**PHY 482 Mid Semester Report**

During this semester I have been continuing my photocatalysis project in the effort to publish my data in *RSC Advances.* Previously I had measured the photonic yield of my photocatalysts and obtained the following data in Table 1:

Table 1. Old Optimal Rate and Photonic Yield of USR and NG Catalysts

|  |  |  |
| --- | --- | --- |
| Catalyst | Optimal Rate (M/min) | Photonic Yield |
| USR AR | 3.96 \* 10-7 | 39.9 % |
| USR 450 | 1.13 \* 10-6 | 114 % |
| NG AR | 3.57 \* 10-7 | 36.0 % |
| NG 450 | 9.23 \* 10-7 | 93.0 % |

However, there was an issue with these photonic yield measurements. The photonic yield should not be able to physically exceed 100%. Additionally previous literature has measured photonic yields of titania catalyst to be between 1-2% so these all seem very high.1 This is most likely due to two experimental constraints; 1) the 385 nm UV-LED was wired in a way that the entirety of the LED could not be inserted into the integrating sphere used to make these photon flux measurements; 2) measurements of the photon flux were only being measured at 385 nm. The UV-LED has a distribution of wavelengths above the band gap that also contribute to the photocatalytic reaction. To account for these issues we solved 1) by using a flat copper wiring and soldering it to the LED so that the entire LED will lay flat and can be inserted into the integrating sphere. We then solved 2) by integrating the calculated photon flux over the total distribution of wavelengths of the 385 nm LED. The updated photonic yields are presented in Table 2.

Table 2. Updated Optimal Rate and Photonic Yield of USR and NG Catalysts

|  |  |  |
| --- | --- | --- |
| Catalyst | Optimal Rate (M/min) | Photonic Yield |
| USR AR | 3.96 \* 10-7 | 1.10 % |
| USR 450 | 1.13 \* 10-6 | 3.15 % |
| NG AR | 3.57 \* 10-7 | 0.99 % |
| NG 450 | 9.23 \* 10-7 | 2.57 % |

These new measurements are physically reasonable compared to the old data set!

It is important to note that 385 nm light is in the UV region and can be damaging to the DNA in our bodies, leading to adjacent bases (thymine or cytosine) to form dimers. This can lead to cancer and other dangerous health implications. As a result, all experiments, photocatalytic reactions and photonic flux measurements, are made using a cover (cardboard box) keeping the light from irradiating on our skin/eyes. The light source is confirmed to be on not by viewing but by an ammeter with a current output.

I have tried to improve my kinetics data for my NG photocatalyst which I have presented in Figure 1.

A graph of different colored points

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Figure 1. Mass Dependence of Photocatalysts Illuminated by 385 nm LED Lamp

It can be seen in Figure 1 that the NG 450 does not follow a clear trend as compared to the USR 450. This is due to the material being very dense and hard to separate out of solution with our current centrifuge. We require a higher rpm centrifuge, however, the one we have borrowed from Karl Bishop is broken and we are currently waiting on it to be fixed to continue these experiments. This has been a challenge and has put this portion of my project on hold.

Figure 2 shows the transient absorption spectroscopy (TAS) data for our photocatalysts. This data indicates charge carrier lifetimes to increase between as received and calcined photocatalysts. The calcined photocatalysts have charge carrier lifetimes that go out to the millisecond to second timescale. This finding is of particular importance for the potential application of these materials in photocatalysis, as many photocatalytic processes are driven by reactive oxygen species that form on the millisecond timescale on TiO2 which could account for the increased photocatalytic activity.

A graph of different colored lines

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Figure 2. Mass Dependence of Photocatalysts Illuminated by 385 nm LED Lamp

References:

[1] M. Qureshi, and K. Takanabe, “Insights on Measuring and Reporting Heterogeneous Photocatalysis: Efficiency Definitions and Setup Examples,” Chem. Mater. **29**(1), 158–167 (2017).

[2] Distinctive Behavior of Photogenerated Electrons and Holes in Anatase and Rutile TiO2 Powders | The Journal of Physical Chemistry C (acs.org)

[3] Where Do Photogenerated Holes Go in Anatase:Rutile TiO2? A Transient Absorption Spectroscopy Study of Charge Transfer and Lifetime | The Journal of Physical Chemistry A (acs.org)

[4] Transient Absorption Spectroscopy of Anatase and Rutile: The Impact of Morphology and Phase on Photocatalytic Activity | The Journal of Physical Chemistry C (acs.org)

[5] Strong Transient Absorption of Trapped Holes in Anatase and Rutile TiO2 at High Laser Intensities | The Journal of Physical Chemistry C (acs.org)

[6] Ab Initio Simulation of the Absorption Spectra of Photoexcited Carriers in TiO2 Nanoparticles | The Journal of Physical Chemistry Letters (acs.org)

[7] TiO2 photocatalysis and related surface phenomena - ScienceDirect

[8] Comparing photoelectrochemical water oxidation, recombination kinetics and charge trapping in the three polymorphs of TiO2 | Scientific Reports (nature.com)