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Supporting information for article:

From the source: Student-centred guest lecturing in a chemical crystallography class

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Table S1 Example of beam time proposals that students submitted for their own research projects.

Title for example of beam time proposal	Beam line
1) Application of Anomalous X-ray Scattering to Zinc-Nickel Trinuclear Clusters 2) Direct Observation of Solid-State Halogen Elimination by Time-Resolved Photocrystallography 3) Effect of Complex Geometry on Halogen Photoelimination Chemistry 4) Multiwavelength Anomalous Dispersion Experiments for the Determination of Oxidation States in Mixed-Valence Clusters 5) Structure Determination of Bioactive Organic Samples Using 'Crystalline Sponge' Method 6) X-ray Determination of Molecular Structure on Microcrystalline Samples	ChemMatCARS, The University of Chicago, and the Advanced Photon Source[†]
1) Determination of Metal Occupancy in Bimetallic Trinuclear Clusters Using Neutron Diffraction 2) Hydrogen Bridged Ni dimeric Complexes for HX splitting	Spallation Neutron Source, Oak Ridge National Laboratory[‡]

[†] The measurements carried out at ChemMatCARS Sector 15 were 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.

[‡] The measurements carried out at the Spallation Neutron Source were sponsored by the Division of Scientific User Facilities, Office of Basic Energy Sciences, U.S. DOE, under contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.

Guest Lecturing from Prof. Philip Coppens	
April 22, 2015	
20:00	Arrive in Boston Logan Airport
April 23, 2015	
9:30	Meet at lobby, Sheraton Commander Hotel
10:00-10:25	X-ray Lab tour
10:30-11:30	Meet with Prof. Daniel Nocera's group
11:45-13:15	Lunch at Faculty Club
13:30-13:55	Meet with Prof. Theodore Betley's group
14:00-15:30	Lecture
15:45-17:15	Meet with students
17:30	Taxis pick up to Boston Logan Airport†

† Prof. Coppens had to get back Buffalo for his own class on Friday (April 24) morning.

Figure S1 An example of schedule for guest lecturing from Prof. Philip Coppens.

Feedback for *Neutron Diffraction Hands-on Workshop*

1. Why did you take the *Neutron Diffraction Hands-on Workshop*?

2. Please name the primary things you have learned from the *Hands-on Workshop* (max. of 3).

3. Please rate how much you learned about how *Neutron Diffraction* may help your research (1 = not much; 5 = very much), and explain.

1	2	3	4	5	not applicable

4. Would you recommend we continue similar *Guest Lecturing* in the future? How could the *Guest Lecturing* be improved?

Figure S2 An example of feedback form for hands-on workshop during the guest lecturing from Dr. Xiaoping Wang.

Customized Question Sets in Course's Evaluation Form

1. Rate the effectiveness of the course in stimulating your interest in crystallography, and explain.

unsatisfactory	fair	good	very good	excellent	not applicable

2. Rate how much you learned in Chem255 (1 = not much; 5 = very much), and explain.

1	2	3	4	5	not applicable

3. We had three invited lectures: Prof. Bruce Foxman -- "Single-Crystal Reactions and Phase Transitions: Methods, Solutions and Puzzles"; Prof. Rachelle Gaudet -- "Data collection and phasing for macromolecular structure determination"; Prof. Anatoliy Volkov -- "Introduction to the X-ray Charge Density Modelling" this spring. Please comment on these guest lectures.

Figure S3 An example of customized question sets that incorporated to course's evaluation form.

Full text of testimonials:

From Kevin Anderton, a first-year graduate student from Prof. Theodore Betley's group in 2017, currently still a graduate student at Harvard University:

> *"Entering our chemical crystallography course with a basic appreciation from my undergraduate education of some simple aspects of crystallography for obtaining structural models of new molecules, my expectation was that I would simply learn more details about the principles and practice of this topic. However, I ended up learning much more, and the lectures by guest speakers were a key part of this. For example, the visit by Xiaoping Wang from the Spallation Neutron Source at Oak Ridge National Lab in 2017 highlighted for me the differences between X-ray and neutron diffraction and the unique experiments enabled by the latter. The guest lecture provided a great opportunity to hear a beamline scientist's perspective on their own field and to ask questions about experimental capabilities, and the workshop introduced us to the basics of the data processing for a simple experiment and emphasized the differences in data processing as compared to a standard X-ray experiment. This inspired me to read further into the literature and learn more about other advanced neutron techniques that could be very useful for my research. As a result of this experience, I am now planning to apply for neutron beam time, and the guest lecture program played a key role in highlighting the usefulness of this advanced technique for me."*

From Michael G. Campbell, a former student from Prof. Tobias Ritter's group, currently an Assistant Professor of Chemistry at Barnard College:

> *"I was involved with Chem255 twice, first as a student auditor, and then as a Teaching Fellow. During these two years, I had the opportunity to see guest lectures from Bruce Foxman, Scott Speakman, Yu-Sheng Chen, and Anatoliy Volkov. I found each of these lectures to be valuable additions to the class, and really great opportunities to learn more about advanced techniques that expanded on the foundational course material. As a student and researcher-in-training, it's exciting to see a direct connection between something you're learning in class, and research being done by leaders in the field. It definitely made me and the other students in the class more engaged, and eager to think about how to use various X-ray techniques for our own research.*
>
> *The knowledge I gained from some of the guest lectures ended up having a direct impact on my research. Before Scott Speakman's guest lecture, I didn't have any exposure to PXRD or thin-film analysis with X-rays; but I ended up using these*

techniques heavily in my post-doctoral research, in which I was fabricating and characterizing devices made with thin films of metal–organic frameworks (MOFs). It was really nice to have a base knowledge of these characterization methods, which enabled me to more easily address new research challenges. As a graduate student, I also collected low-temperature diffraction data on microcrystalline samples using synchrotron radiation at APS, with help from our class' guest lecturer Yu-Sheng Chen. Without the opportunity to learn about these techniques, and to meet the guest lecturers and make valuable connections, I wouldn't have been able to pursue these kinds of directions in my research. And now, at the beginning of my independent research career, I am grateful to have a working knowledge of advanced X-ray techniques that I gained from the guest lectures in Chem255."

From Harbing Lou, a former graduate student from Prof. Roy Gordon's group, currently working at T-Mobile Inc.:

"I have benefited a lot from the guest lectures organized in Chem255. Shao-Liang had created this great tradition to invite a variety of experts from both academic and industrial institutions. The broad scope of X-ray crystallography opened by guest lecture series had changed my thesis direction.

Since our department purchased a new 2D XRD system, Shao-Liang invited one of its inventors, Dr. Bo He, as the guest speaker. Dr. He had introduced the philosophy of this novel technology when he designed it. This is the knowledge that could never be shared in any of the publications. Moreover, the following conversations with Dr. He had led to a series important experiments that supported my main findings in my thesis.

In 2014, Shao-Liang learned that our group members are interested in advanced thin film X-ray analysis. Thus he invited Dr. Scott Speakman, a distinguished thin film X-ray expert in both academia and industry, as the guest speaker. Dr. Speakman not only provided an insightful introduction to the characterization technology but also shared a lot of valuable personal experience, which I had applied to my own studies."

From Brian J. Malbrecht, a former graduate student from Prof. Theodore Betley's group, currently working at Dow Chemical Company:

"As an inorganic chemist, X-ray crystallography is a fundamentally necessary tool for my research. In particular, the chemical structures of the small, paramagnetic molecules that researchers in my field routinely prepare are almost impossible to characterize in the absence of single crystal X-ray diffraction experiments. Fortunately, the use of X-ray crystallography as a structural characterization technique is widespread. Software that facilitates processing diffraction data and producing an atomic model from that data is accessible and generally accompanied by good documentation. As a result, basic X-ray crystallography experiments that allow the user to prepare structural models are highly accessible and can be independently conducted by users who are not experts in the field.

By contrast, this is not true for advanced X-ray crystallography techniques, such as charge density analysis. Software tools and documentation that enable and direct these experiments are generally less approachable, and the barriers to understanding the theory and proper execution of these techniques are such that most novices will not choose to attempt them. In this situation, one of the best ways for a novice to learn how to use these techniques is through workshops with an expert in the field. The expert can rapidly review the theory necessary to understand how the technique works, suggest a data collection strategy, and direct first-time users to the appropriate software for working up the data. Given enough time, the expert can even walk new users through a guided work-up of previously collected data. Moreover, the workshop setting provides distinct advantages to the expert, who will experience a significantly reduced time burden by training multiple users at one time."

From David Powers, a former post-doctoral fellow from Prof. Daniel Nocera's group, currently an Assistant Professor in the Department of Chemistry at Texas A&M University:

"Not only did guest lectures during the graduate crystallography course significantly broaden my exposure to advanced crystallographic techniques and modern applications of chemical crystallography, these lectures directly impacted my independent research program. As a post-doctoral fellow, I was engaged in developing new coordination compounds to serve as platforms for energy-storing halogen-elimination photochemistry. One of the major goals of these efforts was to develop new inorganic complexes that participated in more efficient photochemical processes. These efforts were guided in large part guided by standard photochemical experiments: steady-state and time-resolved absorbance spectroscopy. While these

techniques provide valuable information about photochemical processes, direct structural information about the structures involved in photoreactions is elusive. In large part influenced by attending Prof. Coppens's guest lecture on advanced crystallographic techniques, we initiated an effort in photocrystallography and obtained direct structural data related to critical photointermediates. The ability not only to attend the lecture but also to interact one-on-one with Prof. Coppens was invaluable to understanding both the theory of photocrystallography as well as the practicalities of executing these challenging experiments. As I transitioned to my independent career, I have continued to rely on photocrystallographic experiments to study reactive intermediates in catalysis. It is rare that a classroom experience so directly impacts research directions, but the exposure to advanced crystallography through guest lectures significantly impacted the toolbox that my group now uses to understand photochemical processes."