1. After running the executable file, the homepage will be shown as in Fig. 1

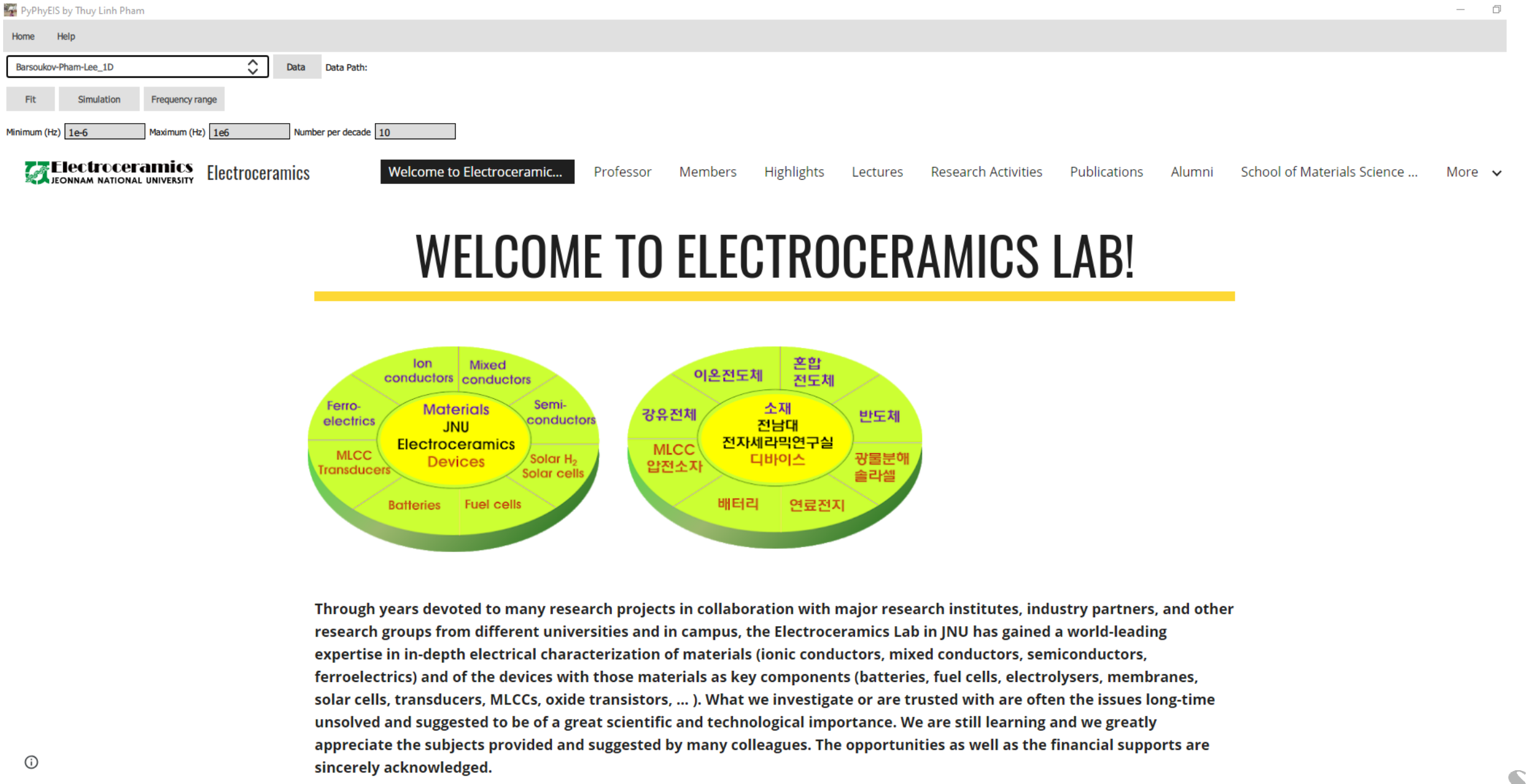


Fig.1: Homepage of PyPhyEIS

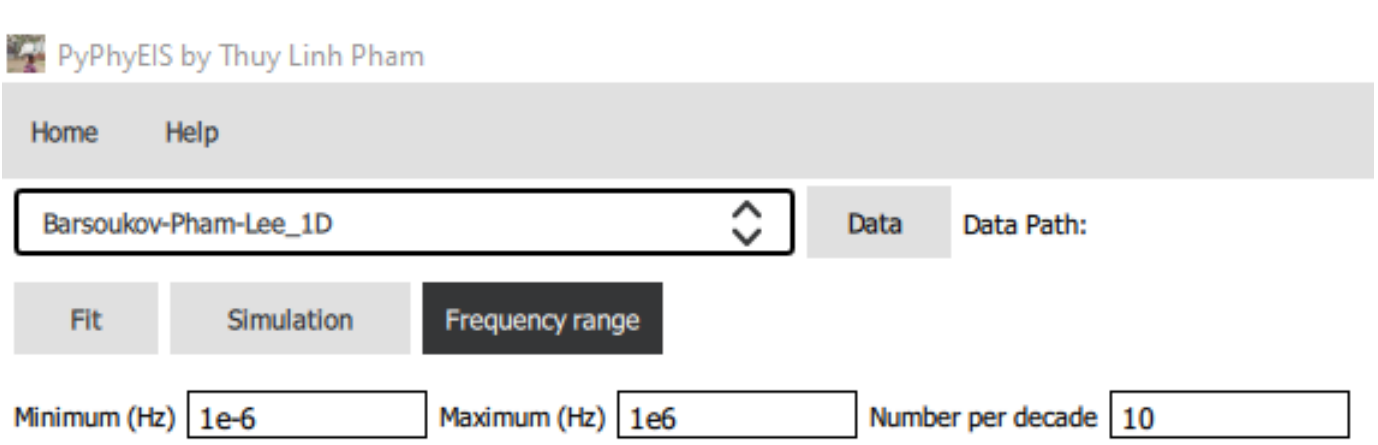
2. Depending on the geometries of your active particles, choose the suitable model:

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

Note that **Barsoukov-Pham-Lee_1D (2D/3D)** are considered only cathode impedance while in **Barsoukov-Pham-Lee_1D (2D/3D)_Full cell**, stray effect as well as Li metal impedance are added.

3.

- Data file for fitting 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.
- For simulation mode, first click “Frequency range” to change the maximum/minimum as well as number of data points per decade. When you are ready to simulate, click on “Simulation”



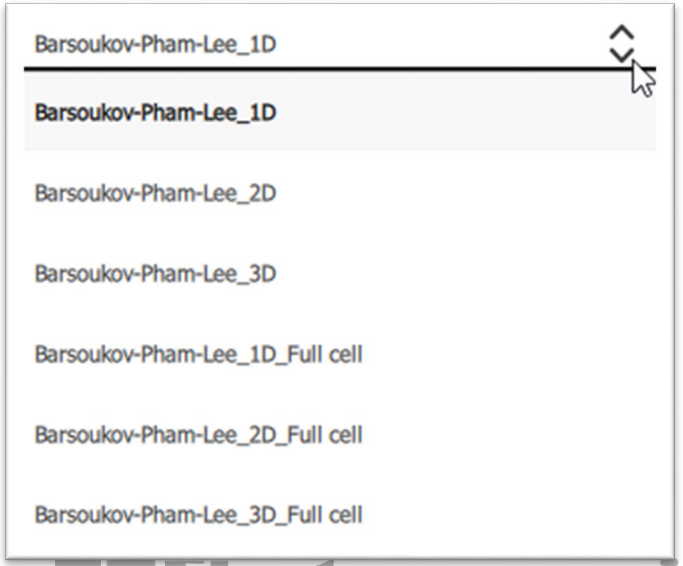
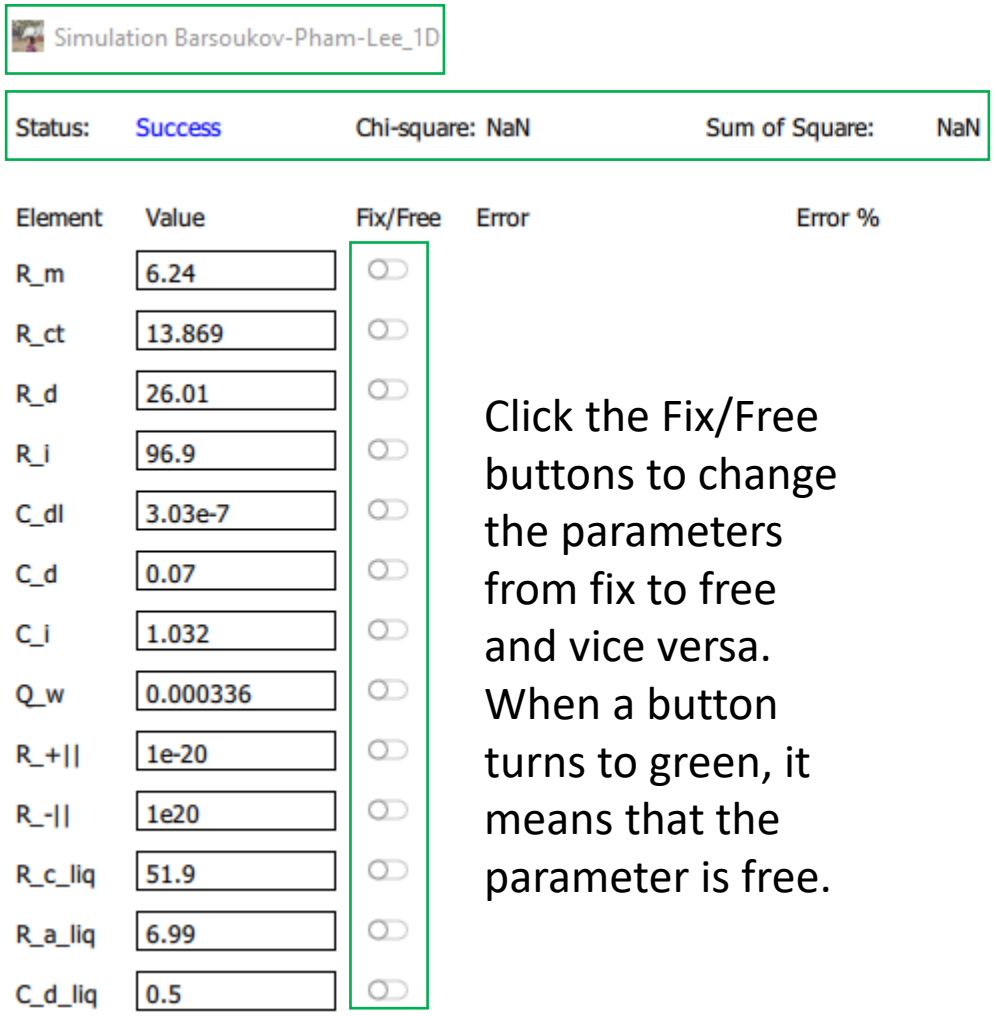


Fig.2: Important features in the task bar

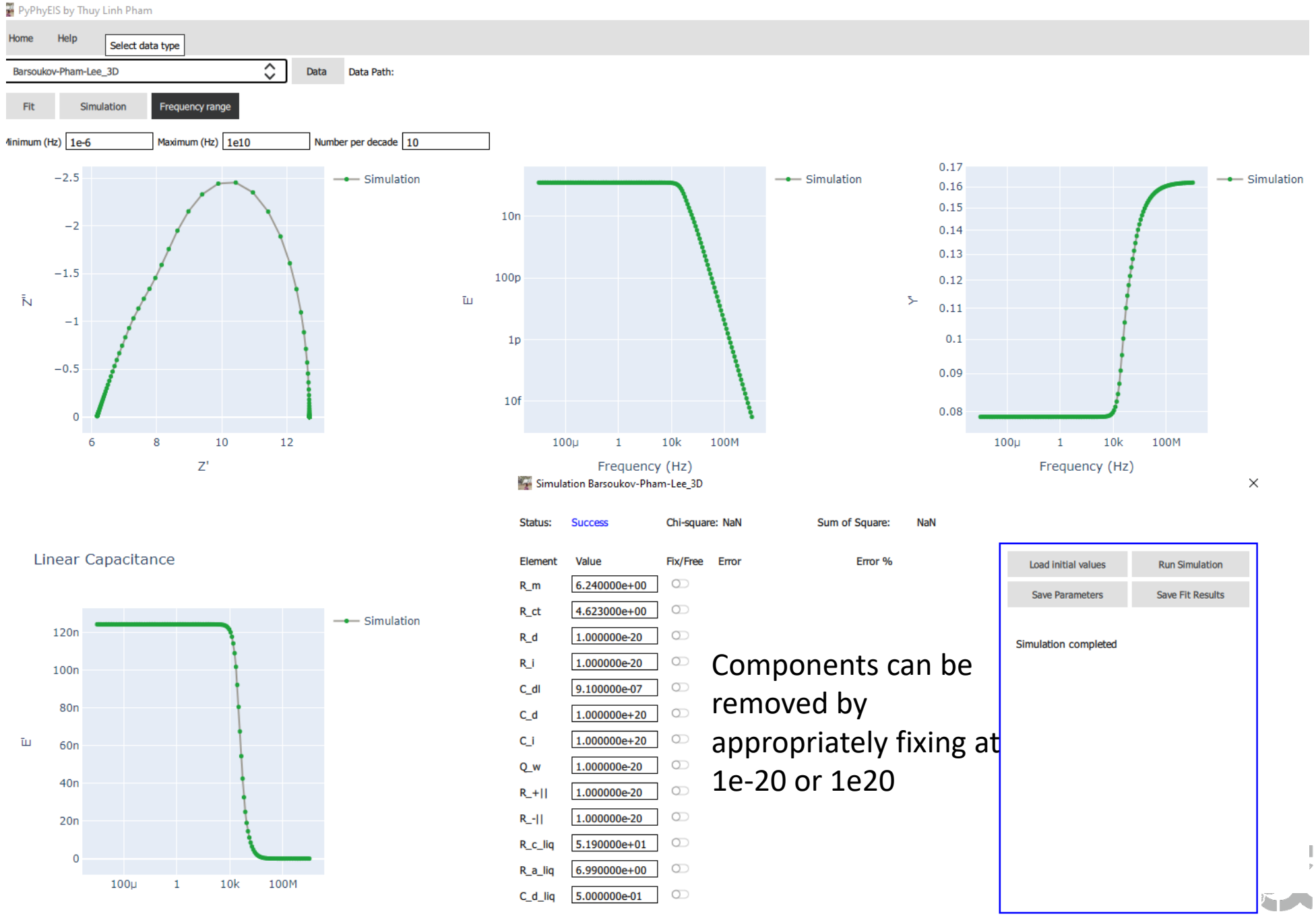


Click the Fix/Free buttons to change the parameters from fix to free and vice versa. When a button turns to green, it means that the parameter is free.

5.

- In here, the example is for model **Barsoukov-Pham-Lee_1D**
- 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.
- “Run Fitting” and “Run 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.

An example of user interface in “Simulation” mode



One can set the frequency range for the simulation file by clicking on “Frequency range” and modify the minimum/maximum frequency along with number of frequency points per decade.

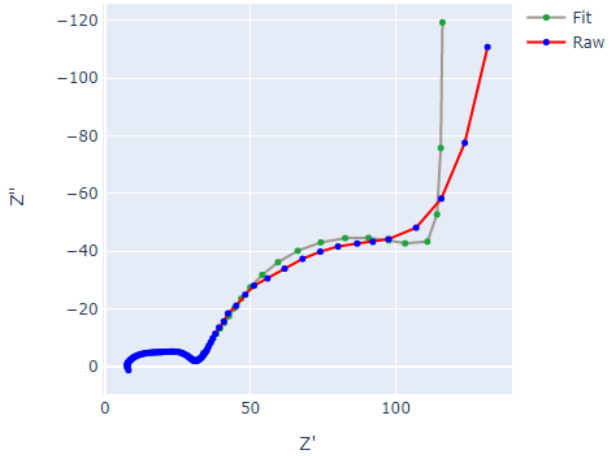
Components can be removed by appropriately fixing at 1e-20 or 1e20

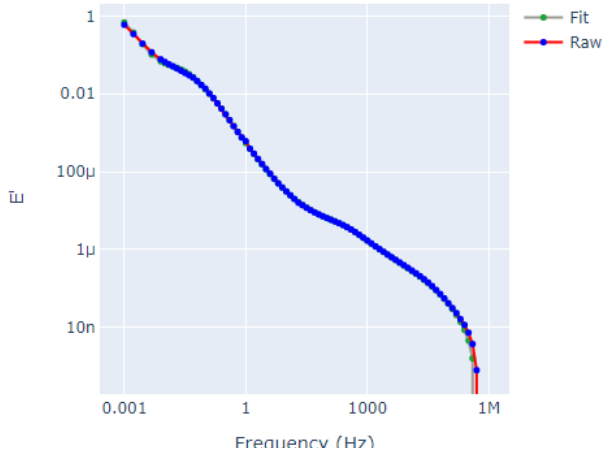
An example of user interface in “Fitting” mode

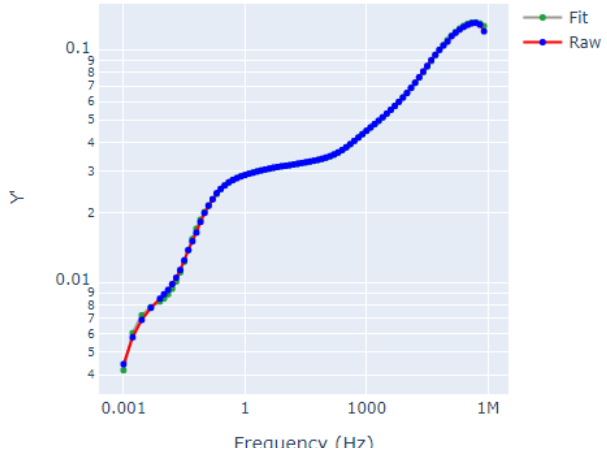
Barsoukov-Pham-Lee_3D_Full cell | Data | T:/4. OLO-LFP/2018/Linh/OLO/GRC2020/Consider Li impedance/Cd no factor Ci new factor/data/20200522/1st charging/G_EIS(26).txt

Fit | Simulation | Frequency range

Minimum (Hz) 1e-6 Maximum (Hz) 1e10 Number per decade 10



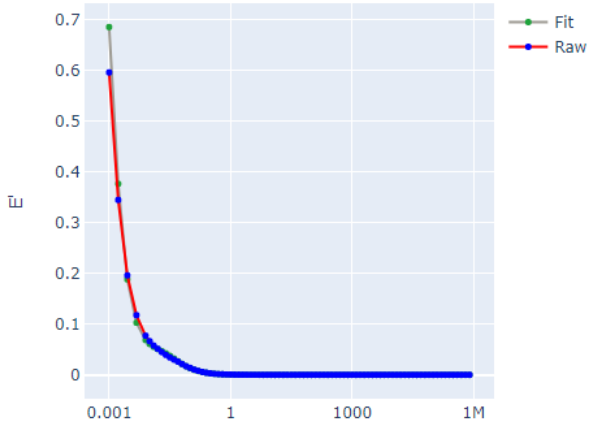




Fitting Barsoukov-Pham-Lee_3D_Full cell

Calc modulus | least_squares | Status: Success | Chi-square: 5.66970e-02 | Sum of Square: 8.78803e+00

Linear Capacitance

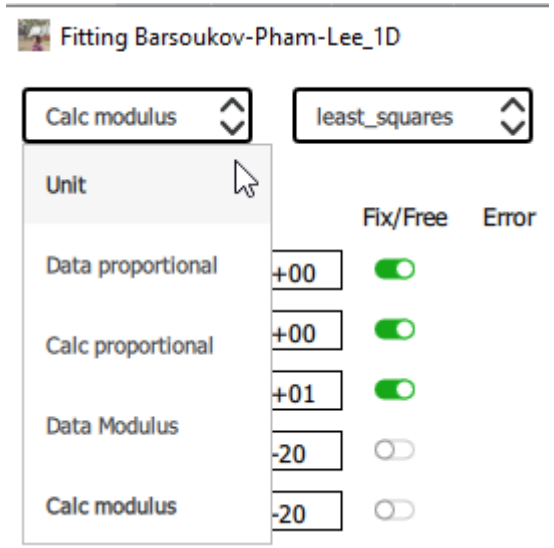


Element	Value	Fix/Free	Error	Error %
L_str	3.854639e-07		3.599671e-08	9.338543e+00
R_str	3.756996e+00		6.512670e-01	1.733478e+01
R_m	8.508027e+00		1.203427e+00	1.414461e+01
R_ct	1.857249e+01		9.527350e-01	5.129817e+00
R_d	8.237766e+00		1.957059e-03	2.375716e-02
R_i	1.069090e+02		6.106851e-02	5.712194e-02
C_dl	1.304944e-06		2.646044e-07	2.027707e+01
C_d	3.403760e-01		7.991222e-04	2.347763e-01
C_i	1.033651e+00		7.239900e-04	7.004200e-02
Q_w	4.830201e-04		6.402496e-05	1.325513e+01
R_+||	1.000000e-20			
R_-||	1.000000e+20			
R_c_liq	1.631728e+01		4.235829e-01	2.595915e+00
R_a_liq	1.005564e+01		3.156228e-01	3.138763e+00
C_d_liq	3.701643e-01		3.459480e-02	9.345796e+00
R_ct_Li	3.703044e+00		7.321700e-01	1.977211e+01
C_dl_Li	1.400279e-04		3.088945e-05	2.205949e+01

Load initial values | Run Fitting

Save Parameters | Save Fit Results

Method: least_squares.
Weighting: calcModulus.
Number of iteration: 31
Success: `xtol` termination condition is satisfied



6.

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