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Python Script in the processing of electrochemical impedance spectroscopy and current transient measurements for the determination of the chemical capacitance

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Big Data is defined in a variety of ways, including a) the search and retrieval of information to make decisions, and b) the science behind the data when these are used to respond any question. On other hand, chemical capacitance (a fundamental thermodynamic quantity related to charge accumulation at an electronic conductor/ionic conductor interface), is conventionally obtained by electrochemical impedance spectroscopy (EIS). Herein, current transients (CT) are proposed as an alternative measurement to determine the chemical capacitance. Thus, we describe a Python script to evaluate whether chemical capacitance can be obtained by CT collected at multiple potentials. The experimental procedure was performed with the redox pair $\text{Fe}(\text{CN})_6^{3-}/\text{Fe}(\text{CN})_6^{4-}$, a model one electron outer sphere process, and applied to the derivation of the chemical capacitance of the redox-active species on a Pt electrode. To validate the methodology here proposed is necessary to organize, process, and matching between these two different types of measurements, like so display information in the form of mathematical models, plots and files. Hence, we develop a protocol to analyze and compare a large amount of data irrespective of time scale. Usually, the experimental data for CT and EIS are analyzed independently and in different ways by computational programs, for instance, repeating the sampling process for different times yields a family of curves named “sampled current-voltammograms”, one for each time scale. In addition, EIS data may be presented in several types of plots (e.g., Bode or Nyquist), which increase the volume of information obtainable from these measurements. Therefore, a `getData` class was created to get and process the experimental data from CT and EIS measurements. To process the experimental data a Python script was used to instantiate two objects: input and data objects. An input object is a JSON-like object where the file name and the potential for experiment data are defined, thereby JSON object was implemented as a Python dictionary. A data object is the instantiated `getData` object with the information contained in the data files referenced in the input object. A Python script containing the input and data objects was created to process experimental data of $\text{Fe}^{\text{III}}/\text{Fe}^{\text{II}}$ redox pair in solution. A total of 64 data files were obtained with NOVA 2.0 software for electrochemistry. Each CT data file contains approximately 15000 experiment numbers, and EIS, 305. With instantiate `getData` object the capacitance curves against potential from EIS and CT was constructed and compared in an easier way than process data with traditional tools used in electrochemistry. It is concluded that at a specific condition of time scale, the integral of CT and EIS measurements give similar results of capacitance.

Biography

Daniel Andres Triana Camacho received the B.S degree in Electronic Engineering from the Technological Units of Santander in 2014, Bucaramanga, Colombia. He is currently Msc. Physics student and researcher at the Science of Biology Materials and Semiconductors CIMBIOS group. His research interests include a design of biomedical devices, condensed matter, data processing, electrochemistry methods, pedagogy models and neural networks.

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