

SLATT UNDERGRADUATE RESEARCH FELLOWSHIP FINAL REPORT

SCHOLAR NAME:	Laura Manukyan
FACULTY ADVISOR:	Professor Emily Tsui
PROJECT PERIOD:	May 24 – Ongoing
PROJECT TITLE:	Organometallic Functionalization of ZnO Nanocrystals
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	<input checked="" type="checkbox"/> Energy Conversion and Efficiency <input type="checkbox"/> Sustainable and Secure Nuclear <input type="checkbox"/> Smart Storage and Distribution <input type="checkbox"/> Transformation Solar <input type="checkbox"/> Sustainable Bio/Fossil Fuels <input type="checkbox"/> 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
Synthesizing ZnO nanocrystals	The colloidal nanocrystalline ZnO were successfully synthesized and characterized by X-ray powder diffraction as well as UV-vis spectroscopy. Nanocrystals were also treated with TOPO to increase solubility in nonpolar solvents such as toluene.	100%
Synthesizing precursor	The organometallic precursor $(\text{NH}_3)_3\text{ZnFe}(\text{CO})_4$ was also successfully synthesized and characterized with IR spectroscopy.	100%
Functionalizing nanocrystals	Efforts are underway to functionalize the ZnO nanocrystalline with the organometallic fragments in different solutions.	50%

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)
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) Summer Undergraduate Research Symposium, Organometallic Functionalization of ZnO Nanocrystals , July 20 th , 2022, University of Notre Dame
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

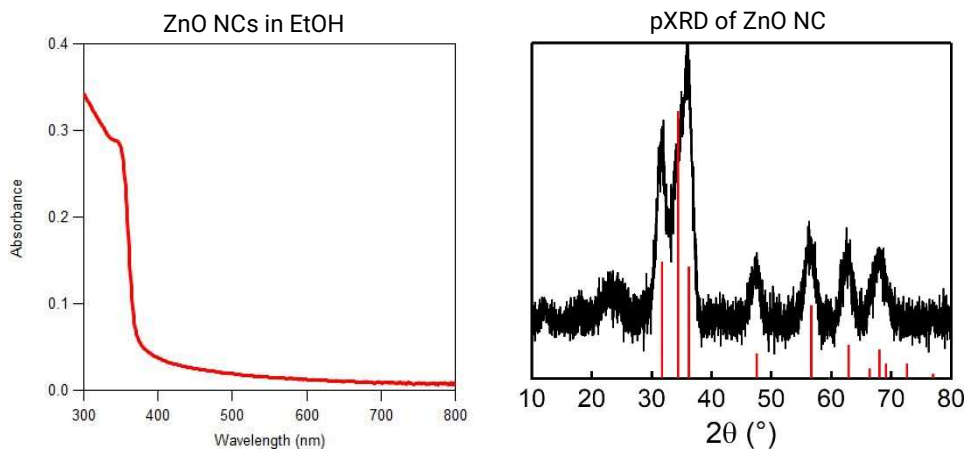
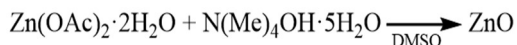
Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

This research opportunity enabled me to become a more efficient researcher and greatly enhanced my lab skills. While I learned many new concepts and gained valuable experience doing research during the semester, being able to work 9am-5pm allowed me to accelerate my work as well as gain some independence in the lab, in turn, increasing my knowledge and skills in the field. The graduate students and P.I. were always patient and willing to thoroughly explain any concepts I had trouble with.

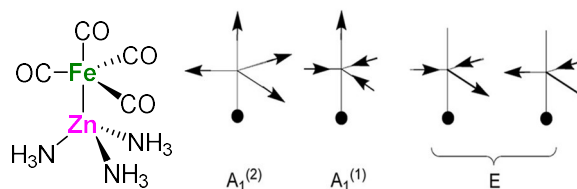
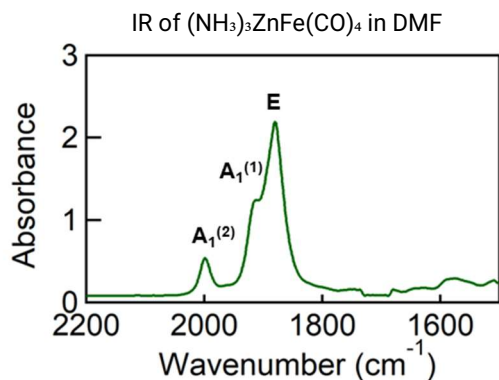
FINAL WRITTEN REPORT

The surface chemistry of colloidal semiconductor nanocrystals is critical to applications such as large-scale solution processing as well as for tunable optoelectronic properties. However, they remain poorly understood. Our group has developed CdSe, PbS, and ZnS and functionalized them with metal carbonyl moieties as surface spectroscopic reporters. This study probes the question whether similar methods can be extended onto metal oxide materials, specifically ZnO. Oxides are much more ionic and chemically different but are of interest for transfer of electrodes and electrochromics. In this research project, I was able to synthesize both the ZnO nanocrystals as well as the organometallic precursor $(\text{NH}_3)_3\text{Fe}(\text{CO})_4$.

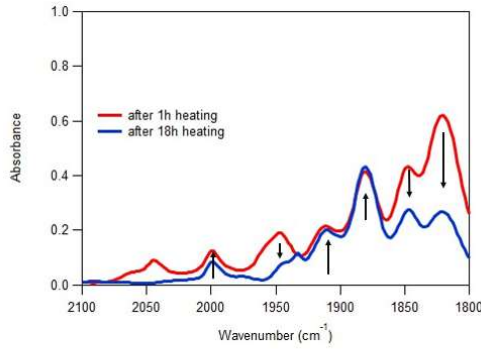
The colloidal nanocrystalline ZnO were characterized by X-ray powder diffraction as well as UV-vis spectroscopy. With pXRD data, the estimated size of a ZnO crystal was determined to be $\sim 6.5 \text{ nm}$. pXRD of the nanocrystalline match literature data indicated with the red lines.



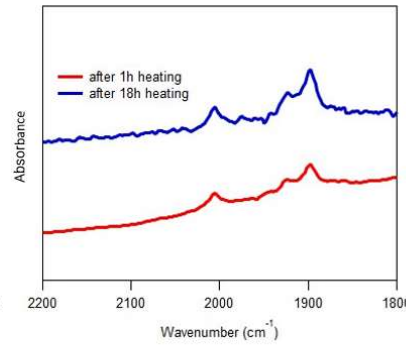
The metal carbonyl $(\text{NH}_3)_3\text{Fe}(\text{CO})_4$ was also synthesized and later characterized with IR spectroscopy.



Currently, efforts are underway to functionalize the ZnO nanocrystalline with the organometallic fragments in different solutions.

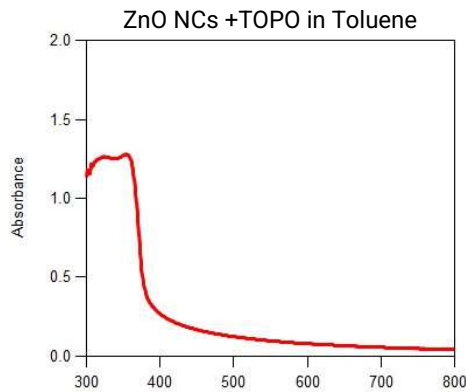
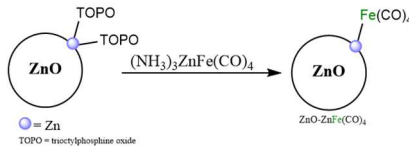


IR of ZnO-ZnFe(CO)₄ in DMF heating aliquots



IR of ZnO-ZnFe(CO)₄ in Toluene heating aliquots

In order to attach these IR-active metal carbonyl fragments to the nanocrystals, I have treated ZnO with trioctylphosphine oxide (TOPO) for stability and resuspended in a nonpolar solvents such as toluene in hopes of successfully synthesizing ZnO-ZnFe(CO)₄.



The synthesized precursor and nanocrystals were later tested with ZnS and (NH₃)₂CdFe(CO)₄ respectively.

