Hydrogen evolution/oxidation electrocatalysts for $\text{H}_2/\text{Br}_2$ energy conversion systems

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North American energy production is, and for the near future will remain, dominated by fossil fuels, however, in the long term, or in other locations in the world, renewables such as wind and solar can play a greater role in the energy portfolio. Renewables’ issue is their reliance on energy storage to match the intermittent supply to demand. Here I discuss the advantages of using $\text{H}_2/\text{Br}_2$ electrochemistry (flow cells as well as artificial photosynthesis) to store electrical energy. The main technological issue for these systems is developing an electrocatalyst that can do hydrogen evolution and oxidation while remaining stable in bromine and bromide. We hypothesize that transition metal sulfides will be stable in hydrobromic acid and bromine, and that they can improved by doping. We have used high throughput screening techniques to identify interesting catalysts, and measurements of hydrogen binding energy to understand the surface chemistry and charge transfer of the electrochemical reactions to see why certain dopants can improve catalyst activity. We also developed a technique to use carbon monoxide to identify the active sites of our best performing catalyst, with the hope to maximize its activity. We have found that certain dopants improve the activity of metal sulfides for hydrogen evolution and oxidation, through improvements in charge transfer, and that to develop an ideal electrocatalyst we will need to maximize the type of active site on our catalyst and improve the conductivity of the semiconductor portion of our catalyst.