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Journal
ECS Meeting Abstracts, MA2020-01(39)

ISSN
2151-2043

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Publication Date
2020-05-01

DOI
10.1149/ma2020-01391751mtgabs

Peer reviewed

(Invited) Virtual Analysis of Gas-Diffusion-Electrode CO2 Electrolyzers

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Abstract

The electrochemical reduction of CO2 (CO2R) to value-added products is an attractive technology for tackling the rising atmospheric CO2 levels and storing intermittent renewable energy into chemical bonds. Fundamental understanding of CO2R has progressed significantly in recent years and is critical in the development of CO2R to liquid-fuel electrolyzers, where gas-diffusion electrodes (GDEs) have been shown to be key enabling architectures. Various designs have been proposed and studied in the literature to enhance overall selectivity, rates, and maximize the conversion of CO2, the latter of which is only now being recognized as a critical issue. In this respect, there is a need to explore the governing phenomena inherent in these architectures to enable optimization. Mathematical modeling is ideally suited to tackle and explore these multiphysics interactions and provide virtual design analysis.

In this talk, we discuss modeling methodologies and physics inherent in these devices and present our recent modeling of GDEs for CO2 reduction. We specifically examine the impacts of multiphase flow and related phenomena on overall cell performance. We then explore the performance and limitations of various cell designs guided by simulation results and examine potential methods for improving water management and tuning catalyst selectivity including the use of different anion-exchange and bipolar membranes. Finally, we discuss the disparities in local environments between aqueous and GDE devices and propose strategies to reduce the gap in knowledge between the two systems.

Acknowledgements

This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993.