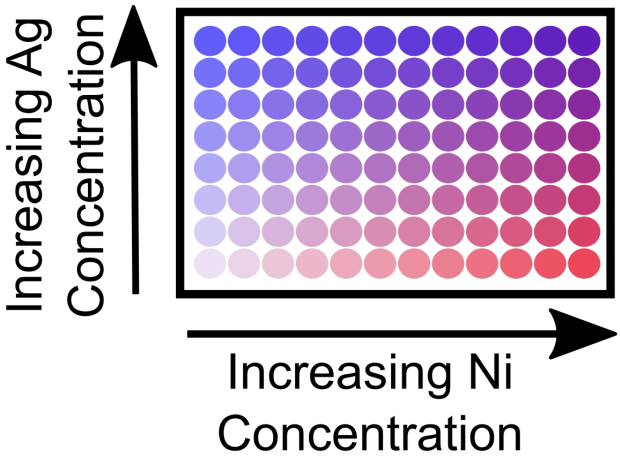
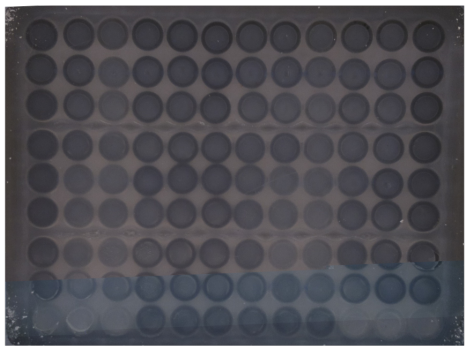
Experimental

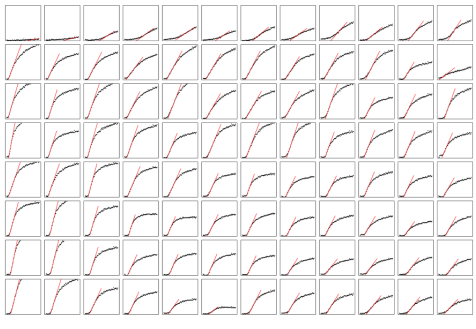
1. Design a wellplate with metals at varying concentrations



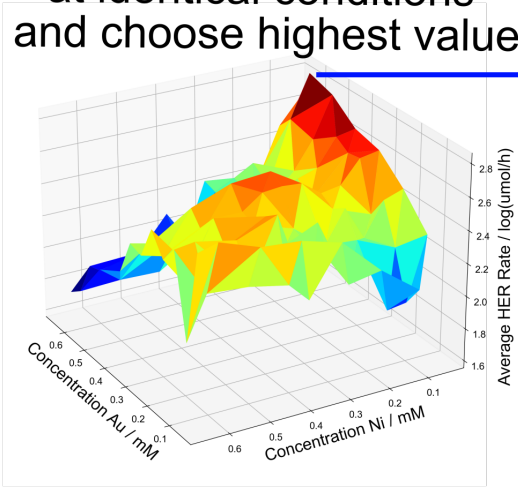
2. Run experiment and observe hydrogen evolution over time



3. Extract maximum rate of hydrogen evolution of each well

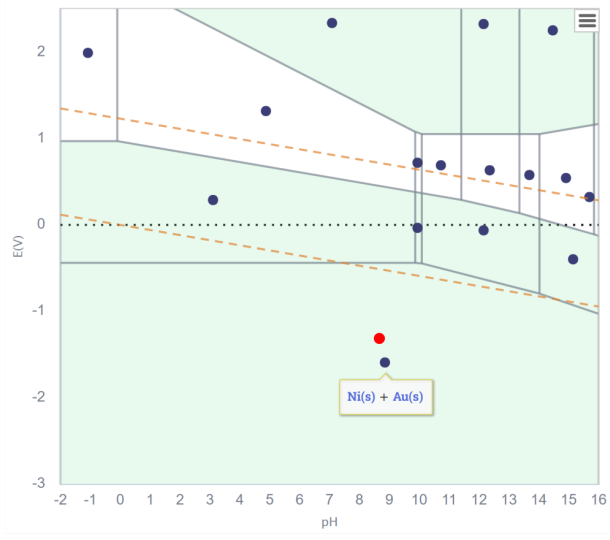


4. Average rates observed at identical conditions and choose highest value

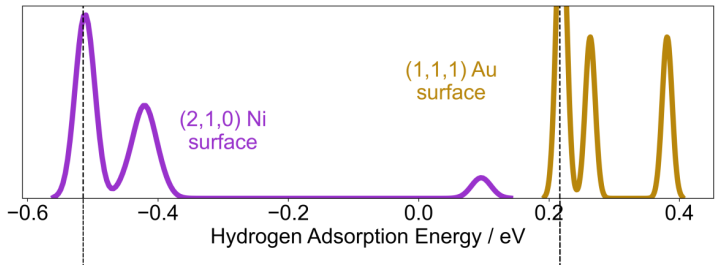


Theoretical

1. Select materials using electrochemical stability threshold



2. Predict H binding on all sites and take minimum per surface (two example surfaces shown)



3. Choose surface closest to HER optimum at -0.24 eV