
BESH2020 Tailoring Hydrogen Evolution Reaction (HER) Catalysts for Operation at Specific pH Values

Principal Investigator: Bianca Ceballos

Organization: University of California, Irvine

Electrocatalysts that can generate renewable fuels under a wide range of pH conditions in water are necessary for renewable energy applications. Metal hydrides are critical intermediates involved in bond-breaking and bond-forming steps in relevant catalytic reactions. Our group relies on thermodynamic hydricity-pH relationships to target reaction conditions for selective hydride transfer for proton reduction to H₂ or CO₂ reduction to formate (HCO₂) in water. Although metal hydricities have been measured for hundreds of transition metal complexes in organic solvents, aqueous hydricities are relatively unexplored.

We report the electrocatalytic activity of [HNi(DHMPE)₂][BF₄] (DHMPE= 1,2-bis(di-(hydroxymethyl)phosphino)ethane) (1) toward hydrogen production at pH 1, with a rate of ~10³ s⁻¹, Faradaic efficiency between 92–105%, and negligible decomposition after 18 hours of electrolysis. We are currently pursuing new nickel diphosphine complexes modified to make stronger metal hydrides for the reduction of substrates such as CO₂ to other C1 fuels.