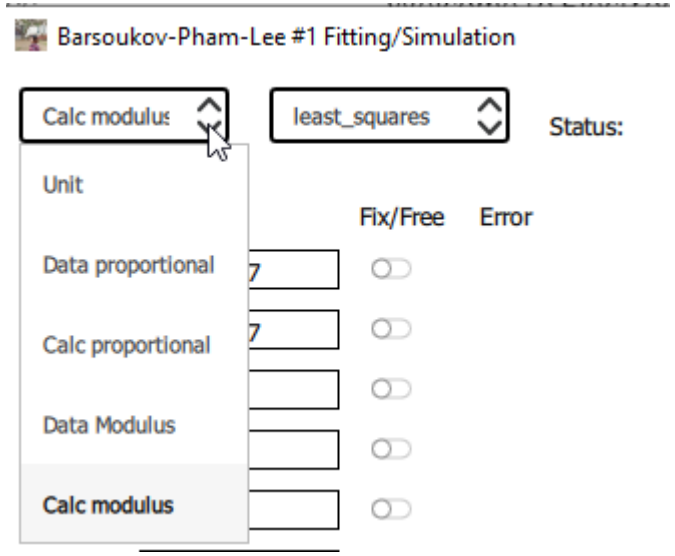
Fig.2: Important features in the task bar



Click the Fix/Free buttons to change the parameters from fix to free and vice versa. When a button turns to green, it means that the parameter is free.

5.

- In here, the example is for model #1.
- Chi-square and sum of square are only calculated in fitting. Otherwise, they will show NaN.
- “Load initial values” is for loading the saved parameters by PyPhyEIS
- “Fit” and “Simulation” are for fitting and simulation the impedance.
- After fitting/simulation, click the “Save parameters” to save the current parameters (with errors if fitting) into csv file (comma-separated values file).
- “Save Fit Results” button to save the impedance which is simulated/fitted from the model. The default file will be in text format.



6.

- There are 5 options of weighting type to choose for fitting.
- The optimization algorithm is least-squares as in SciPy.