

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

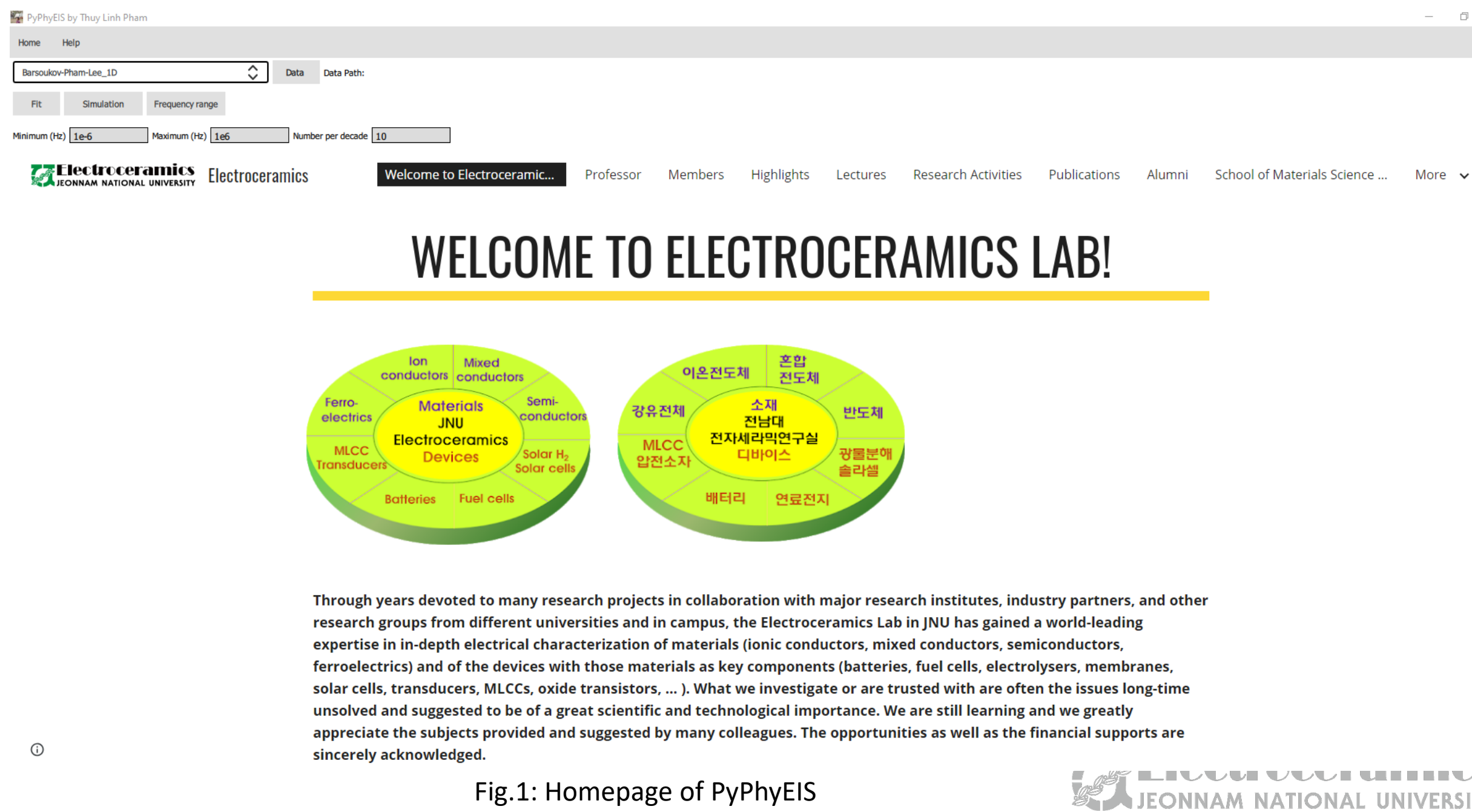


Fig.1: Homepage of PyPhyEIS

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”

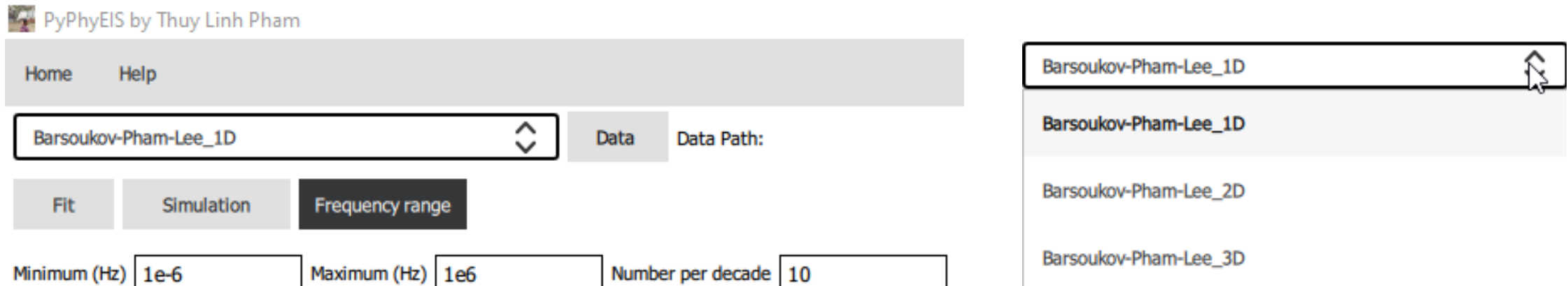


Fig.2: Important features in the task bar

Status: Chi-square: Sum of Square:

Element	Value	Fix/Free	Error	Error %
R <sub>ohm</sub>	6.16	<input type="radio"/>		
R <sub>m</sub>	6.24	<input type="radio"/>		
R <sub>ct</sub>	13.869	<input type="radio"/>		
R <sub>d</sub>	26.01	<input type="radio"/>		
R <sub>i</sub>	96.9	<input type="radio"/>		
C <sub>dl</sub>	3.03e-7	<input type="radio"/>		
C <sub>d</sub>	0.07	<input type="radio"/>		
C <sub>i</sub>	1.032	<input type="radio"/>		
Q <sub>W</sub>	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

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.

Calc modulus	least_squares	Status:
Unit		
Data proportional	7	<input type="checkbox"/>
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.