SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Seryeong Lee
FACULTY ADVISOR:	Emily Tsui
PROJECT PERIOD:	Aug 2020-December 2020
PROJECT TITLE:	
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** **( ) 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
Coding of vibrational spectroscopy	Successfully modeled spectra using Cotton's GF Matrix Method	100
Synthesize different nanomaterials and new organometallic compounds to attach to their surfaces	Synthesized CdSe quantum dots and coordinated both $(Me_3Si)_2Fe(CO)_4$ and $(Et_3Si)Co(CO)_4$ to the surface Reacted $CdSCo(CO)_4$ with triflic acid and studied the product made spectroscopically	70

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	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS RECEIVED	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s) Inorganic Chemistry, "Metal Carbonyl Functionalized CdSe Nanocrystals: Synthesis, Surface Redox, and Infrared Intensities"; Prather, Keaton; Lee, Seryeong; Tsui, Emily; Submission Date: 13 Dec 2020
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	(Event, Presentation Title, Presentation Date, Location)
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	(Purpose, Title, Date Received)
INTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
EXTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
WEBSITE(S) FEATURING RESEARCH PROJECT	(URL)
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	(Please describe each item in detail)

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?

This experience helped me learn about the culture and expectations in a synthetic inorganic chemistry lab. I learned new techniques, such as using a Schlenk line and a glove box. Lab personnel were helpful in teaching me how to be independent and adaptable to new situations. I hope to continue learning how to be a more efficient researcher and read scientific literature more critically.

FINAL WRITTEN REPORT

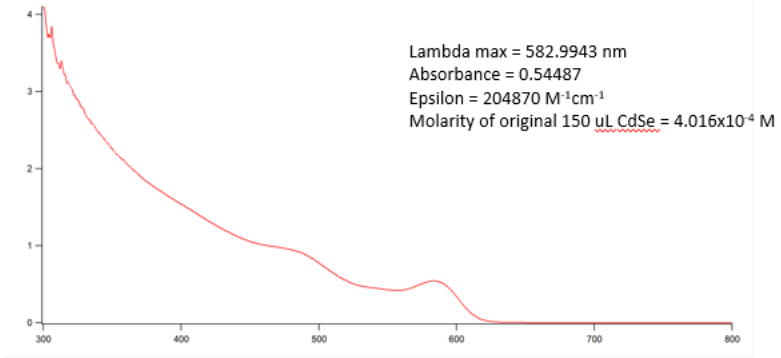
(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

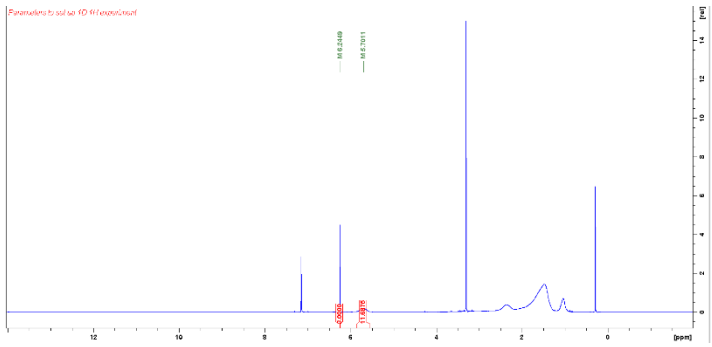
One of my project goals was to model FTIR spectra of organometallic fragments coordinated to the surfaces of semiconductor nanocrystals. This work is important in understanding the coordination geometry of individual surface sites in nanomaterials, and consequently, the understanding of optoelectronic properties of these materials in energy applications such as photocatalysis or photovoltaics. Professor Tsui referred me to a method of obtaining internal coordinates for a vibrating molecule called the GF Matrix method. This method uses a G matrix (the linear internal coordinates) and a F matrix (the harmonic potential energy) to obtain the relationship between the vibrational frequency, the group dipole moment, and the intensities.

The compound we are interested in has a symmetry of C_{3v}. The SALCs of this molecule produced a GF matrix that looks as follows:

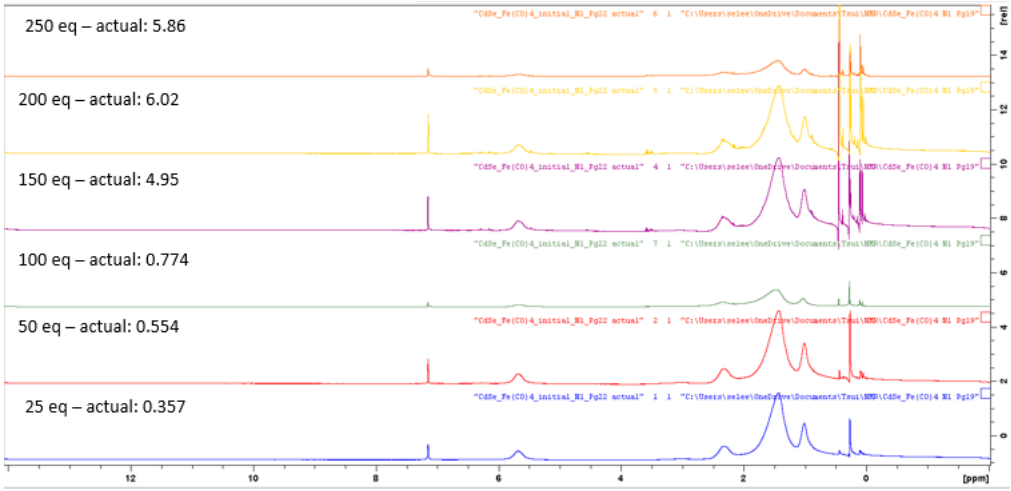
$k_1\mu - \lambda$	$\sqrt{3}k_c\mu$	0	0
$\sqrt{3}k_c\mu$	$\mu(k_2+2k_c') - \lambda$	0	0
0	0	$\mu(k_2-k_c') - \lambda$	0
0	0	0	$\mu(k_2-k_c') - \lambda$

Moreover, upon my return to in-person instruction at Notre Dame, I began work on synthesizing different nanomaterials and new organometallic compounds to attach to their surfaces as well as studying the surface chemistry at these quantum dots spectroscopically. I synthesized the CdSe quantum dots and took a UV-Vis and ^{1}H-NMR of the dots.





We hypothesized that additional surface Cd^{2+} sites could be identified at higher equivalents of $(Me_3Si)_2Fe(CO)_4$ per nanocrystal. I used varying equivalents of $(Me_3Si)_2Fe(CO)_4$ as a reagent in functionalizing CdSe nanocrystal surfaces with iron tetracarbonyl fragments. However, I kept running into trouble getting the exact equivalents I wanted on the nanocrystal surfaces. The following stacked ^{1}H NMR spectra are of the varying equivalents.



I realized eventually that my calculations were incorrect, which is why I kept adding the incorrect equivalents. Through this experience, I learned the importance of keeping an organized lab journal to help me save time and effort in the future when I review the work I did.