

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

PyPhyEIS by Thuy Linh Pham

File Edit Help

Barsoukov-Pham-Lee #1

Data

Run Fit/Simulation

Data Path:

Electroceramics
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Welcome to Electroceramics Lab!

Professor

Members

Highlights

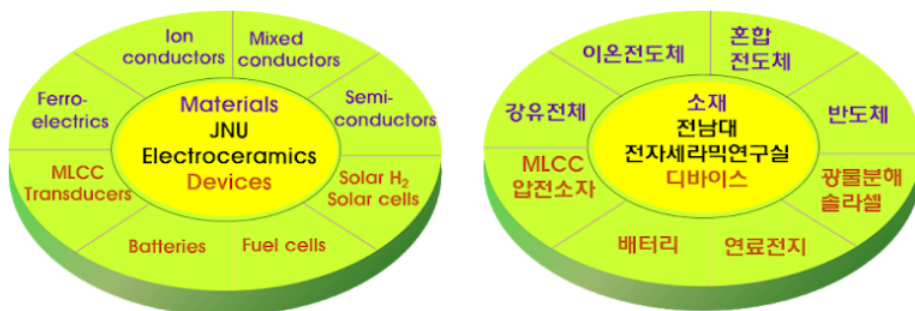
Lectures

Research Activities

Publications

Alumni

Welcome to Electroceramics Lab!



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: 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

Barsoukov-Pham-Lee #1 Fitting/Simulation

Calc modulus

least_squares

Status:

Chi-square:

Sum of Square:

Element	Value	Fix/Free	Error	Error %
L	2.0717e-7	<input type="radio"/>		
R	1.2565e-7	<input type="radio"/>		
R_OHM	6.314	<input type="radio"/>		
Rm	34.68	<input type="radio"/>		
Rct	22.29	<input type="radio"/>		
Rd	27.37	<input type="radio"/>		
Cdl_CO	5.1388e-6	<input type="radio"/>		
Cdl_HNC	3.542e-5	<input type="radio"/>		
Cdl_HNT	0.0003955	<input type="radio"/>		
Cdl_HNP	1.0	<input type="radio"/>		
Cdl_HNU	0.75983	<input type="radio"/>		
Cd_CO	0.048411	<input type="radio"/>		
Cd_HNC	0.97414	<input type="radio"/>		
Cd_HNT	134.9	<input type="radio"/>		
Cd_HNP	1.0	<input type="radio"/>		
Cd_HNU	1.0	<input type="radio"/>		
CPE_B_T	0.023301	<input type="radio"/>		
CPE_B_P	0.5	<input type="radio"/>		

Load initial values

Fit

Simulation

Save Parameters

Save Fit Results

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.

- 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.

Calc modulus	least_squares	Status:
Unit		
Data proportional	7	<input type="checkbox"/> Fix/Free <input type="checkbox"/> Error
Calc proportional	7	<input type="checkbox"/>
Data Modulus		<input type="checkbox"/>
Calc modulus		<input type="checkbox"/>

6.

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