

2018 GSRAC Visit Summary

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Single-crystal X-ray diffraction of Ln-containing coordination complexes of interest for single-molecule magnetism

This past summer, I was privileged to conduct research at NSF's ChemMatCARS as a recipient of the 2018 Graduate Student Research Award (GSRAC). This was my second visit to this sector of the Advanced Photon Source (APS) to conduct x-ray diffraction experiments. Last summer, my Professor Dr. Skye Fortier and myself made a 2-day trip to ChemMatCARS to run experiments as participants in another program offered by ChemMatCARS, FaSTRAC. It was during that visit that I learned about the GSRAC and expressed my interest in the program. In January 2018 I was notified that I had been accepted to the 2018 GSRAC program and begin planning for my visit in the month of July.

My major research project coming into the GSRAC program was to conduct single crystal x-ray diffraction experiments on a series of Ln containing coordination complexes. These complexes have shown some interesting magnetic properties, including single molecule magnetism, and it was important for me to determine, with high accuracy, the chemical structure of these materials. Unfortunately, due to inherent disorder in the structure, and the unusually small crystal size, good data was not obtained at my home institution. The instrumentation and the x-ray source available at ChemMatCARs are ideal for overcoming these issues.

Dr. Yu-Sheng Chen, beamline scientist at NSF's ChemMatCARS was my host at the lab and helped me devise, prepare and execute experiments during my stay. In addition to Dr. Chen, Suyin Grass Wang, Jr. Beamline Scientist at ChemMatCARS, was very helpful in instructing me on use of the diffractometer and some best practices for determining the quality of data from the experiment. With both Yu-Sheng and Grass's help, I was instructed on the use of specialized crystallographic techniques, like low-temperature (liquid helium) crystallography and the use of laser for photocrystallography – both of which are the facilities at ChemMatCARS is uniquely equipped to do. After a brief training on the instrument, I was able to pick, mount and execute experiments on single crystals that I had for analysis. Using the software available at Sector 15ID, and given the quality of the data I collected, I was able to solve high resolution structures during my visit which are publication ready.

I came to the APS this summer with the intention of collecting data for my samples, I accomplished this and much more. I encountered several other students and professors who were also involved in summer research programs supported by ChemMatCARS, who were conducting experiments on materials quite different than mine. From them, I was able to learn much about different approaches to collecting and analyzing data from single crystal x-ray diffraction experiments. Additionally, I had many delightful conversations with them about their science, universities and their various career experiences and future goals. Already, I am seeing some of the work from this visit making an impact.

Some of the structures which came from data I collected in my July 2018 visit are already included in a prepared manuscript which will be sent to a peer-reviewed journal in the coming weeks.

I feel that beyond the good data I gathered during my GSRAC visit, I have gained a broader perspective on what career paths are available to individuals in the science field. After my visit, I now see that careers at national laboratory facilities can be just as creatively rewarding experiences as those at academic research institutions. In the future, I will use my experiences at with ChemMatCARS to inform my career path after completion of my current graduate work.

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