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

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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 H<sub>2</sub> or CO<sub>2</sub> reduction to formate (HCO<sub>2</sub>) 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)<sub>2</sub>][BF<sub>4</sub>] (DHMPE= 1,2-bis(di-(hydroxymethyl)phosphino)ethane) (1) toward hydrogen production at pH 1, with a rate of ~10<sup>3</sup> s<sup>-1</sup>, 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 CO<sub>2</sub> to other C1 fuels.