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

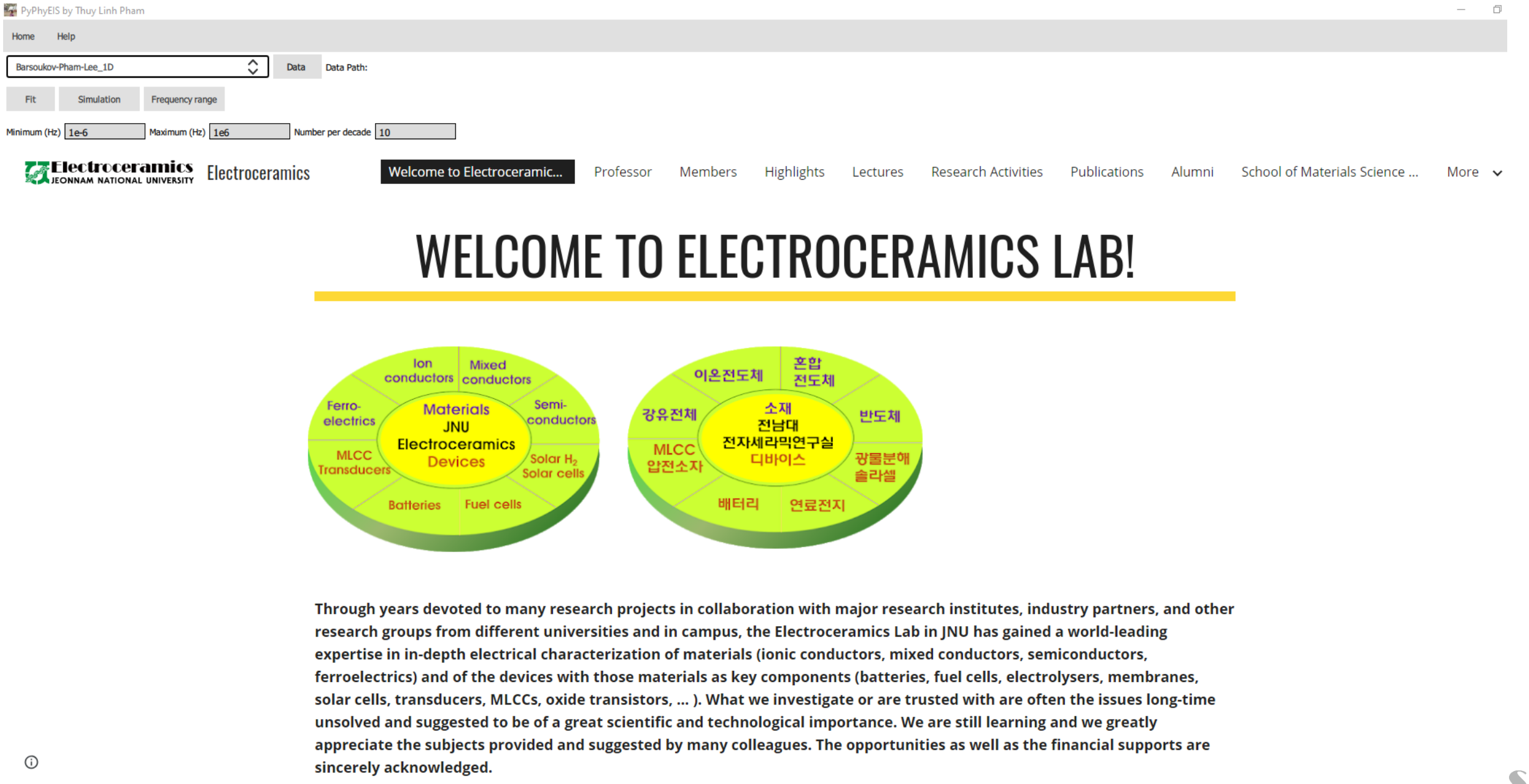


Fig.1: Homepage of PyPhyEIS

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

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”

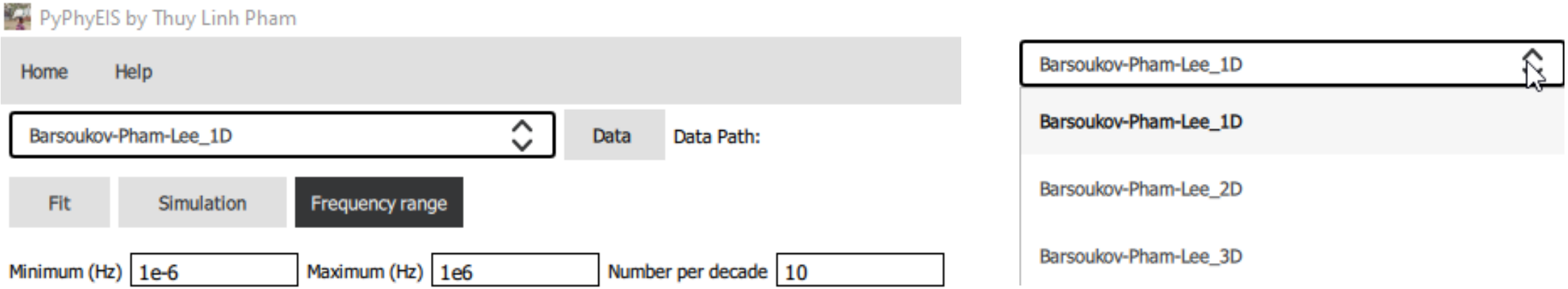
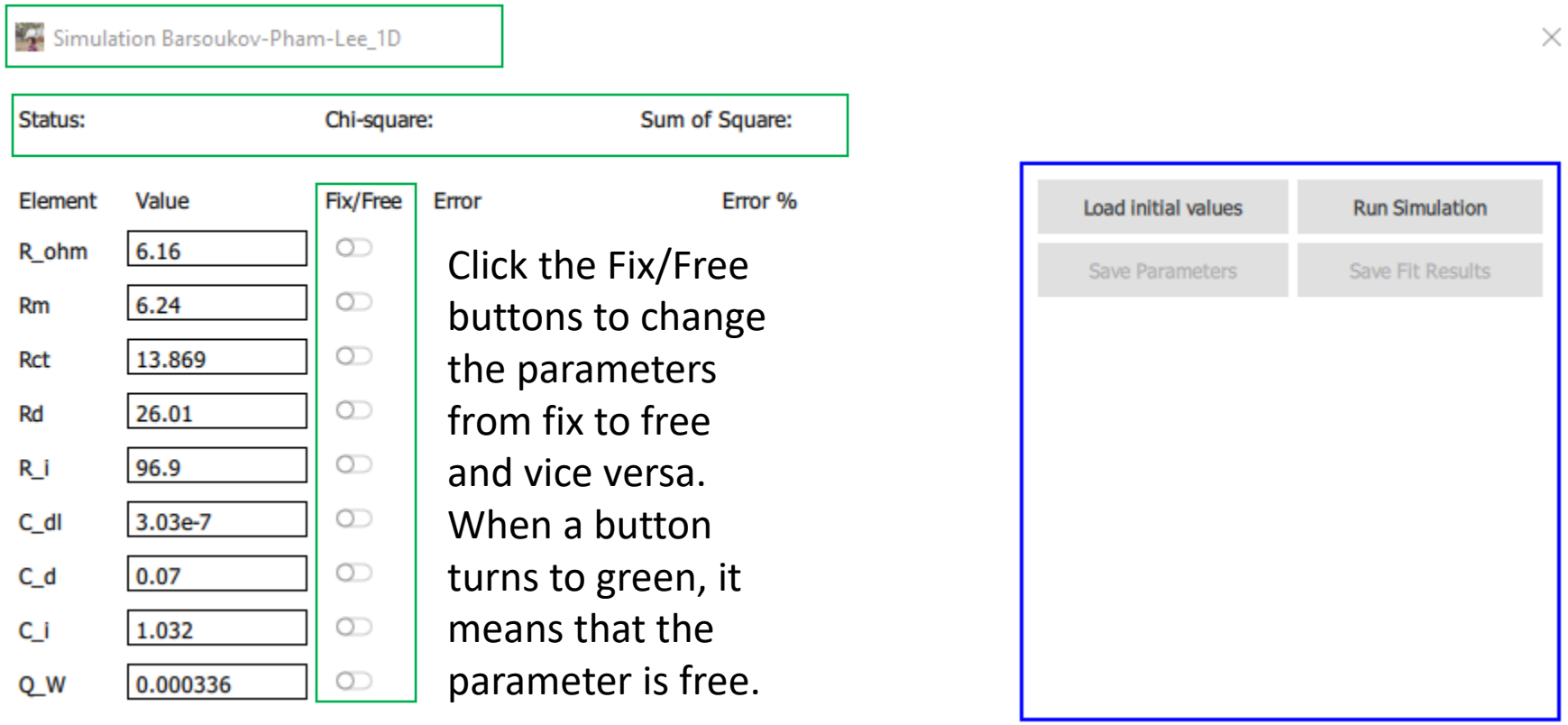


Fig.2: Important features in the task bar

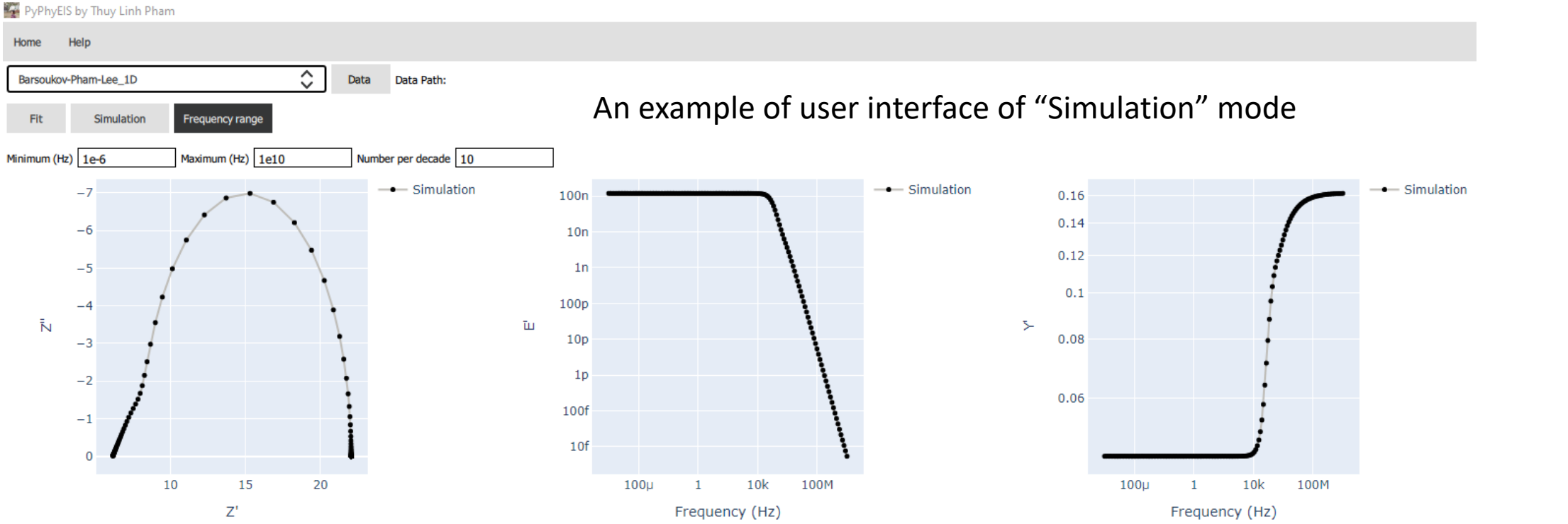


Click the Fix/Free buttons to change the parameters from fix to free and vice versa. When a button turns to green, it means that the parameter is free.

5.

- In here, the example is for model 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 of “Simulation” mode



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

PyPhyEIS by Thuy Linh Pham

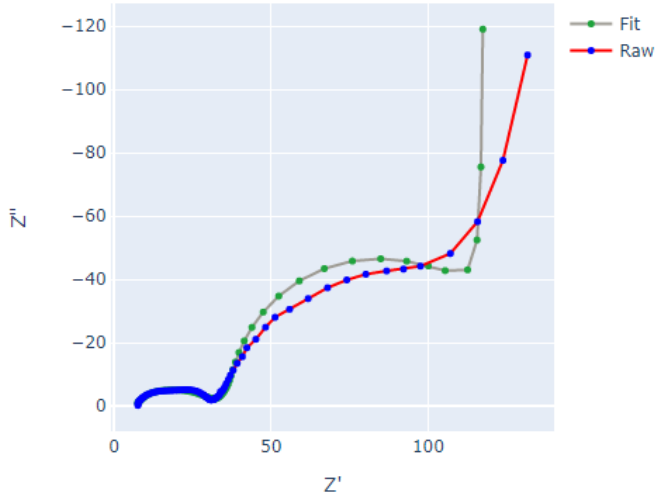
Home Help

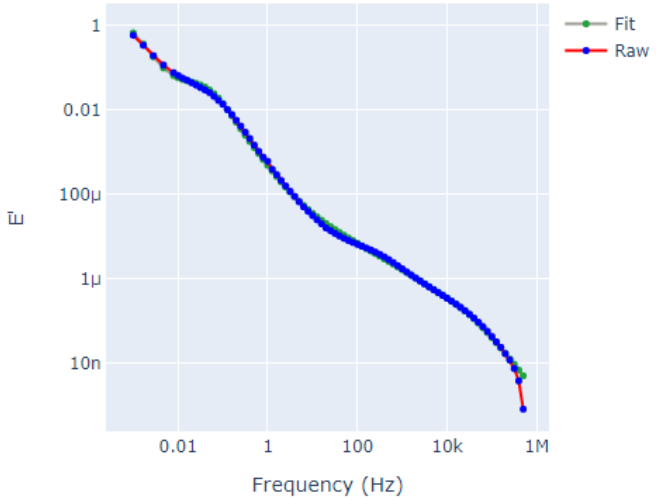
Barsoukov-Pham-Lee_3D | Data | T:/4. OLO-LFP/2018/Linh/OLO/GRC2020/DX30 with Zd geometries/For battery paper/Cd no factor Ci new factor/PyPhyEIS_20200516_for GitHub_most updated/G_EIS(26).txt

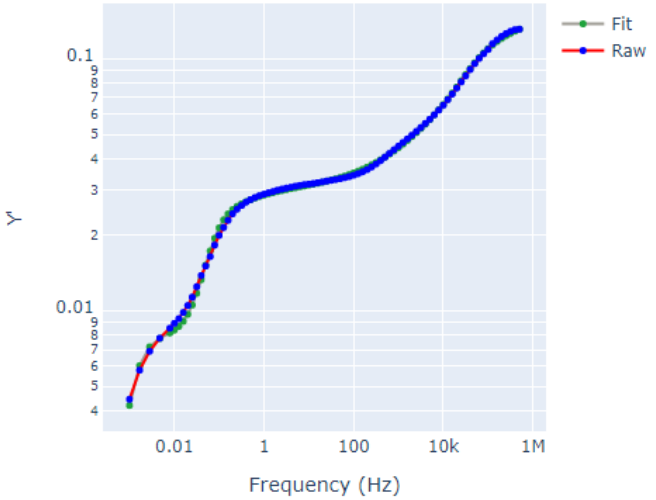
Fit | Simulation | Frequency range

Minimum (Hz) 1e-6 Maximum (Hz) 1e6 Number per decade 10

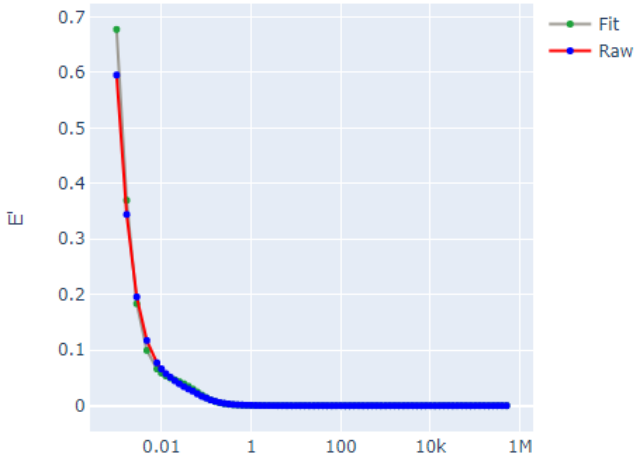
An example of user interface of “Fitting” mode







Linear Capacitance



Fitting Barsoukov-Pham-Lee_3D

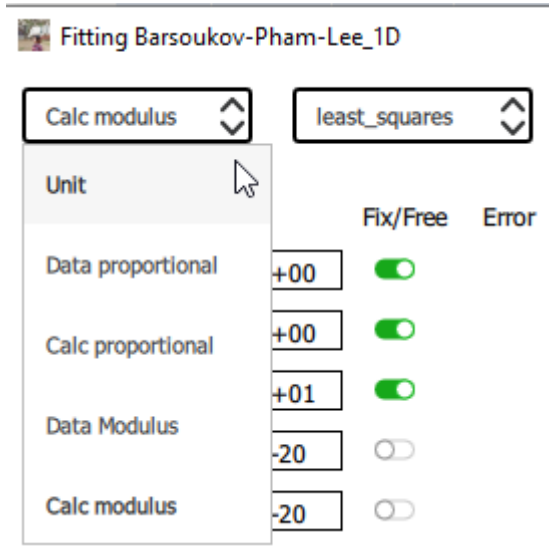
Calc modulus | least_squares | Status: Success | Chi-square: 1.33137e-01 | Sum of Square: 2.09025e+01

Element	Value	Fix/Free	Error	Error %
R_ohm	6.630209e+00		9.669089e-02	1.458338e+00
R_m	9.932292e+00		1.018489e+00	1.025432e+01
R_ct	2.271755e+01		3.694381e-01	1.626223e+00
R_d	2.480381e+01		2.610286e-01	1.052373e+00
R_i	1.090635e+02		1.784287e+00	1.636007e+00
C_dl	1.951875e-06		2.765119e-07	1.416648e+01
C_d	2.807623e-01		1.907820e-03	6.795143e-01
C_i	1.093646e+00		9.750320e-03	8.915430e-01
Q_W	6.306394e-04		5.432792e-05	8.614736e+00

Load initial values | Run Fitting

Save Parameters | Save Fit Results

Method: least_squares.
Weighting: calcModulus.
Number of iteration: 39
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.