SLATT UNDERGRADUATE STUDENT FELLOWSHIP
CHECK ONE: ☐ UPDATE ☐ FINAL REPORT

SLATT SCHOLAR:	Corey Atwell
FACULTY ADVISOR:	Prashant V. Kamat
REPORT PERIOD:	Summer 2018
PROJECT TITLE:	Influence of Annealing On the Controlled Growth of $CsPbBr_3$ Nanocrystals
CONNECTION TO ND ENERGY'S RESEARCH AREAS (CHECK ALL THAT APPLY):	**(✓) Energy Conversion and Efficiency ( ) Sustainable and Secure Nuclear** **( ) Smart Storage and Distribution (✓) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels ( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS:

List your major research goals and provide a brief description of your accomplishments (1-2 sentences). Indicate the percentage completed for each goal. Please use a separate sheet to share additional details, technical results, charts, and graphics.

MAJOR RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Find energy of activation for the transition of $CsPbBr_3$ nanocrystals to bulk film	Undetermined whether a saturation curve is in effect, however a value was obtained with unknown certainty. More points were taken near the end of the summer in hope to better our understanding of the saturation.	75%
Determination of the mechanism by which the crystals grow during the transition	In the beginning we assumed that the small nanocrystals self-sacrificed to the larger in order for the larger crystals to grow. However, since there are two peaks in the photoluminescence we have become unsure.	90%
Track and measure the physical and photophysical properties of the film with time	Using Photoluminescence and SEM we were able to correlate average particle size with the change in the peak intensity of the photoluminescence.	100%

RESEARCH OUTPUT:

CATEGORY	INFORMATION
EXTERNAL PROPOSALS	N/A
EXTERNAL AWARDS	N/A
JOURNAL ARTICLES	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s) Chemical Communications, Influence of Annealing on the Controlled Growth of CsPbBr3 Nanocrystals, Rebbeca A. Scheidt, Corey Atwell, December 1st, N/A, N/A, N/A
BOOKS AND CHAPTERS	N/A
PUBLIC PRESENTATIONS, SEMINARS, LECTURES	N/A
AWARDS, PRIZES, RECOGNITIONS	N/A
INTERNAL COLLABORATIONS FOSTERED	N/A
EXTERNAL COLLABORATIONS FOSTERED	N/A
WEBSITE(S) FEATURING RESEARCH PROJECT	N/A
OTHER PRODUCTS AND SERVICES	N/A

RESEARCH EXPERIENCE:

The research I did this summer was a great opportunity for me to get involved in a real research lab. I was able to get a feel for what it would be like to work 9am-5pm in a lab and it helped me gauge how strong my passion for research was while also learning a lot of new material. I was treated as an independent researcher and was given some freedom on how to pursue the project which I very much enjoyed. All of the grad students were patient and always took the time to thoroughly explain new concepts to me. I realized that as the summer went on I began to become a more efficient researcher and my lab skills sharpened. In the last 3 weeks of my research I obtained more useful data than in the first 7. This has nothing to do with the lab or how I was taught but more to do with my lack of experience as a researcher. I learned so much and gained valuable experience, this past summer went better than my expectations.

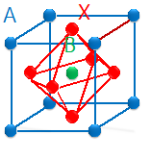
MAJOR GOALS AND ACCOMPLISHMENTS
(Additional Details, Technical Results, Charts and Graphics)

Influence of Annealing On the Controlled Growth of CsPbBr3 Nanocrystals

Corey Atwell, Rebecca A. Scheidt, and Prashant V. Kamat
Radiation Laboratory, Department of Chemical and Biomolecular Engineering, University of Notre Dame

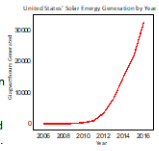
What is a perovskite

- Perovskites are cubic FCC crystals
- They have a form of $A^{2+}B^{4+}X^{2-}{}_3$
- $CsPbBr_3$ is the perovskite used in this research
- Great potential in photovoltaic devices due to its tunable bandgap
- Long charge carrier diffusion lengths.



Why are they useful?

- Solar energy production growth is exponential
- Silicon based solar cells dominate current market
- Requires extremely clean environments for construction
- Not flexible and high energy synthesis
- Perovskites are a cheaper and more manageable alternative.



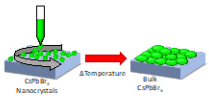
Goals

- Energy of activation for the transition of $CsPbBr_3$ nanocrystals to bulk film through annealing
- Determination of the mechanism by which the crystals grow during the transition
- Track and measure the physical and photophysical properties of the film
- Elucidate strategies to create more pristine bulk films towards solar cell applications

Method of measurement

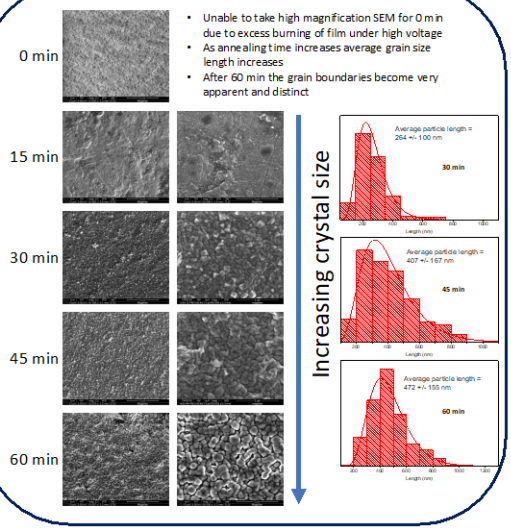
- **SEM images** to track nanocrystal diameter growth
- **Photoluminescence** to measure the nanocrystals' peak intensity (used in **calculation of activation energy** due to reproducibility among other factors)

Scheme

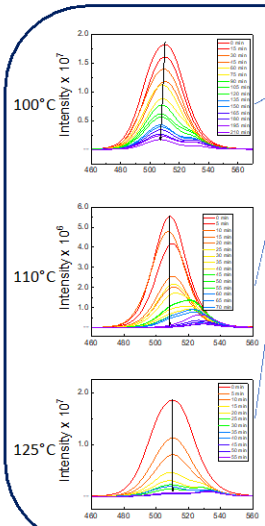


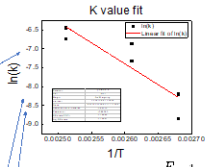
SEM Images

- Unable to take high magnification SEM for 0 min due to excess burning of film under high voltage
- As annealing time increases average grain size length increases
- After 60 min the grain boundaries become very apparent and distinct



Photoluminescence





$$\ln(k) = \ln(A) - \frac{E_a}{R}\frac{1}{T}$$

$$E_A = 92\,\frac{kJ}{mol}$$

- Increasing annealing time shows decrease in 509 nm peak
- Growth of 530 nm peak with increasing annealing time, indicating appearance of larger crystal phase
- Intensity of 509 nm peak plotted against time to find exponential decay of the intensity
- Rate of change used in Arrhenius Equation
- Energy of activation found through Arrhenius Equation

Conclusion

- Changes in physical properties were tracked over time using SEM
- Size of nanocrystals increases with annealing time until they become bulk film with defined grain boundaries
- Photoluminescence decreases with annealing time
- Change in photoluminescence tracked to find energy of activation

References

"SAS Output." Chinese Coal-fired Electricity Generation Expected to Flatten as Mix Shifts to Renewables - Today in Energy - U.S. Energy Information Administration (EIA). Accessed July 23, 2018. https://www.eia.gov/electricity/annual/html/epa_03_01_b.html.

Further Work

- Repeat experiments to improve data evaluation
- Transient absorption spectroscopy for change in charge carrier dynamics
- TCSPC for change in photoluminescence lifetime
- UV-Vis absorption to show increase in excitonic peak with longer annealing time and transition to bulk film

Here is the poster I submitted for the undergrad poster symposium. This poster contains all relevant data and graphs to my project!