Deep Learning-Enhanced Parameter Extraction for Equivalent Circuit Modeling in Electrochemical Impedance Spectroscopy

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***Abstract*—Reliable and automatic parameter extraction in equivalent circuit modeling of electrochemical impedance spectroscopy (EIS) could be a challenge as the common circuit fitting method, complex nonlinear least-squares (CNLS), heavily depends on the initial guesses. To prevent the adjustment of the initial guess that demands extra time and experience, we propose employing a deep learning-based convolutional neural network (CNN) to perform the pre-fitting of the measured impedance spectrum. This approach not only facilitates the convergence dynamics of CNLS but also manifests a notable enhancement in parameter extraction fidelity, especially when benchmarked against conventional methodologies. The improvement of 25% in fitting success rate is demonstrated on an open-source impedance dataset by comparing to CNLS with random initials and the traditional stochastic methods including differential evolution and simulated annealing. Thus, we believe the proposed pre-fitting method can provide a useful tool for reliable parameter extraction with the uncertainty minimized to explore the underlying mechanism from EIS and automate this process for the analysis of a large amount of data.**

***Index Terms*—Equivalent Circuit, Electrochemical Impedance Spectroscopy, Deep Learning, Convolutional Neural Network.**

I. Introduction

Electrochemical impedance spectroscopy (EIS) is a non-invasive method measuring the sinusoidal response of a linear time-invariant system under a stimulus of a spectral of frequencies. The characterization of the system under test can be reflected in the resulting impedance spectra, offering the possibility of studying these insight properties. The advantages of EIS make it a common tool in a variety of areas including monitoring electrochemical processes or providing biological information [1], [2]. Its typical applications range from corrosion analysis and battery diagnosis to biomedical sensing and bio-analyte detection [3], [4]. To interpret the EIS data from measurements, the equivalent circuit model (ECM) method is widely employed to simulate the impedance spectra by a combination of electrical circuit components that parameterize the physical and chemical characteristics of the real system [1], [5]. By fitting the impedance of the ECM to the measured data, an optimal set of parameters for the circuit components can be extracted for further quantitative evaluation of the system under test [6].

While the complex nonlinear least-squares (CNLS) method [7] is usually performed to optimize and obtain the parameters of the defined ECM, it can be unreliable and time-consuming due to its dependency on initial guesses [5]. As this optimization algorithm requires a starting point to kick off, an initial far from the global solution or near a trap of a wrong local minimum can introduce errors and uncertainties in estimated parameters or failure in convergence. Thus, manual adjustment to manage parameter calculation is required for each measurement, placing additional demands on time and experience and preventing the fast or automatic analysis of a large size of EIS data.

To tackle the initial guess issue of inverse parameter extraction from impedance spectra, some stochastic methods have been proposed, including particle filter [8], simulated annealing [9], and differential evolution [10]. These methods search a specific range instead of optimizing a given input of initial parameters. However, in cases where the ECM topology is complicated and a large number of component parameters need to be evaluated, the fitting accuracy and computation time cannot be guaranteed. Moreover, measurement errors and noise or inaccuracies of the ECM may lead to extracted parameters that do not match the impedance spectra [5], [11].

In order to optimize the reliability and robustness of the parameter extraction process in ECM-based EIS analysis and automate it for large-scale data, in this paper, we propose an impedance pre-fitting method using a deep learning method, Convolutional Neural Network (CNN) [12], to generate the initial parameters for CNLS regression. Due to the different circuit topologies and components, a specific CNN regression model should be trained for each defined ECM. This can be done with the randomly generated parameters of the circuit components and their corresponding impedance spectra obtained from the simulation of the ECM. The trained model can analyze the measured impedance spectra and roughly estimate the ECM parameters, which are subject to a certain degree of errors but are appropriate as starting values for CNLS with further optimization. Thus, the proposed method can solve the initial guess problem of CNLS and achieve automatic and fast extraction of ECM parameters.

The proposed method is validated using the synthetic spectra from the GitHub repository, AutoECM [13] and its performance can outperform the traditional curve fitting and optimization method including CNLS with random initials, differential evolution, and simulated annealing. Equivalent circuit modeling of impedance spectroscopy is an essential analytical method in a wide range of technical applications, where the proper exploration of physical mechanisms relies on

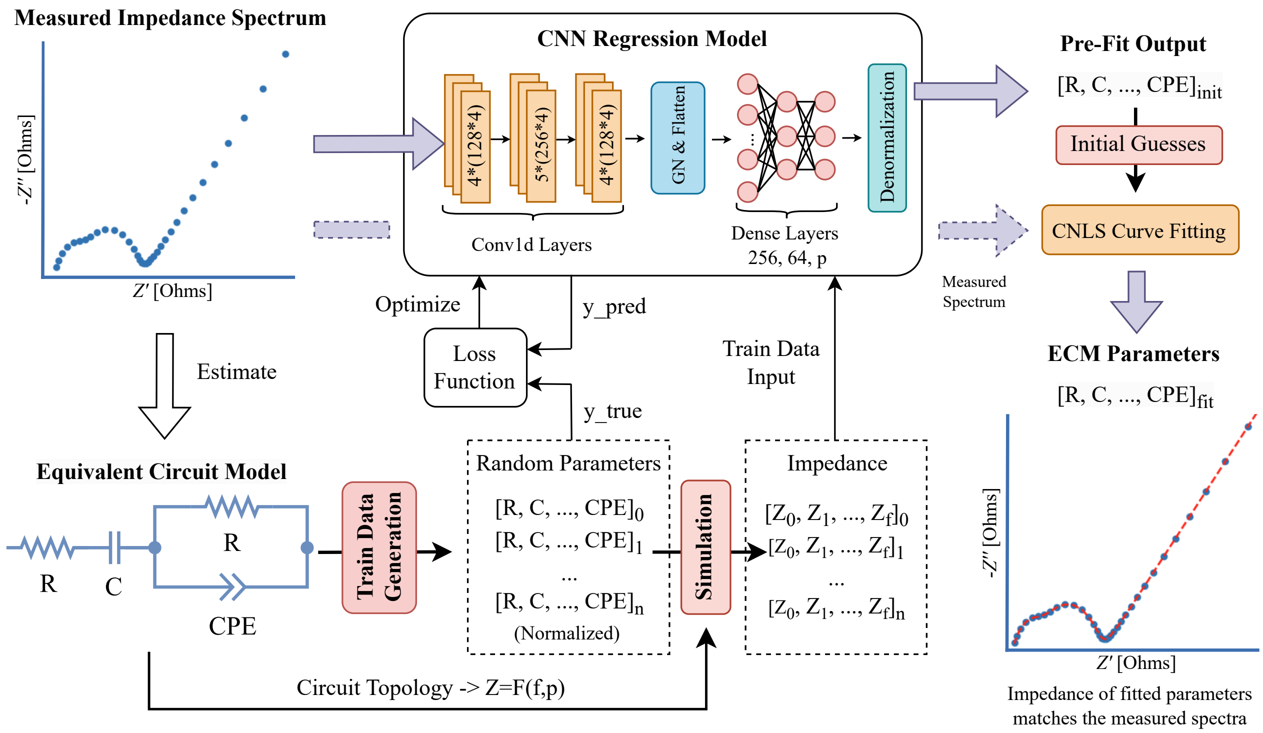


Fig. 1. Equivalent circuit parameter extraction procedures by CNN pre-fitting with CNLS.

the proper electrical circuit fitting. We believe this paper offers a reliable tool for parameter extraction from the impedance spectra by solving this inverse problem with fitting errors minimized, and thus brings automation and convenience to future EIS and ECM-based studies.

II. Background

The complex nonlinear least-squares (CNLS) method is an efficient method for curve fitting and thus equivalent circuit fitting [7]. Considering a defined ECM with N circuit parameters $p_1, p_2, ..., p_N$, its impedance spectrum is given by $\boldsymbol{Z} = \boldsymbol{F}(\boldsymbol{f}; p_1, p_2, ..., p_N)$, where $\boldsymbol{f}$ represents the M sampling frequencies $f_1, f_2, ..., f_M$ and the $\boldsymbol{F}(\cdot)$ is determined by the circuit topology. The task is to find an optimal set of circuit parameters so that the impedance of ECM can closely fit the measured impedance spectrum $(f_1, z_1), (f_2, z_2), ..., (f_M, z_M)$. This can be implemented by the Levenberg-Marquardt algorithm [14] which minimizes the mean squared error (MSE):

$$MSE = \frac{1}{M} \sum_{m=1}^{M} (z_m - Z_m)^2. \tag{1}$$

The advantage of the CNLS method is that its calculation of error minimization process is precise and so are the parameters obtained. However, to start the optimization relying on the derivation, a set of initial guesses (i.e., a set of circuit parameters) is mandatory while the fitting results are sensitive to the choice of initial values. It has been reported that the strong nonlinear behavior of the ECM and the presence of measurement noise may further deteriorate the convergence of CNLS regression [5], [11].

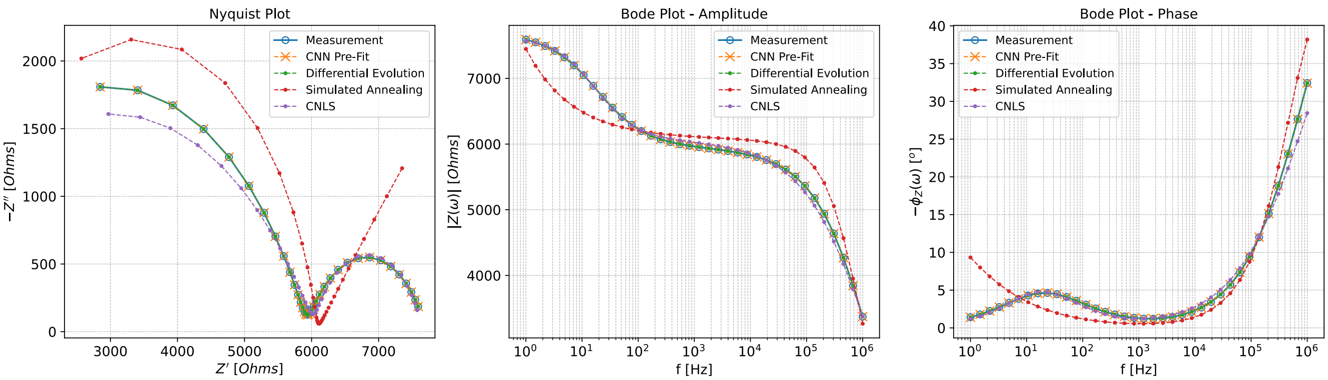
Considering the pros and cons of the CNLS method, it is beneficial to combine it with the deep learning-based regression model [15]. The AI-driven model can estimate values that have a high probability of being around the global optimum and act as initials to facilitate CNLS regression to precisely compute the optimum with minimum MSE.

III. Methods

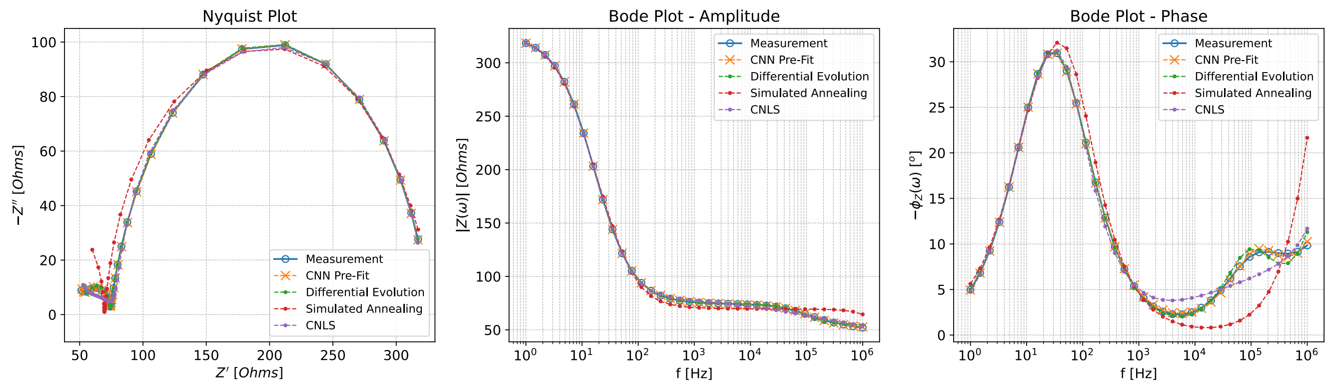
A. CNN Pre-Fitting

Recent studies and developments of deep learning have demonstrated its powerful ability to facilitate the analysis of data for in-depth investigations. In this paper, we propose leveraging the Convolutional Neural Network (CNN) as a regression model to solve the inverse identification problem of extracting parameters from impedance spectra.

The overall parameter extraction program through CNN pre-fitting integrating into CNLS curve fitting is illustrated in Fig. 1. The role of the CNN regression model is to provide a set of reliable initial guesses for CNLS to compute accurate circuit parameters. To train the CNN model, a data set of impedance with its corresponding circuit parameters as the ground truth is needed. Based on the defined ECM estimated from the measured impedance spectra, parameters of circuit components can be randomly generated within a controlled range and the respective impedance can be calculated by circuit simulation. A prior knowledge of the ECM and measured EIS is preferable to narrow down the range for random generation



(a) L-R-RCPE-RCPE



(b) R-C-RCPE-RCPE-RCPE

Fig. 2. Samples of fitted impedance spectra through the proposed and comparative methods along with the measurements, based on two types of ECMs: (a) L-R-RCPE-RCPE, (b) R-C-RCPE-RCPE-RCPE.

of circuit parameters, which can improve the accuracy of the regression. Furthermore, the parameters for training need to be normalized while the output of the CNN model should be normalized considering the values can differ with various component types.

The CNN model in this work consists of three 1-dimension (1D) convolutional layers and three densely-connected (dense) neural network layers. They are cascaded through a Flatten layer and a Gaussian Noise (GN) layer with a standard deviation of 0.05 to improve the generalizability. The convolutional layers take the input of impedance in 4 channels (real, imaginary, absolute, and phase values of the impedance data) and extract the features with 128, 256, and 128 filters and the kernel length of 4, 5, and 4, separately. The densely-connected layers comprise 256, 64, and N units, respectively, and p is the number of ECM components. Each layer uses the Rectified Linear Unit (ReLU) [16] as the activation function, which is written as:

$$\mathrm{ReLU}(x) = \max(x, 0). \tag{2}$$

Finally, the regression loss is evaluated by MSE comparing the predicted parameters p' from CNN and the ground truth circuit parameters, which is given as:

$$Loss = MSE_{CNN} = \frac{1}{N}\sum_{n=1}^{N}(p'_n - p_n)^2. \tag{3}$$

The weight of the model is optimized by the Adam algorithm of 0.001 learning rate according to the loss.

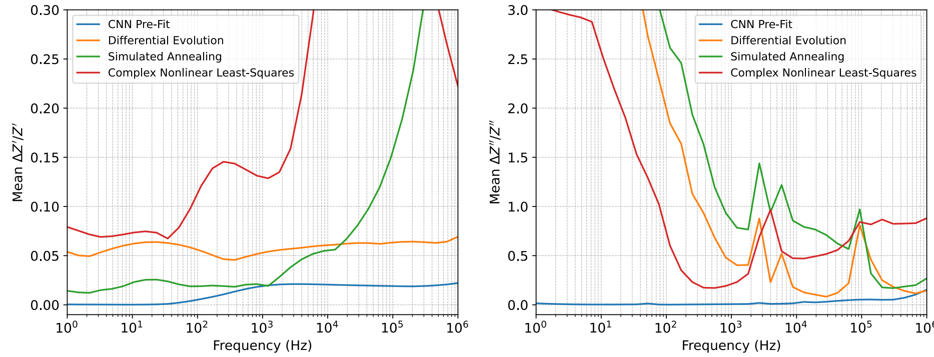
In this work, the training and test of pre-fitting by CNN is performed on MacBook Pro M1 with TensorFlow-macOS 2.9.0. The simulation of circuit impedance is based on the Python repositories `impedance.py` [17].

B. Differential Evolution and Simulated Annealing

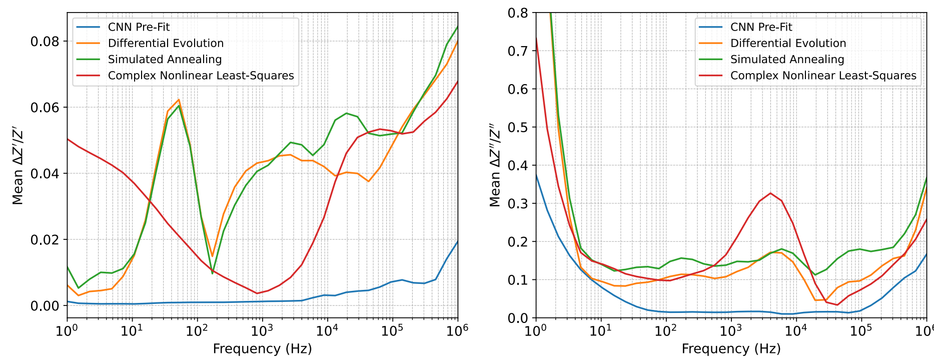
Two typical optimization methods are selected for comparison in fitting performance, which are differential evolution and simulated annealing.

The differential evolution algorithm simulates the evolution process in natural selection by randomly evolving a population of candidate solutions through multiple generations of iterations. For each iteration, evolution occurs by applying mutation, crossover, and selection to create new candidate solutions based on an objective function.

Simulated annealing is another stochastic method mimicking the annealing in metallurgy. This algorithm is likely to accept a worse solution defined by the objective function.



(a) L-R-RCPE-RCPE



(b) R-C-RCPE-RCPE-RCPE

Fig. 3. Real and imaginary residual error ratio across measured frequencies.

TABLE I
COMPARISON OF FITTING SUCCESS RATE AND TIME CONSUMPTION.

Methods	Initial Guesses	Time	Fitting Success Rate
CNN Pre-Fit	Not Required	95s + 921s (Test + Training)	0.875
Differential Evolution	Not Required	390s	0.7
Simulated Annealing	Not Required	2107s	0.45
CNLS	Required	122.7s	0.7

The acceptance probability is given by a function depending on the "temperature", so that it may get rid of local optima and locate the global optima at an early stage. As this iteration processes with the decrease in the "temperature", the acceptance probability of a worse solution drops, allowing an optimal solution to be computed.

Instead of asking for initial values, these two optimization algorithms require rough search ranges for the circuit parameters. In this paper, they are both implemented for performance comparison by the `scipy` package on Python [18].

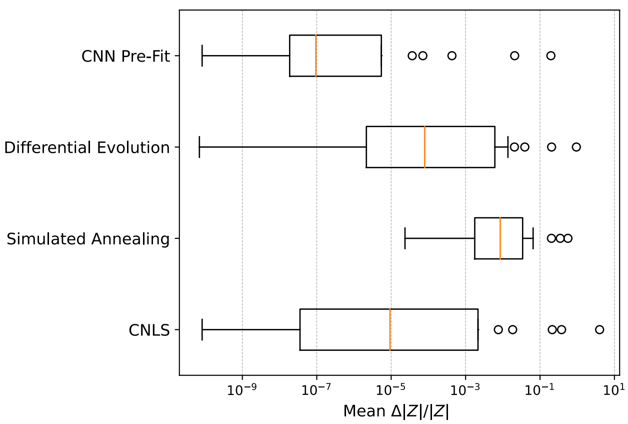
IV. RESULTS

A. Metrics

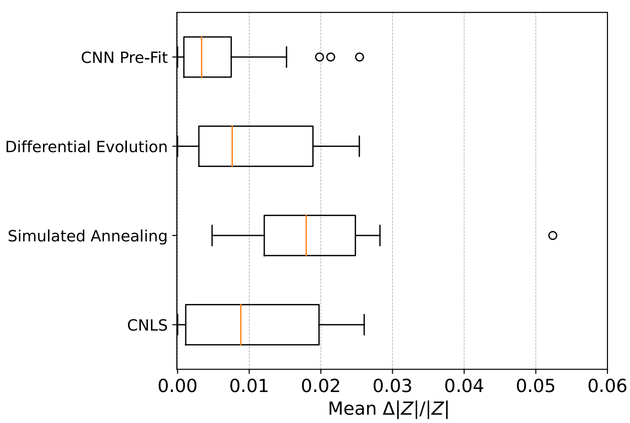
To validate the benefits of the CNN pre-fitting approach, we utilize open-source EIS data from a GitHub repository, AutoECM [13] to perform equivalent circuit fitting and extract component parameters. The impedance spectra to test include 20 sets of data based on the ECM of L-R-RCPE-RCPE and 20 sets based on the ECM of R-C-RCPE-RCPE-RCPE. The strings describe the circuit topology, where L, R, C, and CPE denote inductance, resistance, capacitance and constant phase element, respectively, and the hyphen represents the serial connection while the combination of two characters represents the parallel connection. The fitting results obtained by the proposed method are examined by comparing with three typical optimization techniques, differential evolution, simulated annealing, and CNLS with random initials.

Fig. 2 presents the Nyquist and Bode plots of two examples of impedance curves corresponding to the ECM parameters extracted by fitting through the proposed method and the comparative methods, together with the original measurement impedance spectra. As an example, the impedance spectra simulated from the parameters extracted by the CNN pre-fitting method can closely match the sampling points of the measurement spectrum, which represents an accurate fitting case.

As the objective of equivalent circuit modeling is to simulate the measurement impedance spectra, to evaluate the fitting performance, it is straightforward to estimate the error between the measured and fitted results instead of the error of the extracted parameters. Fig. 3 indicates the residual error ratio of the real and imaginary parts of the fitted impedance at each measured frequency, which is given by $\Delta Z'/Z'$ and $\Delta Z''/Z''$, respectively. For each tested impedance spectrum, the accuracy



(a) L-R-RCPE-RCPE



(b) R-C-RCPE-RCPE-RCPE

Fig. 4. Box plot of mean absolute percentage error (MAPE).

of the fitting approaches is assessed by the mean absolute percentage error (MAPE):

$$\mathrm{MAPE} = \frac{1}{M}\sum_{m=1}^{M}\frac{|z_m - Z_m|}{|z_m|}. \tag{4}$$

The MAPE for the performance of the tested methods on two selected types of ECM is illustrated in the form of the box plot in Fig. 4. Furthermore, the success rate of fitting is summarized in Table I as well as the computation time, where a successful fitting of the tested impedance spectrum is defined by its MAPE lower than 0.01.

B. Discussion

As the presented residual error ratio plots shown in Fig. 3, the proposed method, CNN pre-fit, can keep the residual errors of the fitted impedance spectra low for both two tested ECMs and thus high accuracy for the extracted parameters. In comparison, other chosen optimization methods may result in much higher error levels, indicating failures of convergence in some regression cases.

Similar patterns apply in Fig. 4, where the box plots summarize the distribution of the MAPE of the tested methods for each type of ECM. The box plot results can imply that for some cases of tested impedance spectra, the comparative methods, differential evolution or CNLS with random initials, may find the global optima with the minimum error, but this is not guaranteed. The greater deviation of these methods indicates that the fitting outcomes are unstable and they have a high probability of getting trapped with local minima, leading to large errors. However, by employing the CNN pre-fit method, the lowest deviation in the MAPE can be gained. These results demonstrate it can be a trustworthy option for automating the process of parameter extraction for a large amount of data.

The overall benchmark is presented in Table I, showing the total accuracy of parameter extraction in the tested dataset, as evidenced by the fitting success rate. The CNN pre-fitting method achieves a success rate of 0.875, which constitutes an improvement of 25% compared to the traditional approaches with only 0.7 success rate. In addition, the proposed method also consumes less time in parameter extraction. It is noticed that the training of the CNN model takes additional time, but this is worthwhile for the processing of a large number of EIS data.

Although the CNN pre-fit method is also based on CNLS regression, influenced by dependence on initial values, CNLS with random starting points may not find the correct global optima and result in a significantly higher residual error ratio due to the failure of convergence. Thus, it can be deduced that introducing the CNN pre-fitting method to generate a set of approximate parameters as the initial can considerably facilitate the accuracy of CNLS-based curve fitting and improve the certainty of extracted parameters.

V. Conclusion

In this paper, we propose a reliable and automatic parameter extraction method for equivalent circuit modeling of EIS, exploiting a CNN-based approach to pre-fit the spectrum and generate initial parameters for the CNLS regression. While other optimization methods are unstable in fitting and the traditional CNLS regression requires initial guess and extra manual adjustment, the proposed method automates the parameter extraction processes and is demonstrated with satisfactory accuracy and low fitting errors. As a result, this deep learning-based method can become an effective solution in equivalent circuit modeling where impedance spectrum fitting is needed and lower the uncertainty in the exploration of the underlying mechanisms. The realization of the fast analysis of massive impedance spectra could advance future EIS-based studies.

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