Discovering Electrochemistry with an Electrochemistry-Informed Neural Network (ECINN)

Haotian Chen[1], Minjun Yang[1], Bedřich Smetana[2], Vlastimil Novák[3],Vlastimil Matějka[4], Richard G. Compton[1,*]

[1]*Departmement of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford*
[2]*Departmement of of chemistry and physico-chemical processes, Faculty of materials science and technology VSB- Technical University of Ostrava*

* *richard.compton@chem.ox.ac.uk*

Machine learning is increasingly integrated into chemistry research by guiding experimental procedures, correlating structure, and function, interpreting large experimental datasets, to distill scientific insights that might be challenging with traditional methods. Such applications, however, largely focus on gaining insights via big data and/or big computation, while neglecting the valuable chemical prior knowledge dwelling in chemists' minds. In this presentation,[1] we introduce an Electrochemistry-Informed Neural Network (ECINN) by explicitly embedding electrochemistry priors including the Butler-Volmer (BV), Nernst and diffusion equations on the backbone of neural networks for multi-task discovery of electrochemistry parameters. We applied the ECINN to voltammetry experiments of Fe^{2+}/Fe^{3+} and $Ru(NH_3)_6^{2+}/Ru(NH_3)_6^{3+}$ redox couples to discover electrode kinetics and mass transport parameters. Evolving from physiscs-informed neural network for electrochemistry,[2-5] ECINN seamlessly integrated mass transport with BV to analyze the entire voltammogram to infer transfer coefficients directly, so offering a new approach to Tafel analysis by outdating various mass transport correction methods. In addition, ECINN can help discover the nature of electron transfer and is shown to refute incorrect physics if imposed. This work encourages chemists to embed their domain knowledge into machine learning models to start a new paradigm of chemistry-informed machine learning for better accountability, interpretability, and generalization.

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References

1. H. Chen, M. Yang, B. Smetana, V. Novák, V. Matějka and R. G. Compton, *Angew. Chem. Int. Ed.*, 2024, **n/a**, e202315937.
2. H. Chen, E. Kätelhön and R. G. Compton, *J. Phys. Chem. Lett.*, 2022, **13**, 536-543.
3. H. Chen, E. Kätelhön and R. G. Compton, *Analyst*, 2022, **147**, 1881-1891.
4. H. Chen, C. Batchelor-McAuley, E. Kätelhön, J. Elliott and R. G. Compton, *J. Electroanal. Chem.*, 2022, DOI: https://doi.org/10.1016/j.jelechem.2022.116918, 116918.
5. H. Chen, E. Kätelhön and R. G. Compton, *Curr. Opin. Electrochem.*, 2023, DOI: https://doi.org/10.1016/j.coelec.2023.101214, 101214.