ElectroKitty: A Python based electrochemical simulator

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To this day almost all electrochemical experiments made to elucidate the underlying mechanism are done on the RDE. However almost all of the reports of the surface mechanism are done qualitatively. The major reason for this is that simulating electrochemical experiments is hard and requires a good understanding in how to solve the set of differential equations, used in describing the observed system. To make the electrochemist's job easier, in quantifying the observed system, I developed an electrochemical simulating tool in Python. We chose Python as it is currently the most popular programming language and is easy to use. Python's another major advantage is that it has a rich repository of various other libraries for data analysis, thus combining ElectroKitty with a data treating package is almost seamless.[1] ElectroKitty is based on an implicit finite difference approximation, making it both stable and efficient in computing an electrochemical signal.[2] The simulator is capable of calculating a current response for virtually any potential input with a predefined mechanism. To demonstrate the workflow and functionality of the simulator, we show a comparison of simulated and experimental data for two well-known systems. First, we show that the simulator can accurately simulate both the CV and alternating-current CV (FTacCV)[3] response of the ferro-ferri cyanide couple. Second, we show that using the PINTS[4] library for parameter inference, we can accurately fit the data for HER on Pt in alkaline. It is the authors hope that such a tool will further help electrochemists in understanding the underlying mechanisms of their systems.

References

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