SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Nathaniel Hiott
FACULTY ADVISOR:	Prashant Kamat
PROJECT PERIOD:	Summer 2022
PROJECT TITLE:	Operational Stability of the 2D/3D Interface in Metal-Halide Perovskites
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	**(x) Energy Conversion and Efficiency** **( ) Sustainable and Secure Nuclear** **( ) Smart Storage and Distribution** **(x) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels** **( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Prepare 2D/3D Films	I optimized a synthesis procedure for 2D, 3D, and films with a 2D/3D interface using spin-coating of methylammonium and lead halide solutions.	100
Heat and Irradiate 2D/3D Interface	I subjected all three film types to up to 100 C heating and visible light irradiation to induce any changes to the interface	100
Analyze Changes to the 2D/3D Interface	I observed that light and heat caused changes in the interface that indicate the 2D layer diffuses into the 3D layer. My analysis of the charge carrier lifetimes suggests that further experiments could increase our understanding of this process.	100
Synthesize 2D colloidal perovskites	I optimized a preparation procedure for single, double, and triple layer 2D colloidal lead-iodide and lead-bromide perovskites.	100
Irradiate 2D Colloidal Perovskites	By irradiating mixed-halide colloidal perovskites, I am seeking to understand the structural changes that cause pure halide forms to appear.	90

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	
EXTERNAL AWARDS RECEIVED	
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	ACS Energy Letters, How Stable Is the 2D/3D Interface of Metal Halide Perovskite under Light and Heat?, Jishnudas Chakkamalayath, Nathaniel Hiott, Prashant Kamat, Submitted October 2022, Published January 2023, Volume 8, Pages 169-171
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	American Chemical Society Spring Meeting, “Operational Stability of the 2D/3D Interface in Metal-Halide Perovskites”, March 2023, Indianapolis IN Summer Undergraduate Research Symposium, “Colloidal 2D Perovskites for Light Harvesting Applications”, July 2022, Notre Dame IN
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	
INTERNAL COLLABORATIONS FOSTERED	
EXTERNAL COLLABORATIONS FOSTERED	
WEBSITE(S) FEATURING RESEARCH PROJECT	
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models,	

curricula, instruments, education programs, outreach for ND Energy and other groups)	

RESEARCH EXPERIENCE

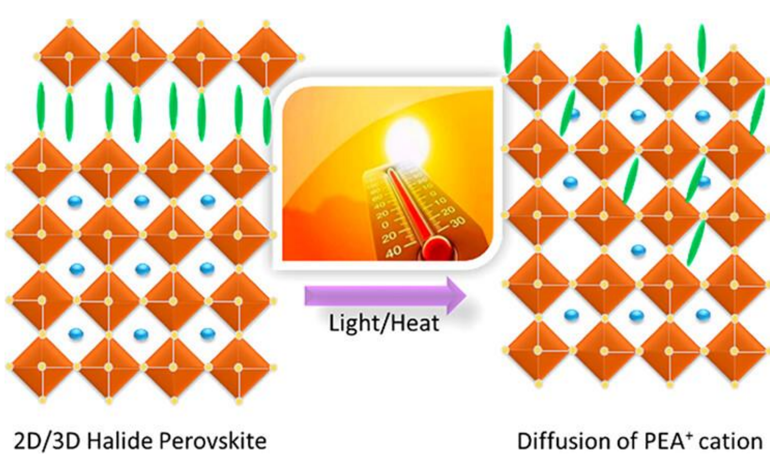
Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

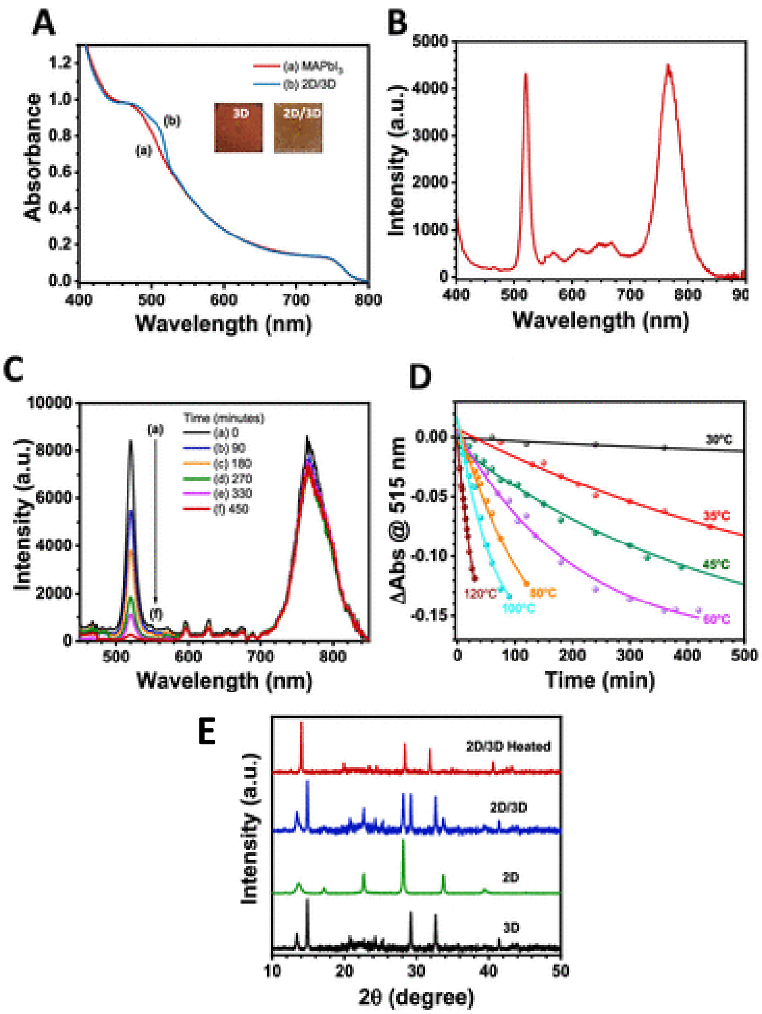
My research experience in the Kamat lab was incredibly useful for preparing me for a career in professional materials science research and for my ability to succeed in graduate school. Over the course of the summer, I gained more independence and ownership over my project as my expertise with the synthesis procedures and the UV-Vis, fluorescence, and transient absorption spectrometers grew. I was partnered with Jishnudas Chakkamalayath, a 4th year graduate student in the Kamat lab, and he was an excellent mentor in training me on the various techniques and tools necessary to complete my project. I met with Prof. Kamat every few weeks to update him on my progress and receive suggestions for additional experiments to attempt, and his support was integral to my completion of the project and publication of my results. I was treated like a part of the lab group during my research experience, with the associated expectations and responsibilities, and this experience will be invaluable to my ability to adapt to graduate level research next year. Because of this research experience, I was well equipped to apply to many top graduate schools for a materials science Ph.D..

FINAL WRITTEN REPORT

I performed my research project with Professor Kamat in the Radiation Laboratory at Notre Dame, and we are investigating a new class of light-harvesting materials called perovskites. Since perovskite research began just 10 years ago, researchers have already produced perovskite cells of efficiencies that are close to the silicon solar cells that make up most commercial solar energy. Perovskites present a promising alternative to silicon solar cells because of their potential for higher performance output and lower production costs. My research looks at addressing the stability challenges that are currently preventing this material from becoming a larger part of our solar energy landscape.

Perovskites are known to be relatively stable in a laboratory setting. However, they need to be stable in the heat and illumination conditions of an outdoor environment for applications in solar cells. My project investigated the claim that the stability of three-dimensional lead-halide perovskites could be improved by using a two-dimensional perovskite as a capping layer. In 10 weeks, I optimized a synthesis procedure for spin-coating 3D, 2D, and 3D capped with 2D perovskite films. I used absorption and emission spectroscopy to confirm the formation of 2D and 3D perovskites and to probe the film response to operational heat and light conditions. I also assisted with using transient absorption spectroscopy to investigate changes in the charge carrier lifetime of the perovskites due to thermal and light stress. I found that operational conditions cause the 2D layer to transform and diffuse within the 3D bulk, passivating defects along the way. I analyzed the samples with X-Ray diffraction to confirm the dissolution of the 2D/3D interface to a pure-3D film. These results indicate that the 2D/3D interface is unstable under operational conditions, meaning that reported stability improvements can be attributed more to the diffusion of an organic cation into the 3D layer. As a result of my findings, I published a paper in the ACS Energy Letters Journal. Another member of the lab will continue investigating the 2D/3D interface by clamping together a 2D and 3D film and heating, to determine if a more stable interface can be produced with this technique.





These graphs describe the production of a 2D/3D interface on the perovskite film and its disappearance under heat stress. (A) Depositing the 2D solution onto a 3D film causes an absorbance increase corresponding with the 2D perovskite peak (515 nm). (B) Fluorescence spectroscopy shows that the films have the emission pattern of a 3D (780 nm) and a 2D (515 nm) perovskite. (C) As the 2D/3D interface is heated, the 2D emission peak decreases while the 3D peak remains stable. (D) Higher temperatures cause quicker decreases in the 2D absorbance. (E) The 2D XRD peaks disappear from the 2D/3D film when heated