JOURNAL OF CHEMICAL EDUCATION

Communication

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Teaching Outside the Classroom: Field Trips in Crystallography Education for Chemistry Students

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Supporting Information

ABSTRACT: Field trips are an underutilized opportunity to provide depth and richness in college-level chemistry courses. The authors have found that a field trip, such as to the Advanced Photon Source (APS) at Argonne National Lab, greatly enhances the impact of a course in X-ray crystallography. Students who attend this field trip report that it is a highlight of the course and develop a lasting interest in the science of X-ray crystallography as a result. We report on our experience in planning these trips, advise on best practices, and demonstrate the positive impact of a field trip on student learning and engagement.

KEYWORDS: *Upper-Division Undergraduate, Graduate Education/Research, Collaborative/Cooperative Learning, Hands-On Learning/Manipulatives, Problem Solving/Decision Making, Crystals/Crystallography, X-ray Crystallography, Inorganic Chemistry, Curriculum*

THE PURPOSE AND BENEFITS OF A FIELD TRIP

College education in chemistry, as well as across the sciences more broadly, generally recognizes the value of practical experience in enhancing the theoretical material that is commonly taught in lecture.[1] This experience is most often earned in laboratory experiments that are designed either to teach specific techniques and concepts or else allow students to recapitulate known research and provide their own analysis of the results.[2−5] Many science departments further extend the opportunity for experiential learning in their curricula by including field trips to sites off the university grounds; however, such experience is almost entirely lacking in undergraduate chemistry education.[6−8] This represents a missed opportunity to expand students' appreciation of chemistry's fundamental utility and of how it may be applied to solving real world problems.[6] Accordingly, we wish to share our experiences in designing and conducting field trips as part of an upper-level undergraduate and graduate level course in X-ray crystallography, with the intention of encouraging and enabling other educators to include field trips in their course curricula.

Our course in X-ray crystallography[9] provides students with an understanding of the fundamental physics underlying X-ray crystallography through traditional lectures, and also allows them to collect and evaluate single crystal diffraction data in a laboratory section. The course also includes a case study component that helps the students learn to think critically about the limits and correct interpretation of single crystal data.[10] We find that the practical experience derived from the laboratory and case study components is particularly useful in turning the students from chemists with an appreciation of single crystal X-ray diffraction into budding crystallographers in their own right. Adding a field trip into the course then allows the students to further develop by exposing them to techniques that are not available in-house, thereby expanding their awareness of the opportunities that advanced X-ray crystallography offers and enabling them to employ advanced X-ray experiments in their own work (*vide infra*).

Planning a Field Trip

Choosing a Destination. The primary consideration when designing an effective field trip is the equipment that is available in-house. In a college that lacks access to single crystal X-ray diffractometers, students may be able to learn the theory of X-ray diffraction and work with previously collected data, but may not gain a full appreciation of how that data was collected. A trip to a nearby college with access to single crystal X-ray diffractometers may then fill in that gap. Alternatively, if the students have already been able to observe the standard in-house equipment that many colleges possess, a trip to an accessible national lab or other facility with access to specialized X-ray techniques may then provide the greatest benefit (Table 1). An additional consideration in choosing a destination may be the available funding for the trip, as travel/transportation costs are likely the most cost-intensive aspect of such a field trip. While financial resources differ from school to school, we suggest two possible options for instructors to consider: first,

Received: February 8, 2016
Revised: June 7, 2016

DOI: 10.1021/acs.jchemed.6b00073
J. Chem. Educ. XXXX, XXX, XXX−XXX

Table 1. Selected National Laboratories with Advanced Crystallography Service in the USA[a]

laboratory	state	light source name	light source type
Lawrence Berkeley National Laboratory	California	The Advanced Light Source	synchrotron, 3rd generation
Argonne National Laboratory	Illinois	The Advanced Photon Source	synchrotron, 3rd generation
SLAC National Accelerator Laboratory	California	Stanford Synchrotron Radiation Lightsource	synchrotron, 3rd generation
SLAC National Accelerator Laboratory	California	Linac Coherent Light Source	synchrotron, 4th generation
Brookhaven National Laboratory	New York	National Synchrotron Light Source II	synchrotron, 3rd generation
Oak Ridge National Laboratory	Tennessee	Spallation Neutron Source	neutron

[a]A more complete list of advanced light sources that may be suitable for crystallography field trips may be found at http://www.lightsources.org/light-source-facility-information.

with advance planning it may be possible to incorporate travel costs into the course budget; second, many schools offer grants to students for research-related travel, and in a small class it may be feasible for students to apply for such grants to cover their travel expenses.

In our case, we chose to design our trip around research that our X-ray laboratory already performs and traveled to Argonne National Lab to visit ChemMatCARS, The University of Chicago, and the Advanced Photon Source (APS). The guidelines described herein were developed based on our experiences in planning our course's field trip over the past several years, and should be generally useful to educators in the field who are interested in using field trips for their own course. In addition to dedicated X-ray crystallography courses, other chemistry courses that incorporate X-ray diffraction (such as advanced inorganic and physical chemistry courses) may find such a trip to be valuable.

The APS at Argonne National Lab is a synchrotron and one of the world's most brilliant and stable sources of X-ray radiation (Figure 1).[11] The unique capabilities that become

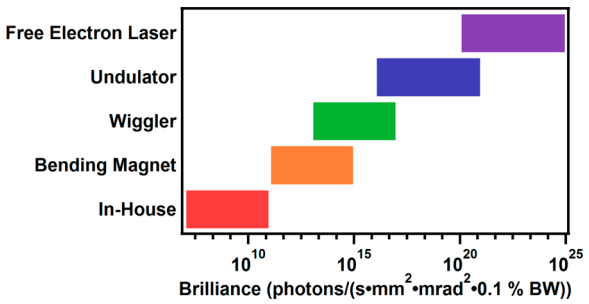

Figure 1. Approximate average brilliance commonly obtained from a variety of X-ray sources. The range of expected values is indicated in color. All sources except in the in-house source represent technologies that are only available at a synchrotron. Data for the figure were obtained from references14 and15.

accessible with such a brilliant beam attract top researchers from academic, government, and industrial institutions around the world. Research at the APS includes not just the determination of small molecule and macromolecular structures but also investigations into areas like the dynamic response of molecules and materials to external stimuli like light or pressure, the effects of soil composition and structure of microbe growth and how this informs effective agricultural practice, and the behavior of uranium dioxide samples under conditions relevant to nuclear fuel storage and bioremediation.[11,12] ChemMatCARS is one of the sectors of the APS and specializes in an array of advanced crystallographic and liquid interface scattering techniques.[13] Each of these investigations is beyond the obvious extensions of the material commonly taught in a standard X-ray diffraction class, and each offers a new opportunity to show students what is possible when the techniques they have begun to learn are pushed to the cutting edge.

Format and Schedule. Field trips have been found to be most effective when they go beyond the simple idea of a lab tour.[8] Accordingly, the trip should include both an active research component and a seminar and tour component to maximize the exposure of the students to new techniques and capture their attention for as long as possible. The research component that is integrated into the field trip not only helps our institution's research groups to complete their own projects and achieve fruitful results,[16−18] but also engages students in a study that is designed to facilitate the students' active involvement. The level of student engagement is substantially enhanced when they can actively participate in solving a problem, and by following the experiment from beginning to end they obtain a deeper understanding of the material than what they might gain from a lecture or tour. Any downtime in the experiment provides the perfect opportunity for tours, lectures, and demos by different staff scientists at the field trip site, with the goal of complementing the relative depth obtained from the focused experimental component with an appreciation of the breadth of experiments that are possible (Table 2 and Figure S1).

Table 2. Example Seminar Titles

1.	Introduction to X-ray Sources
2	Application of the Synchrotron X-ray Source
3	Design and Set Up for Photocrystallography Experiment
4.	Experimental Aspects of Charge Density Studies
5.	High-Pressure Crystallography

With this type of schedule in mind, the timing of the field trip becomes quite important since the students must be well versed in the basic collection and modeling of X-ray diffraction data prior to the field trip. This timing is also subject to the scheduling requirements of the students' other courses, in that it cannot overlap with any of their mandatory activities. Spring break, being both late in the semester and a time when we expect the students to be available, is one of the few times of the year that fulfill both of these requirements and has been our constant choice for field trip timing. Should this time not prove feasible then a weekend trip may be an acceptable alternative, though the students' opportunity to interact with staff scientists at the field trip site may be reduced by the absence of weekday working hours.

From the early stages of field trip planning, it is critical to work closely with staff members at the field trip facility since they can provide advice about any formal application process

DOI: 10.1021/acs.jchemed.6b00073
J. Chem. Educ. XXXX, XXX, XXX−XXX

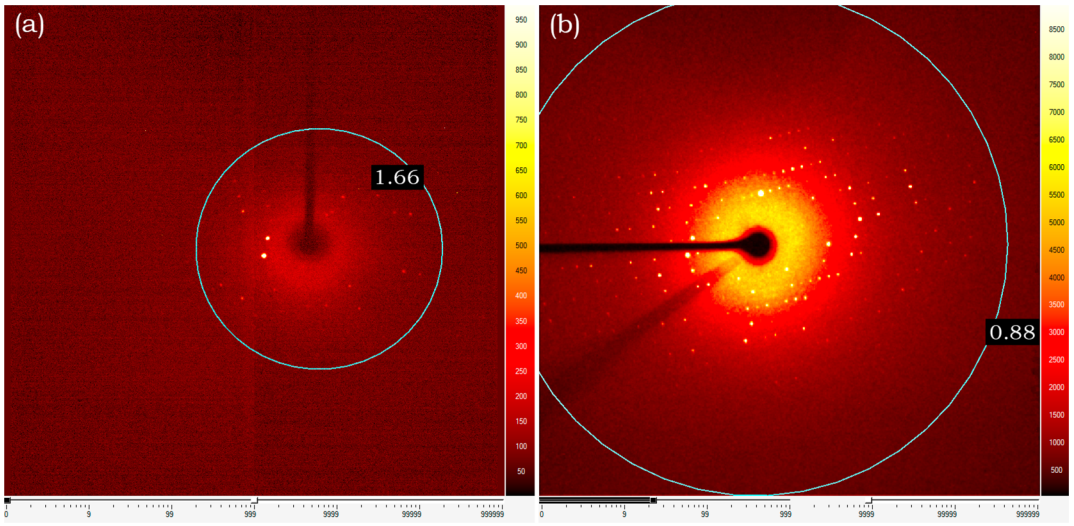

Figure 2. A comparison of two frames from crystallography experiments for the same micron-sized crystal conducted (a) in-house using a 120 s exposure time on a D8 VENTURE single-crystal diffractometer equipped with a PHOTON-100 CMOS detector and high brilliance IμS Mo X-ray source (wavelength of 0.71073 Å) and (b) at ChemMatCARS using a 0.5 s exposure time on a APEX II CCD detector and X-rays from the APS (wavelength of 0.40651 Å). The white circle and corresponding number in each frame provide an approximate representation of the resolution limit (in Å) of the data available from that frame, indicating the superior resolution obtained from data collected at a synchrotron source. Data are from E. N. Jacobsen.

that is necessary for the field trip and will often act as hosts during the field trip. A trip to the APS, for example, requires one to successfully apply for access to a segment of beamline time. This process involves writing a good research proposal that justifies use of the time-limited synchrotron radiation for the period required by the research component of the trip, and must be started months in advance in order to complete all steps of the administrative cycle before the field trip begins. Early contact with a staff scientist, then, is crucial in quickly learning about the application process, the time and effort it entails, and what is required from a successful research proposal. Each of the national laboratories listed in Table 1 has information available on their websites to guide users through the proposal writing and submission process, including information specifically for first-time users.

Once the timeline of the trip is established, the process of filling out the trip schedule begins, with a focus on allowing ample time for both the experimental and seminar components of the trip. The experimental part of our field trips has usually focused on microcrystallography studies at ChemMatCARS, and we have found that including the students in these experiments does not introduce additional planning requirements beyond those that are fundamental to the experiment itself. The microcrystallography component is particularly advantageous since the short experiment time (Figure 2), often less than 1 h per sample, allows each student to conduct at least one full experiment on their own and then model the results using skills already learned in the course. The seminar component requires considerably more work: this is again where a positive relationship with the staff at the field trip destination can be helpful, since they can readily suggest the scientists who might be most willing to present their work to students and provide introductions between the field trip planners and the proposed presenters. This part of the planning is made much easier if the institution being visited has, like Argonne,[19] an educational component of its mission that encourages its staff to engage in teaching opportunities.

Safety and Travel Considerations. Finally, with the trip scheduled and planned we begin preparing the students to access the field trip site. All laboratories utilizing X-ray radiation present some hazards and the students must undergo training that prepares them to behave safely in the field trip's environment.[20,21] At national laboratories like Argonne this training is often a prerequisite to site access and must be completed by the students in advance of the field trip. We also make ourselves aware of any additional access requirements and help the students fulfill them, paying particular attention to international students who may be subject to stricter requirements than their American peers. Additionally, there are legal implications to taking students off site and it is important that students sign an appropriate release form to indicate their informed consent to the trip and any hazards that it may present.[22]

Post-Trip Activities. In order to enhance the lasting benefits of the field trip, as well as to spread the benefits of the field trip to any students in the class who were unable to attend, we require those students who attended the field trip to make a short presentation about one of the techniques learned.[7] Doing this gives the students the opportunity to review and further improve their familiarity with the ideas and techniques that they were exposed to. We also ask students to fill out an evaluation form (Figure S2) so that we can incorporate their feedback to improve future field trips.

IMPACT

The benefits of introducing the students to an environment that constantly puts X-ray techniques to practical use are immediately obvious. Students who attend the trip have the opportunity to network with their hosts (e.g., the staff scientists at the APS) and maintain these connections as valuable resources long after the course is done. These students are typically keen to take advantage of the opportunities that they now know are available, and often submit their own research proposals to apply for beam time and use the facility for their own research projects.[23−29] Written feedback from the students

DOI: 10.1021/acs.jchemed.6b00073
J. Chem. Educ. XXXX, XXX, XXX−XXX

(*vide infra*) paints a remarkable picture of the impact that the field trip has had and underscores the potential contribution of fields trips to education in chemistry

We also find that there are distinctly human benefits to our field trip. Our students, by the very nature of the trip, are obliged to spend about 50 or 60 hours in close proximity, discussion, and collaboration and we see friendships being formed or strengthened as a result. The students themselves recognize this, and this less tangible course outcome may prove just as valuable to them over the long-term.

Testimonials

Former student participants have been very enthusiastic in their support and evaluation of the trip. An excerpt of reviews from former participants may be found below, and the full text is available in the Supporting Information.

> *"There were a few parts of this course that were my favorite and that I will remember for a long time. The first was our trip to APS··· I was fortunate to be able to have tours of the Center for Nanoscale Materials and ChemMatCars··· as well as hearing some lectures··· and going around the beamline and reading posters from all the other research groups that work at APS··· It was really interesting to learn about lots of other applications of the synchrotron source··· It will be awesome that I can apply such techniques into my research one day."*

[Casey Brodsky, a first-year graduate student in 2015, currently still a graduate student at Harvard University]

> *"That trip was more than I could have hoped for out of an academic class··· teaching me an incredible amount about advanced crystallographic techniques··· this trip was incredibly valuable for my education as a crystallographer and was an unparalleled opportunity to forge close friendships with certain members of the class···"*

[Matt Condakes, a junior undergraduate in 2013, currently a graduate student at the University of California, Berkeley]

> *"I learned more about what other fields were doing with X-ray experiments as the entire facility was littered with posters and various groups all utilizing the synchrotron source··· we got to interact with the synchrotron itself, setting up samples and seeing the power that the machine had for determining crystal structure of complex molecules. This experience was truly great and further encouraged me in my path to be a chemist."*

[Doug Evans, a senior undergraduate in 2015, currently a graduate student at Texas A&M University]

> *"The excursion was an exceptional opportunity to meet and make friends with a number of other students and scientists at different stages of their career and life··· I had many chances to learn from older students, not only about crystallography, but about organic chemistry, biology, society, and popular culture··· Another aspect of this trip that I found to be extremely rewarding was the exposure to state-of-the-art technologies and the frontiers of research in crystallography and spectroscopy··· these experiences have had a significant impact on my own research interests and inspired me to explore new projects in physical and analytical chemistry··· I credit this experience in particular with reigniting much of my interest in chemistry."*

[Richard Liu, a sophomore undergraduate in 2013, currently a graduate student at the Massachusetts Institute of Technology]

CONCLUSION

We have found that a field trip is an invaluable addition to the learning experience that a crystallography course can offer. Though field trips are rarely used for teaching chemistry at the college level, they deliver many opportunities that are difficult to replicate in a lecture hall or teaching lab. The students see real world applications of their learning, including applications far beyond simple solid-state structure determination. Consequently, they are made aware of the opportunities that the field presents and may be drawn to work in one of these areas. They are also more inclined to look to advanced crystallography techniques to solve problems that arise in their own research and will have formed contacts whom they may consult to determine if and how the techniques that they saw can deliver answers to their questions.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.6b00073.

> The full text for the testimonials presented here, a representative schedule, and example evaluation form (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

We wish to acknowledge and thank Mati Meron, Kathleen Carrado Gregar, Rick L. Stevens, Julie A. Smagacz, Rosemarie Wilton, Peter J. Chupas, Saul H. Lapidus at the APS, Argonne National Lab, who have helped organize the APS tours. We thank the Teaching Fellows and the students of Chemistry 255, as well as Allen Aloise, Theodore Betley, Eric Jacobsen, Elizabeth A. Lennox, and Gregory Tucci at Harvard for their support in helping us develop and improve the field trip design for our class. B.J.M. thanks the Natural Sciences and Engineering Research Council of Canada (NSERC) for financial support. M.G.C. thanks the DOE SCGF and the Dreyfus Foundation for graduate and postdoctoral fellowship support, respectively. ChemMatCARS Sector 15 is principally supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1346572. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

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DOI: 10.1021/acs.jchemed.6b00073
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