

# Introduction to ImpedanceFitter

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- Multiple impedance spectra have been recorded
  - Visualization
  - Validity check
  - Fitting, data analysis
- An impedance model is available
  - Expected impedance in a defined frequency range
  - Decomposition of the model
  - Estimating dielectric properties

## Advantages

- High-level interface, batch processing
- Flexible choice of fitting algorithm
- Many relevant models implemented

- Prerequisite: Python  $\geq 3.6$  installed, download from <https://www.python.org>. **Make sure that Python is added to the PATH variable on Windows!**
- Ideally: Jupyter installed (to have Jupyter notebooks) from <https://jupyter.org/>
- Installation is a one-liner:

**`pip install impedancefitter`**

- Bugs? Please report them to me!
- Documentation on the website:  
<https://impedancefitter.readthedocs.io>
- Feedback is highly appreciated!

- The impedance measured in electrochemical impedance spectroscopy (EIS) is assumed to be the linear response of the system
- ⇒ Only linear models (equivalent circuits) considered
- The impedance is modelled by a series or parallel connection of circuit elements and pre-defined circuits
- Realisation in ImpedanceFitter: model is defined in a string and parsed
- Example: Randles circuit

```
1 model = 'R_s + parallel(R_ct + W, C)'  
2 model = 'Randles'
```

# The model

- The model is connects elements in series by + and in parallel by `parallel(a, b)`
- Example: Randles circuit

```
1 model = 'R_s + parallel(R_ct + W, C)'  
2 model = 'Randles'
```

- Question: find out more about the implementation of the Randles circuit and its parameters on the website
- To compute the impedance: generate an equivalent circuit and evaluate it

```
1 Z = lmfit_model.eval(omega=2. * numpy.pi *  
    frequencies, ct_R=Rct, s_R=Rs, C=C0, Aw=Aw)
```

! If you are new to Python please don't hesitate to ask questions!

# Post-processing the model data

- Various functions to plot the data are available:

`'plot_admittance', 'plot_bode', 'plot_cole-cole', 'plot_comparison_dielectric_properties', 'plot_complex_permittivity', 'plot_dielectric_dispersion', 'plot_dielectric_modulus', 'plot_dielectric_properties', 'plot_impedance', 'plot_resistance_capacitance'`

⇒ Documentation on website or through docstrings

- Every device has a frequency independent unit capacitance  $C_0$ , which relates the impedance to the dielectric properties

$$Z = \frac{1}{j\omega\hat{\epsilon}C_0} \text{ with } \hat{\epsilon} = \epsilon_r - \frac{j\sigma}{\omega\epsilon_0} . \quad (1)$$

⇒ Function: `impedancefitter.utils.return_diel_properties`

# EIS data analysis: loading the data

- Available file formats:

<https://impedancefitter.readthedocs.io/en/latest/examples/fileformats.html>

- ! Reach out to me if you want other file formats to be implemented

- General idea: fixed frequencies in one file, probably multiple impedance spectra (real and imaginary part)
- Other representations (polar, R-C, etc.) need to be converted before loaded
- Simplest starting point:

```
1 fitter = impedancefitter.Fitter('CSV')  
2 fitter.visualize_data()  
3 fitter.visualize_data(allinone=True)
```

# EIS data analysis: validating the data

- Impedance data have to fulfil Kramers-Kronig relations
- Test based on general equivalent circuit<sup>1</sup>
- Automated algorithm is implemented<sup>2</sup>
- Simple interface:  

```
results, mus, residuals = fitter.linkk_test()
```
- Test: let's check two exemplary files

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<sup>1</sup>Boukamp, B. A. (1995). A Linear Kronig-Kramers Transform Test for Immittance Data Validation. Journal of The Electrochemical Society, 142(6), 1885–1894.

<sup>2</sup>Schönleber, M., Klotz, D., & Ivers-Tiffée, E. (2014). A Method for Improving the Robustness of linear Kramers-Kronig Validity Tests. Electrochimica Acta, 131, 20–27.



# EIS data analysis: fitting the data

- 1 Choose a model
- 2 Run the fit
- 3 If real or imaginary part are close to zero, it is better to check the residual with respect to the absolute value of the impedance
- 4 If the impedance varies a lot with frequency, it is advised to use a weighting algorithm
- 5 The fit result should be scrutinised by checking the errors of the variables and their correlations in the fit report

# EIS data analysis: post-processing the data

- The fit result can be used to compute the impedance of the model and sub-models
- The data can be exported straightforwardly
- If much data has been fitted: ImpedanceFitter can be used to generate histograms (not shown here, please be referred to online documentation)

Zimmermann, J., et al. (2021) Using a Digital Twin of an Electrical Stimulation Device to Monitor and Control the Electrical Stimulation of Cells in vitro. *Front. Bioeng. Biotechnol.* 9:765516.

- EIS of a stimulation device
- Extraction of different parameters related to electrical, thermal and (electro-)chemical effects by fitting
- Computation of impedances as input for models

Zimmermann, J., & van Rienen, U. (2021). Ambiguity in the interpretation of the low-frequency dielectric properties of biological tissues. *Bioelectrochemistry*, 140, 107773.

- Comparison of measured data and a parametric model
- Data analysis and model analysis
- Suggested correction (see `Correction-Ambiguity.ipynb`)