ELECTROCHEMICAL MATERIALS DISCOVERY AND INTELLIGENCE

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Design and implementation of efficient and cost-effective electrochemical devices is a complex challenge. It hinges on big-data driven knowledge at the frontiers of multi-disciplinary efforts in materials discovery and design. These massive data–driven processes, however, require intensive cognitive, yet expensive systems, including human, to determine the best design decisions. A novel approach towards Artificial Intelligence (AI) and Machine Learning (ML) algorithms can overcome the complexity of selecting advanced new materials with the predictable and desired properties. Focusing on advanced electrocatalysts for CO2 conversion as a use case, we demonstrate an AI-driven “Virtual Materials Intelligence” platform (beta) for materials data management and intelligent design equipped with an advanced user interface and predictive capabilities in view of materials properties and function. The platform combines information originating from large data sets of different origins. The data storage, data analysis, and advanced analysis algorithms enable efficient and secure data flow between several different simulation and characterization activities. The cloud-based platform ultimately aims to manage all available materials databases and relevant modeling, simulation, performance, cost, and characterization data and how they can be communicated to materials fabrication and design teams.