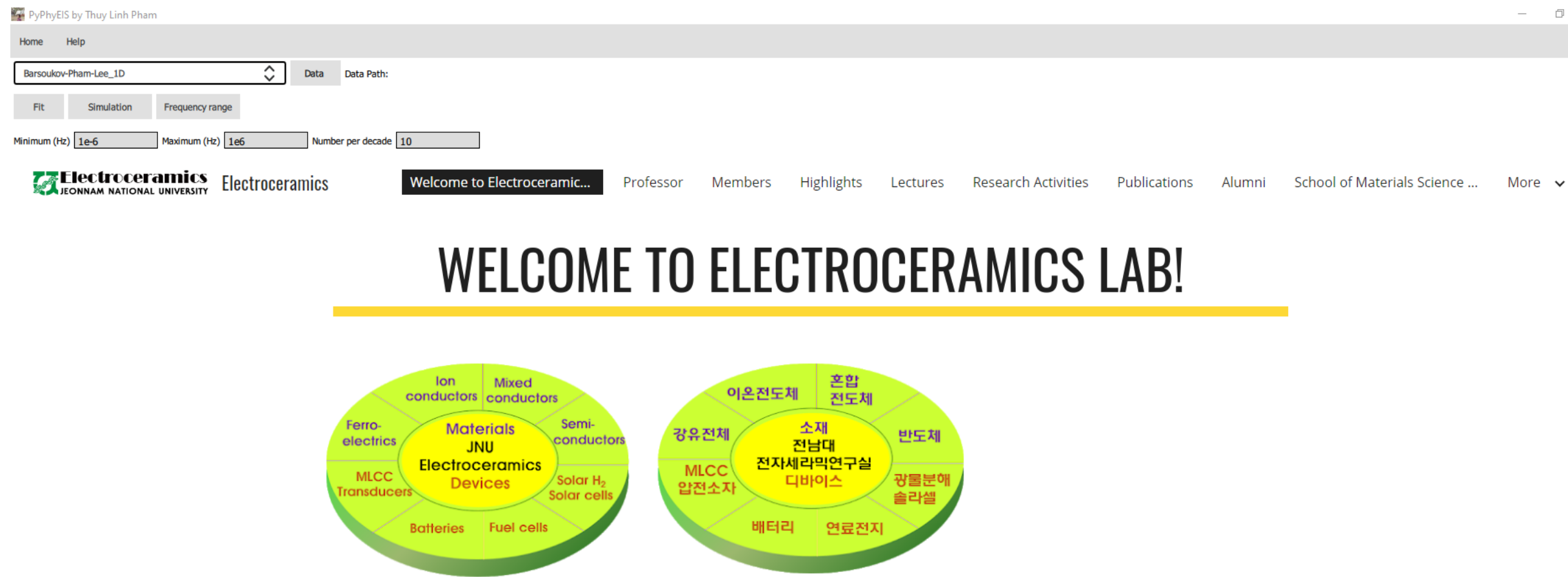


1. After running the executable file, the homepage will be shown as in Fig. 1



Through years devoted to many research projects in collaboration with major research institutes, industry partners, and other research groups from different universities and in campus, the Electroceramics Lab in JNU has gained a world-leading expertise in in-depth electrical characterization of materials (ionic conductors, mixed conductors, semiconductors, ferroelectrics) and of the devices with those materials as key components (batteries, fuel cells, electrolyzers, membranes, solar cells, transducers, MLCCs, oxide transistors, ...). What we investigate or are trusted with are often the issues long-time unsolved and suggested to be of a great scientific and technological importance. We are still learning and we greatly appreciate the subjects provided and suggested by many colleagues. The opportunities as well as the financial supports are sincerely acknowledged.

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”

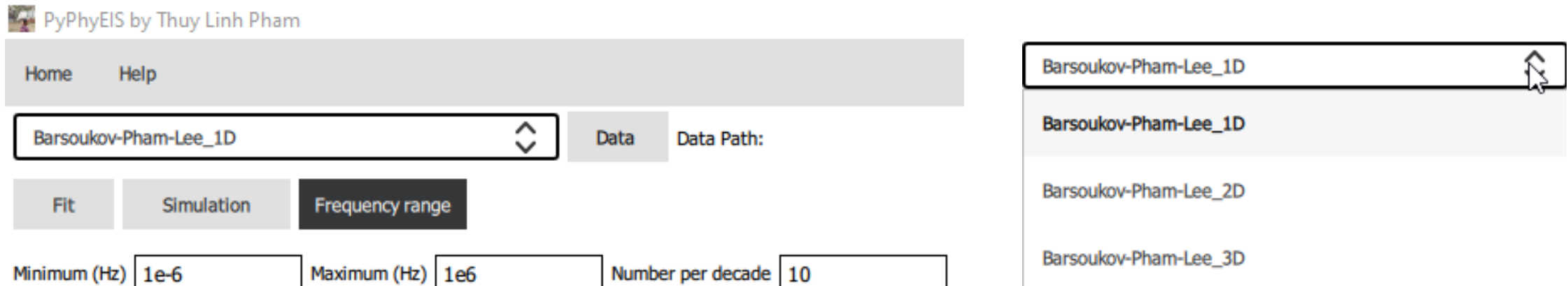


Fig.2: Important features in the task bar

Status: Chi-square: Sum of Square:

Element	Value	Fix/Free	Error	Error %
R_ohm	6.16	<input type="radio"/>		
Rm	6.24	<input type="radio"/>		
Rct	13.869	<input type="radio"/>		
Rd	26.01	<input type="radio"/>		
R_l	96.9	<input type="radio"/>		
C_dl	3.03e-7	<input type="radio"/>		
C_d	0.07	<input type="radio"/>		
C_l	1.032	<input type="radio"/>		
Q_W	0.000336	<input type="radio"/>		

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.

Load Initial values

Run Simulation

Save Parameters

Save Fit Results

- 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.

Barsoukov-Pham-Lee_1D

Data

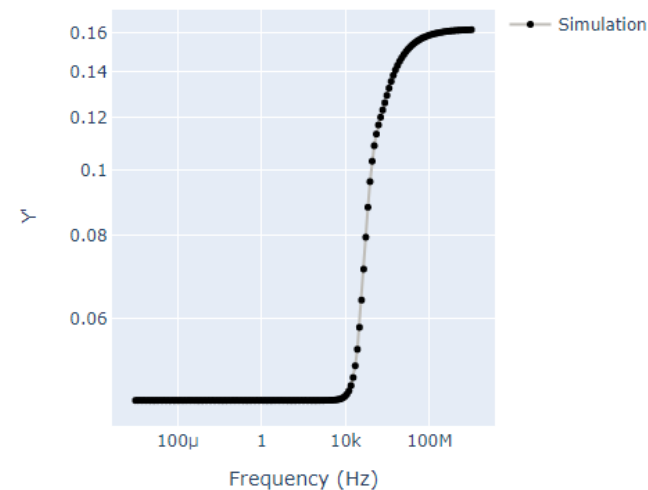
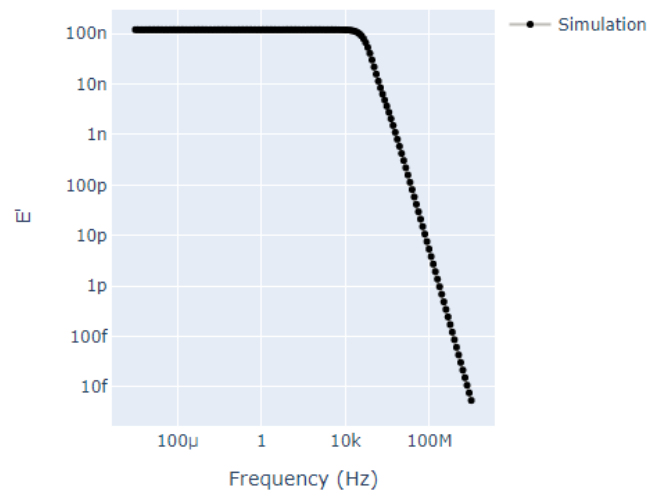
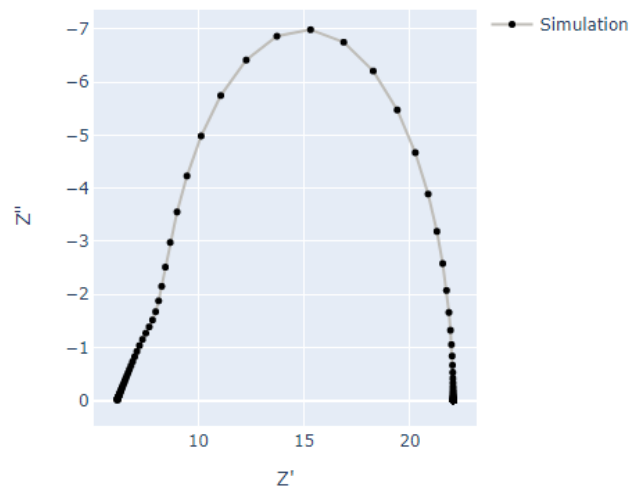
Data Path:

Fit

Simulation

Frequency range

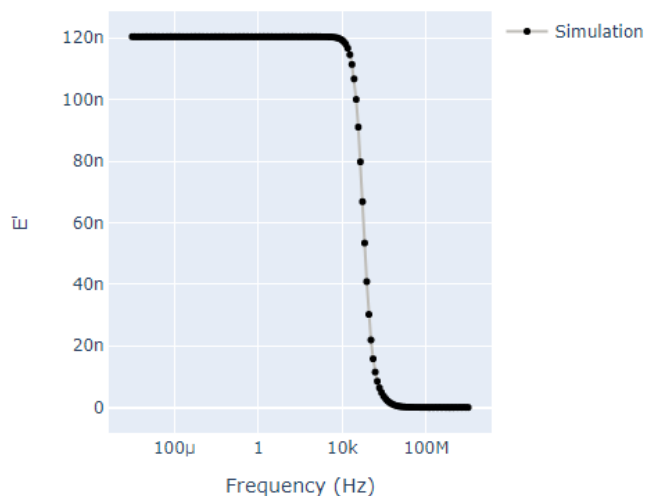
Minimum (Hz) 1e-6 Maximum (Hz) 1e10 Number per decade 10



Simulation Barsoukov-Pham-Lee_1D

X

Linear Capacitance



Status: Success

Chi-square: NaN

Sum of Square: NaN

Element	Value	Fix/Free	Error	Error %
R_ohm	6.160000e+00	<input checked="" type="checkbox"/>		
R_m	6.240000e+00	<input checked="" type="checkbox"/>		
R_ct	1.386900e+01	<input checked="" type="checkbox"/>		
R_d	1.000000e-20	<input type="checkbox"/>		
R_l	1.000000e-20	<input type="checkbox"/>		
C_dl	3.030000e-07	<input checked="" type="checkbox"/>		
C_d	1.000000e+20	<input type="checkbox"/>		
C_l	1.000000e+20	<input type="checkbox"/>		
Q_W	1.000000e-20	<input type="checkbox"/>		

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

Load initial values

Run Simulation

Save Parameters

Save Fit Results

Simulation completed

Barsoukov-Pham-Lee_3D

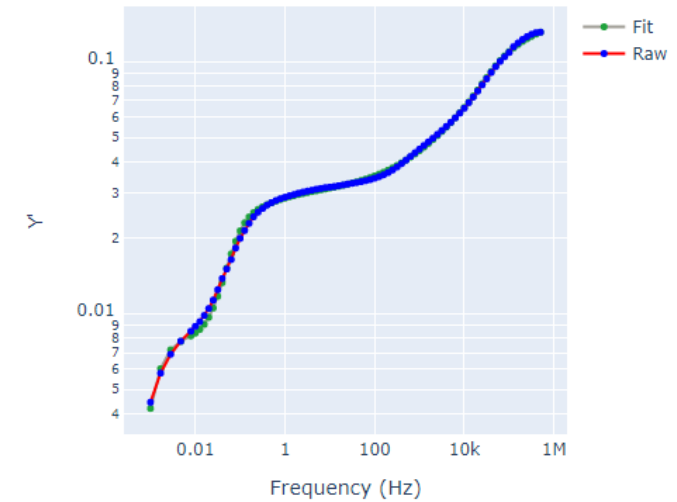
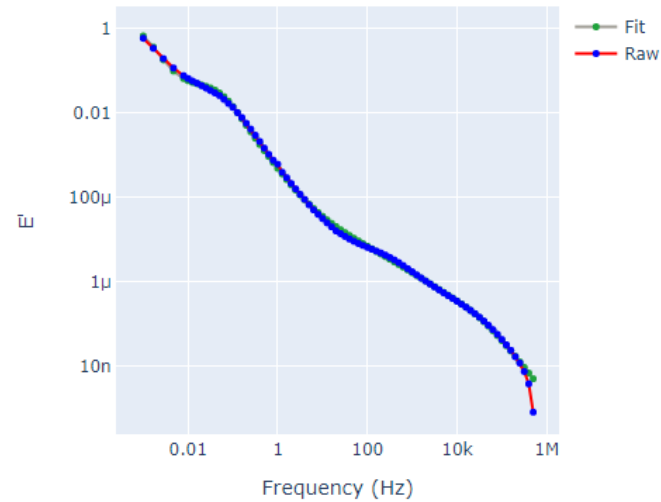
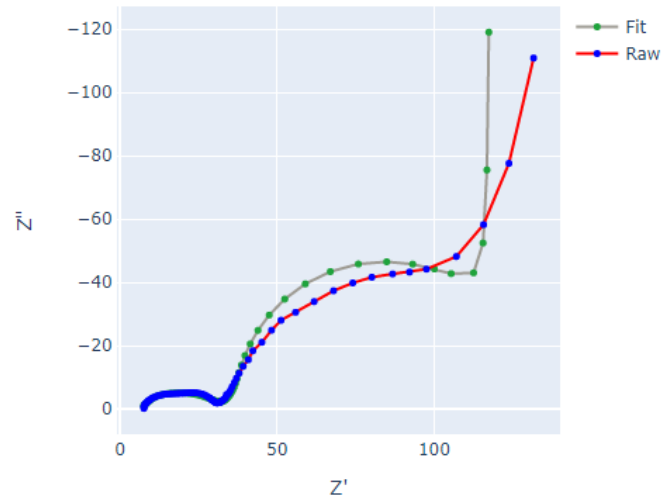
Data

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

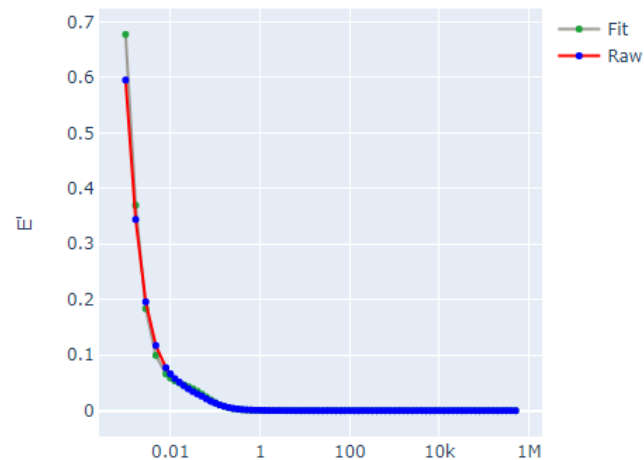
Simulation

Frequency range

Minimum (Hz) Maximum (Hz) Number per decade 

An example of user interface of “Fitting” mode

Linear Capacitance



Fitting Barsoukov-Pham-Lee_3D

Status: Success
Chi-square: 1.33137e-01
Sum of Square: 2.09025e+01

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

Method: least_squares.
Weighting: calcModulus.
Number of iteration: 39
Success: 'xtol' termination condition is satisfied

Fitting Barsoukov-Pham-Lee_1D

Calc modulus least_squares

Unit		Fix/Free	Error
Data proportional	+00	<input checked="" type="checkbox"/>	
Calc proportional	+00	<input checked="" type="checkbox"/>	
	+01	<input checked="" type="checkbox"/>	
Data Modulus	-20	<input type="checkbox"/>	
Calc modulus	-20	<input type="checkbox"/>	

6.

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