Software Development for HER High-Throughput Experiments

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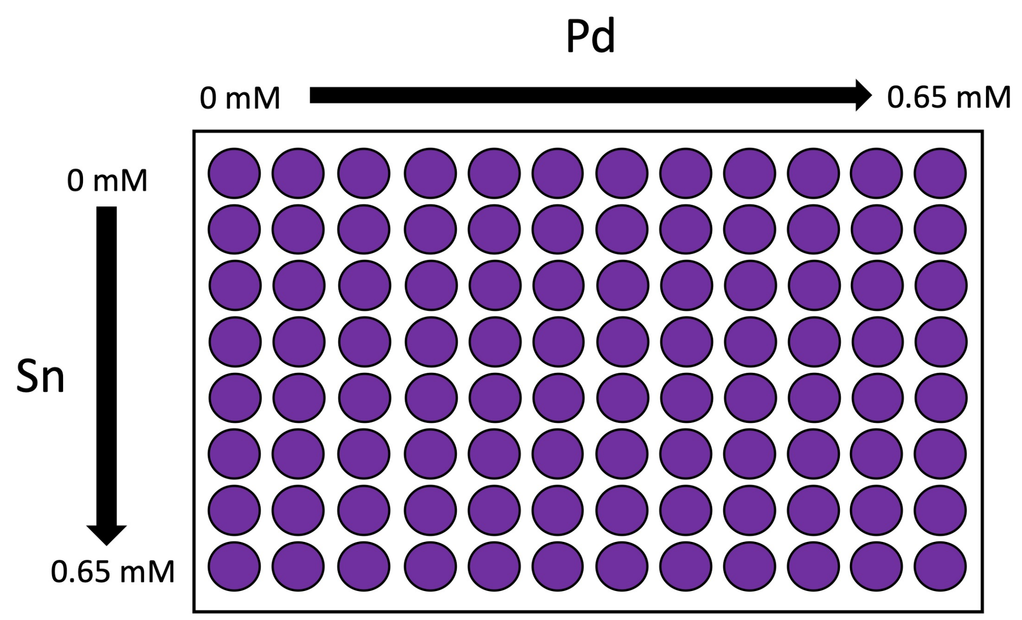
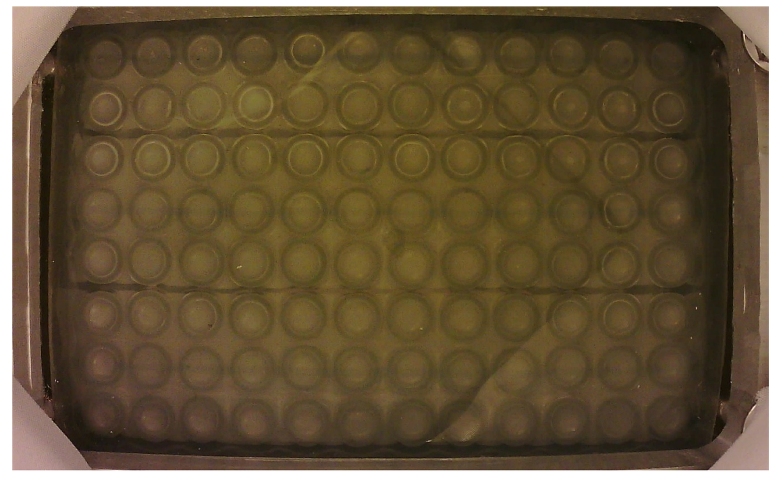
A high-throughput 96 well plate experimental setup has been used to drastically increase the screening rate of bimetallics for HER. The data is then analyzed using a series of software tools that have been developed (pure Python data analysis pipeline).

Experimental Setup

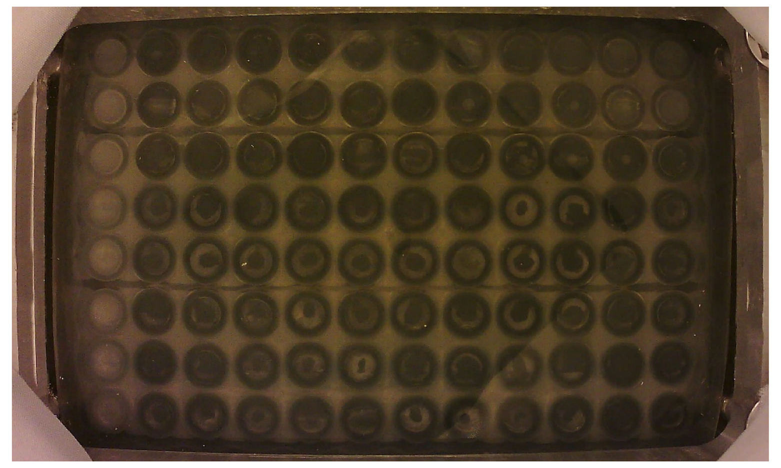
- The general experimental setup is shown below.



- Throughout the experiment, images are taken of the plate every ~10 minutes to quantify the results.



Time = 0 min.

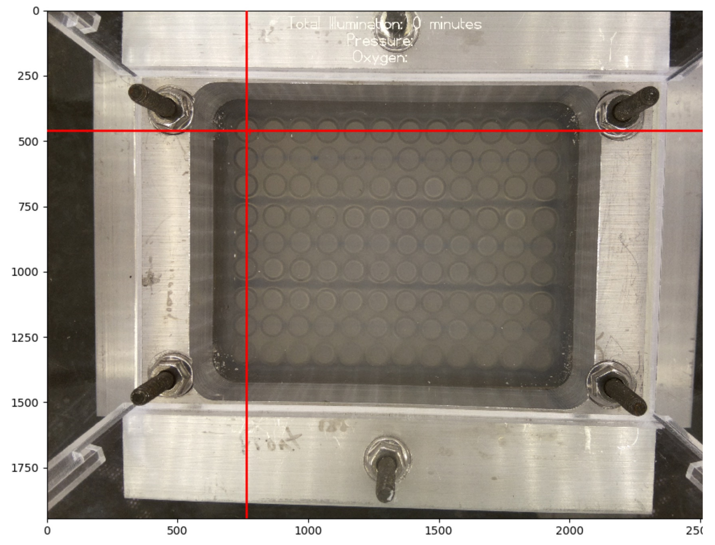


Time = 1180 min.

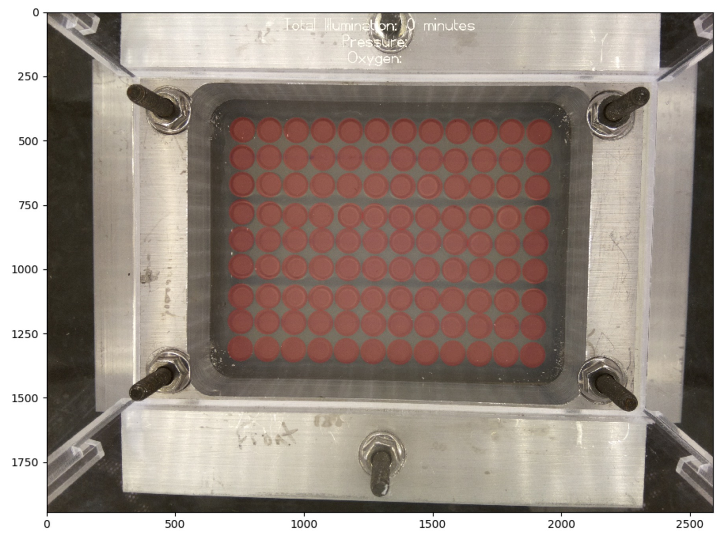
Image Analysis Tools

During an experiment, changes in the darkness of any wells on a plate indicate hydrogen production. To quantify the change in darkness in each of the wells, a binary mask must be created from the first image. This was being done manually in Mathmatica, but a more efficient method was produced with Python as shown below:

1. Interactively click the 4 corners of the first image.
2. The Python script linearly interpolates between the rows and columns (which works even when the pictures were tilted). After the script attempts to identify the locations of the wells, the user has an opportunity to interactively move any wells that are not in the correct location.

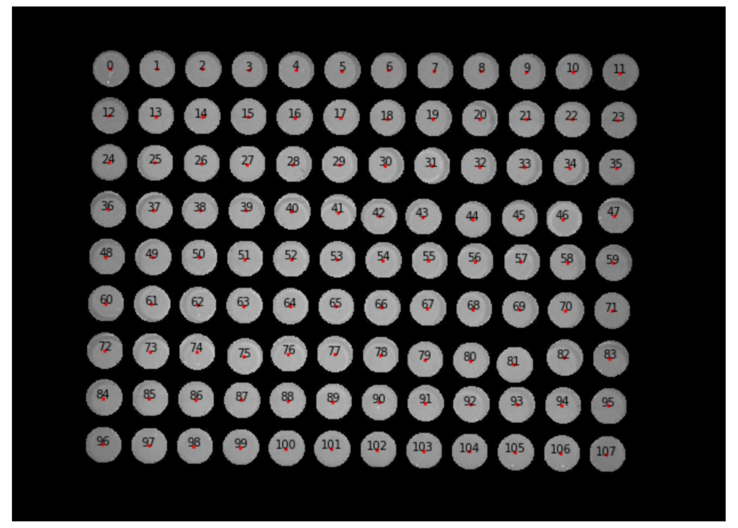


Step 1

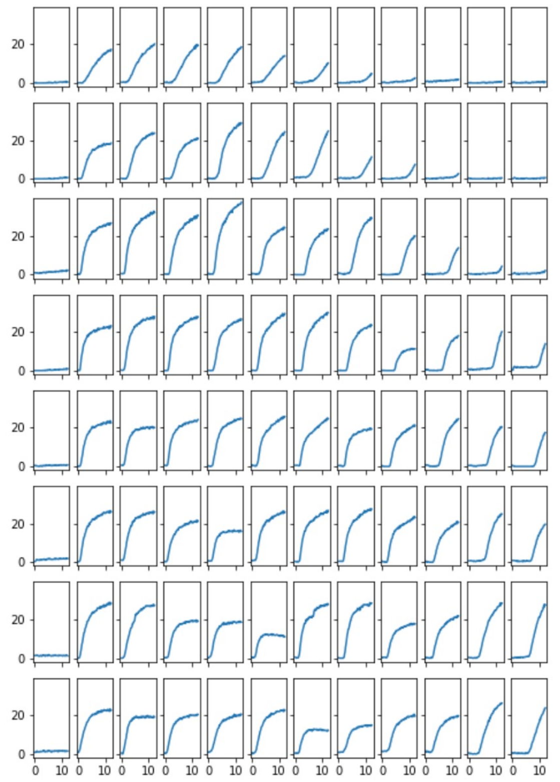


Step 2

3. The binary mask is now finished, and a Python script quantifies the changes in darkness for each of the wells.



Description: Binary mask created in step 2 with each well center location being identified.

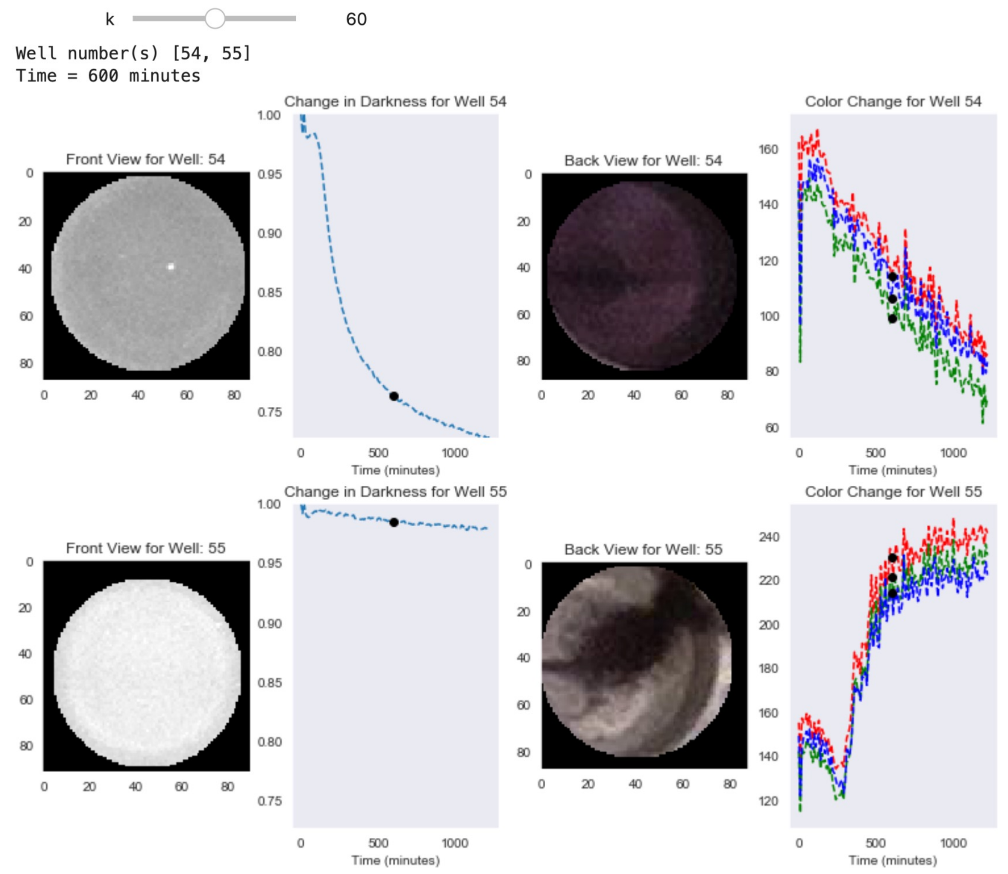


Description: Grid plot of the hydrogen production of each well vs time.

Step 3

Image Analysis Tools (Extended)

A third generation of experiments were conducted, where images of the bottom of the plates were also taken. These images were not of the same quality so they could not be used for quantifying the amount of hydrogen produced, but they did show changes in color. An interactive tool was made to select a well (or a series of wells) and evaluate how the color and darkness of the well(s) changed with time.



File Management – *nb_search*

A script was created to automatically create report notebooks for each of the bimetallic combinations. These were stored at NERSC, a government run database. As the files in the database grew, the time taken to locate data from a specific bimetallic became a nuisance. A Python package, *nb_search*, was developed to efficiently sort through, locate and open the report files. An additional feature allowed tags to be added to files that were urgent or had hard deadlines.

```
[1]: from nb_search import *

[2]: files = search_todo()

     %TODO No due date
    ./Notebooks/Test_notebook3.ipynb
     Optional Description 1 (Due in: 8 days)
    ./Notebooks/Test_notebook1.ipynb
     Late (Past due by: 10 days)
    ./Notebooks/Test_notebook2.ipynb
```

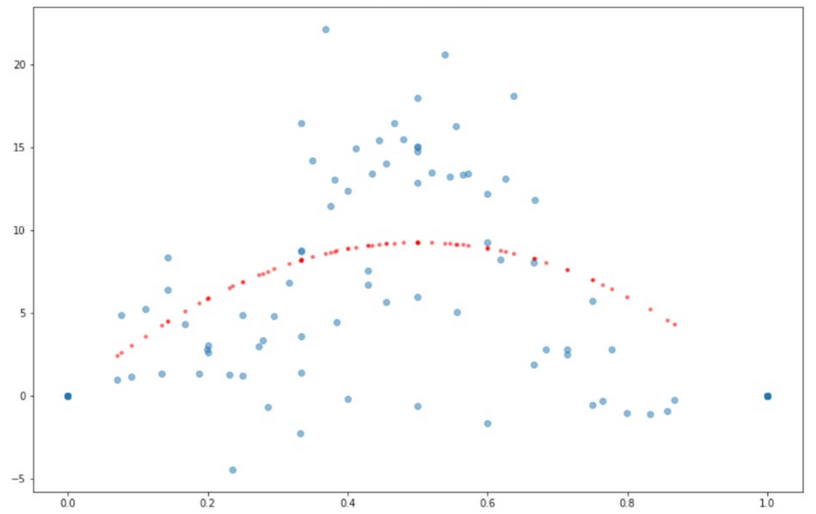
Description: *nb_search* finding TODO tags in any notebook under the current directory. More features can be found at http://github.com/loevlie/nb_search.

Quantitative Groupings

Five groupings of the 31 bimetallics tested became obvious once visualizations of the synergy between the bimetallics were analyzed. These groupings are listed below:

1. Positive Synergy
2. Negative Synergy
3. Positive and Negative Synergy (with a trend)
4. No Synergy
5. Evenly Distributed Positive and Negative Synergy (no trend)

A quantitative method for clustering those synergy plots was created; this was validated with a qualitative grouping of the bimetallics. This method involved fitting the plots with a simple Margules type equation. The equation and an example of a positive synergy plot are shown below.



$$x(1-x)\left(A_{12}x + A_{21}(1-x)\right)$$

Conclusion

In conclusion, the software tools developed have helped improve a few areas of the post experimental computations and evaluation. Getting quantitative information about the experiment from the images taken has become more efficient. Visualizing the individual wells, how they change with time and how they may differ from one another has become easier. Sorting through and locating the data has become simpler. Finally, grouping different bimetallic combinations based on their synergy no longer requires any human input.