Discovering the origin of catalyst performance and degradation of electrochemical CO_2 reduction through explainable artificial intelligence

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Catalyst degradation poses a substantial hurdle for the commercialization of electrochemical CO2 reduction, leading to diminished activity and selectivity. The significant experimental cost associated with catalyst characterization limits the in-depth understanding of this degradation. Machine learning has emerged as a promising tool to bypass these costly procedures, though its limited interpretability has often complicated its application. This study introduces an interpretable machine learning framework capable of accurately predicting catalyst conditions using linear sweep voltammetry (LSV) in sub-seconds, while also shedding light on identifying the origins of catalytic degradation. Based on a comprehensive dataset of 5236 LSV experiments, a convolutional neural network was trained and demonstrated superior predictive capabilities for total current and faradaic efficiency. The insights derived from the model are further elucidated through explainable artificial intelligence (XAI), pinpointing key degradation factors. To validate the XAI interpretation, surface analysis experiments were conducted, underscoring the reliability of the proposed approach. This novel framework offers potential applications in various catalytic processes, battery degradation, and chemical process monitoring, indicating its potential for rapid and reliable performance monitoring.