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Ab-initio modeling of electrochemical processes for hydrogen production

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Recent progresses in predictive modeling methods together with high-fidelity experimental characterization techniques that take device operation condition into consideration led to significant advancements in understanding how microscopic interfacial processes propagate to macroscopic device behavior. In this talk, we will overview our computational modeling efforts, wherein the state-of-art characterization techniques are fully leveraged for the reliability of out interpretation. As examples, we will present our recent activities to improve understanding about the mechanisms that dictate performance and durability of hydrogen production devices, where considering operating conditions and integration with experimental characterization often played critical roles.

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