

Efforts to enhance coverage of crystallography in United States secondary education

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Because crystallography has often been regarded as an ‘experts only’ science, requiring advanced mathematics and physics, it has been eliminated from many science curricula. In the United States, high school is a critical time when students are exposed to science at a more significant level, preparing them for university, and it is when they make career choices. A contemporary secondary science teaching credential must qualify teachers to present topics in substantive ways, to attract talented and enthusiastic young people to science, and to develop scientific literacy in the future workforce. Education and training policies put forward by the United States National Committee for Crystallography and the American Crystallographic Association recommend that molecular structure awareness should begin in K-12 (kindergarten through 12th grade) education as a core component for implementing established national science standards. Furthermore, many contexts exist in which crystallography can be incorporated into secondary education with minimal disruption. Following these guidelines, preparation of secondary teachers should include professional development in crystallography, providing them with knowledge (fundamental and practical), learning units, tools and modern examples to incorporate into their curricula. This article describes activities whose objective is to enhance secondary education by raising crystallography awareness through workshops, summer schools, student/teacher research internships and remote-enabling technologies.

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1. Background and significance

Crystallography has often been regarded as an ‘experts only’ science, requiring advanced mathematics and physics to explain the underlying principles. This has kept crystallography education out of wide parts of the curriculum in the United States, as the subject has been considered too difficult and too advanced to introduce until graduate level university classes. Academic, government and industrial researchers alike have recognized the danger inherent in this interpretation, as students tend to choose subjects for study with which they have some level of familiarity.

One of the early proponents of teaching crystallography was Wally Cordes at the University of Arkansas. He felt that every lecture – whether to K-12 (kindergarten through 12th grade), undergraduate or graduate students – had to include a model, any model that would foster interest, dialog and a basis for understanding. Even the crudest of models could be used to demonstrate a concept, like the Ewald sphere, the lattice model or symmetry elements. The ‘glide-planes’ model

demonstrates just how clever a teacher he was, using actual model airplanes, and the asymmetry of the bottom to the top, as a guide to understand the glide-plane symmetry operation (Fig. 1). He encouraged all of us to use common objects around us to demonstrate these simple principles.

In 2005, recognizing the opportunity to communicate to the broader scientific community the research opportunities afforded by crystallography, as well as the value of crystallographic information, the education committees of the American Crystallographic Association (ACA) and the United States National Committee for Crystallography (USNCCr) organized a crystallography education summit. The outcome of this forum was a consensus policy statement on crystallography education and training, directed towards our scientific colleagues, who may also be practicing crystallographers, as well as education policy makers of the major scientific societies (<http://sites.nationalacademies.org/pg/biso/IUCr/>). This document recognizes that, with advances in computing, the World Wide Web and instrumentation leading to more widespread access and use of crystallography, it is

crucial to educate the next generations of crystallographers. To do so involves introducing students to crystallography at an appropriate level throughout their education. This can be accomplished by recognizing that crystallography has a significant visual component, which can be exploited to connect with students of all ages. Crystallography and molecular structure awareness can and should begin in K-12 education as core components for implementing the established national science standards for all students. Further, many contexts exist in which crystallography can be incorporated into secondary and undergraduate education with minimal disruption to current courses.

In the United States, high school (grades 9–12) is a significant period in the education of students. It is during this critical time that students are exposed to science at a more significant level, preparing them for university, and it is when they make career choices. A contemporary secondary science teaching credential must qualify teachers to present topics in substantive ways, to attract talented and enthusiastic young people to science, and to develop scientific literacy in the future workforce. Preparation of secondary teachers should include opportunities for professional development in crystallography, where we in the crystallographic scientific community provide them with knowledge (fundamental and practical), learning units, tools and modern examples to incorporate into their curricula.

National Science Education Standards expect science curricula in grades 9–12 to develop students' understanding

and abilities aligned with the concepts and processes associated with (a) systems, order and organization; (b) evidence, models and explanation; (c) form and function. High school chemistry classes include substantial content on ionic and molecular structure and chemical bonding, and biology classes include content on protein and DNA structure, all which can be elucidated within the context of crystallography. One of the content standards, *properties of materials*, can be explained through the use of crystal structures. *Order and organization* can be explained with crystals and crystal growth examples. The results of protein crystallographic analysis may be used to develop content standards such as the *molecular basis of heredity and biological evolution* and *matter, energy and organization of living systems*.

Discussions about crystallography may also be used to develop students' understanding of science and technology. According to the National Science Foundation, education in the next decade will take place in ubiquitous learning environments encompassing classrooms, laboratories, libraries, workplaces, homes and other locations. As we undergo this transformation, traditional educational components, including the sum of primary and secondary education, K-12, will become highly leveraged constituents of the open learning world of today's World Wide Web, where everyone is a life-long learner. Open learning in the sciences is made possible by technologies such as social networking and web conferencing applications, which build virtual learning communities, and remotely enabled instruments, which facilitate collaboration, consultation and distributed expertise. This article describes activities whose objective is to enhance secondary education by raising crystallography awareness through workshops, summer schools, student/teacher research internships and remote-enabling technologies.

2. Research opportunities for high school students

2.1. University of Toledo

Over the past six years, the Lind laboratory at the University of Toledo has hosted four high school students who have participated in research projects involving crystallography. Three of these students have become co-authors on peer-reviewed publications, clearly demonstrating the feasibility of introducing high school students to crystallography. All projects utilized powder X-ray diffraction techniques. The concept of periodic building blocks is intuitive to most students based on their everyday experiences (e.g. walls). The basic principles of X-ray diffraction were introduced to the students using a laser and gratings. This simple experiment elegantly introduces important properties of reciprocal space to the students without requiring complex mathematics. Discussion of wave properties and constructive and destructive interference was based on visual examples like water ripples caused by rocks tossed into a lake. Finally, Bragg's law could also easily be derived using high school mathematics concepts. This equipped the high school students with enough background knowledge to accept that the peak positions in a

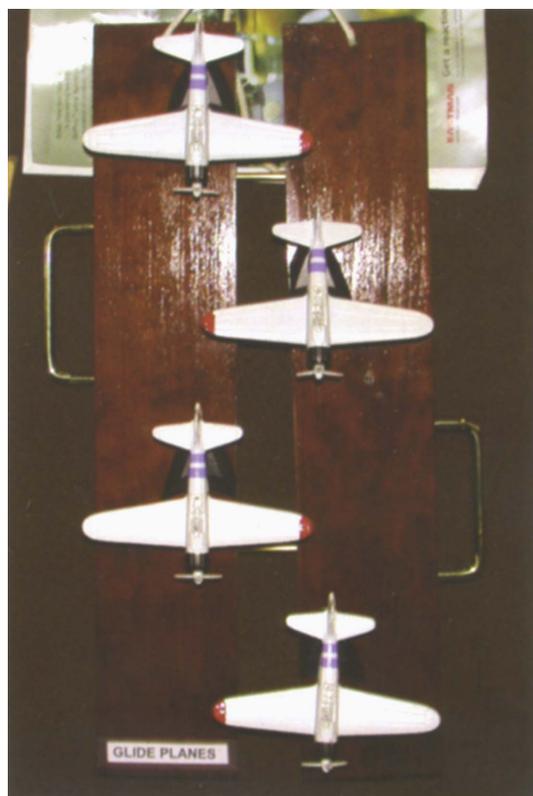


Figure 1
'Glide planes.' From Wally Cordes poster on teaching crystallography at the American Crystallographic Association Meeting, 2002.

powder pattern arise from different sizes of the periodic building blocks. Phases in the powder patterns were identified using search/match software and the International Centre for Diffraction Data PDF database. This allowed students to judge whether they had unreacted starting materials left in their samples and whether they had obtained single-phase products.

Experiments are often complemented with scanning electron microscopy (SEM). SEM images are visually appealing and allow high school students to fully participate in the imaging part of the project. As crystal habits are related to crystal structure, SEM images often reveal distinct particle shapes for multiphase samples. Combining elemental analysis of individual particles by energy dispersive X-ray spectroscopy with visual information from the images allows the assignment of specific particle shapes to the phases identified by powder X-ray diffraction. In many cases, the shape can be explained by the crystal system, reinforcing the concept that the unit-cell structure of materials is important in determining their properties.

Three of the high school students completed summer internships supported through ACS Project SEED. Projects were related to the synthesis of negative thermal expansion oxides. In all cases, target crystal structures were known and could be matched with PDF view cards of isostructural materials.

One student conducted a science fair project in the Lind laboratory. Intrigued by reading about polymorphism and its importance in pharmaceuticals, he wanted to explore how different crystal polymorphs could be prepared. To ensure the feasibility of the project, the student was directed to explore the crystallization of CaCO_3 instead of pharmaceuticals, as CaCO_3 is known to form several well defined polymorphs under different synthetic conditions. Samples were prepared hydrothermally in water/ethylene diamine mixtures to investigate the influence of solution composition on crystallization. The student found that crystalline CaCO_3 could only be obtained for solutions with less than 50 vol.% ethylene diamine. Crystalline aragonite was recovered from pure water, mixtures of aragonite and calcite were obtained for 10 vol.% ethylene diamine, and vaterite was the major polymorph at 25 vol.% ethylene diamine. In addition to powder X-ray diffraction, samples were analyzed by light microscopy. The different crystalline phases resulted in distinct crystal shapes, allowing correlation of crystal structure with crystal habit.

2.2. Keck Center for Molecular Structure

Each summer for the past seven years, students from the Troy Tech Magnet Program in Science, Mathematics and Technology in Fullerton, CA, have spent a year-long internship working on research projects at the Keck Center for Molecular Structure (CMoS) under the mentorship of Katherine Kantardjieff (Fig. 2). The goals of the program are to provide secondary students with a hands-on education in the technology of the 21st century workplace, and to offer them opportunities for career exploration through a variety of

internship experiences and technical classes emphasizing both theory and application. Students have worked with Kantardjieff on a variety of sophisticated projects directly involving crystallography or its application in drug design and protein engineering. Many have co-authored publications and won regional and national science awards, including the California Science Fair and the national Siemens Westinghouse Science Competition. Projects have included determining structures of lactate dehydrogenase, developing cholinesterase inhibitors as potential Alzheimer's therapeutics (Law *et al.*, 2007), determining structures of tuberculosis drug targets, structure-guided design of potential antitubercular drugs (Kantardjieff *et al.*, 2005) and engineering enzymes for synthetic advantage as part of industrial green chemistry efforts (Szocs & Kantardjieff, 2009).

2.3. University of Alabama Huntsville

The Laboratory for Structural Biology at the University of Alabama in Huntsville (UAHuntsville) is situated in a city known for the rocket technology that powered the Apollo mission to the Moon and which is used for the US space-shuttle program. Therefore, it was thought only fitting to conduct an education outreach program that couples space to structural biology.

Alex McPherson was one of NASA's principal investigators, engaged in the study of protein crystal growth in microgravity. Prior to the last Columbia space-shuttle flight, the laboratory of Joseph Ng collaborated with McPherson's team to invite high school students and teachers in the southeastern US to prepare proteins for crystallization on board the International Space Station (ISS) *via* the US space shuttle as part of McPherson's nationwide NASA education outreach activity. Since 1984 the McPherson laboratory at the University of California at Irvine has been engaged in experiments dealing



Figure 2
Troy Tech Interns. Summer student interns from the Troy Tech Magnet Program in Science, Mathematics and Technology working with their mentor, Katherine Kantardjieff, at the Center for Molecular Structure in the California State University.

with the crystallization of proteins, nucleic acids and viruses in the weightless environment of space using the enhanced dewar system (Barnes *et al.*, 2002). The enhanced dewar is an extremely inexpensive, simple, high-capacity system for the crystallization of different samples of many macromolecules in space aboard a space shuttle or the ISS.

Preparation of crystallization samples is technically very simple, requiring limited manual skills and very limited training. The process is so simple that high school students could likely assist in the fabrication of protein crystallization samples in the dewar system, and in that way, they could directly participate in flight experiments aboard the ISS. Students could be enlisted to make protein crystallization samples for this program, under strict supervision and guidance by professionally trained and experienced personnel, and these samples can be frozen in liquid nitrogen and carried into space. The samples would be returned to the classrooms, after being on the ISS for two–four weeks, to the students who prepared them for examination. The experiments would, therefore, provide a student flight experience, but at the same time also be part of an important, ongoing scientific investigation.

2.3.1. What do we hope the students learn? In this program, we hope that students learn about the nature of biological macromolecules and, in particular, what proteins are and why they are important. The program further describes what a protein crystal is and why it is important to crystallize proteins. Why do we want to grow crystals of proteins at all, and in particular, why do we want to grow them in space? Similarly, it was our endeavor to use the classroom and space experience to provide teachers with the opportunity to display and illustrate a broad range of new and significant ideas in the areas of biology, physics and chemistry.

The workshop program consisted of four principal demonstrations of laboratory and research techniques used in

structural biological studies within different stations. The students were divided into small groups and spent about 1–2 h (depending on the station) with a real investigator at each station showing (1) protein purification and characterization; (2) vapor diffusion and batch crystallization; (3) fundamentals of X-ray diffraction; and (4) three-dimensional viewing of a protein molecule with computer graphics (Fig. 3). Since the emphasis of the workshop was focused on protein crystallization, most of the hands-on experience was setting up protein crystallization.

2.3.2. Explanation of microgravity. In space, protein crystallization can occur in a virtually convection-free environment. It was explained to the students that convection can be understood by our observation of a flame on a candle. The burning flame on a candle wick produces hot gas as the result of energy release by combustion. The hot gas that is produced becomes less dense than the cooler gases around it. On Earth the hot gas is directed upwards by the denser surrounding environment and, as the gas rises, stirring is created by a ‘buoyancy-induced flow’, otherwise known as convection. Consequently, the unburned fuel, oxidizer and other burning products are mixed. In a microgravity environment, the stirring is eliminated, allowing the scientist to examine phenomena obscured by the effects of gravity.

Sedimentation is another gravity-driven phenomenon occurring when materials separate as a result of their unequal densities. Particles in a liquid droplet, for example, having a greater density than its environment can sink, creating an asymmetrical flow around the dropping material. Under microgravity, fluids stay more homogeneous, without uneven collision or dispersion of the particles under investigation.

In microgravity, the elimination of sedimentation and convection can also enhance protein crystallization (for example, Ng, 2002; Lorber *et al.*, 2002; Ng *et al.*, 1997). Crystallization droplets have a more uniform concentration of protein, meaning that all surrounding particles in the solution are more evenly distributed. During the nucleation event, the solution in the immediate vicinity of the growing crystal becomes depleted of protein molecules as the crystal nucleates and begins to grow. Therefore the local supersaturation on the surface of the growing crystal is decreased, favoring crystal growth over nucleation. In other words, the growth of pre-existing crystals predominates over the initiation of new crystal formation, resulting in larger and fewer crystals. When a new protein molecule comes out of solution to align itself on the surface of a growing crystal, its movement is solely dictated by free diffusion rather than by convective sources. Therefore, protein molecules traverse the crystallization droplet at a very slow rate, providing more time for crystal lattice alignment and thus producing a higher-quality crystal.

Along the same line, space-grown crystals have less incorporation of large impurities. Many impurities are combinations of protein molecules that are amorphous or denatured. These are often two–three times larger than protein molecules and as a result diffuse much more slowly. The slower diffusion time thus reduces the chance of their incorporation onto the surface of the crystal, which may impede its growth. Under



Figure 3 Highlights of the structural biology workshop emphasizing protein crystal growth in microgravity. Instructors are working with students in showing how proteins are prepared, crystallized and subsequently analyzed by X-ray diffraction.

microgravity, crystals also tend to remain stationary in the mother liquid and do not settle to the bottom of the container as they would on Earth owing to gravity. Consequently there is no asymmetrical flow around any dropping particles.

It is believed that eliminating convection during the crystal-growth process and the lack of sedimentation produce higher-quality crystals. As a result, higher-quality crystals can provide better X-ray diffraction images, allowing more information for the determination of a high atomic resolution structure.

2.3.3. Return from space. Both ground and space experiments were conducted in parallel in the same type of reactors and with the same solutions. All samples underwent identical transport and handling conditions during the pre-launch and post-landing phases of the missions. Exposure to microgravity was experienced either for about ten days aboard the space shuttle or for a few weeks on the ISS.

Samples from space were received at the space-shuttle landing sites, mostly in Florida and occasionally in California. The dewar was usually hand-delivered directly from the landing site to the UAHuntsville laboratories, where immediate analysis was performed. The quality of the crystals was determined by visual inspection and X-ray diffraction. Space-grown crystals were compared with those obtained on Earth by measuring the crystal's volume under a visible microscope and the extent of X-ray diffraction in terms of intensity over background as a function of resolution. Selected protein crystals were subsequently used for structure analysis as well. All results were posted on the web for students to analyze and report. In half of the proteins prepared, improved crystals were obtained from the samples that were space grown.

2.3.4. Overall goals. Participation in a flight experiment was a worthwhile experience in itself, as it had the effect of stimulating an interest in science and inspiring secondary school children who might not otherwise have the opportunity to carry out real research. Moreover, it was an aim of the project to use the opportunity to participate in a flight experiment as a mechanism to encourage young students to think seriously about structural biology: the structures of proteins, nucleic acids, complexes of macromolecules and large macromolecular assemblies. We wanted to develop an appreciation as well that protein crystallography is an essential element of the broader disciplines of biochemistry, biotechnology and molecular biology.

3. Pre-college community outreach and workshops

3.1. American Crystallographic Association

In 2004, the ACA hosted a community outreach workshop aimed at high school students and teachers from the Chicago Public Schools system. The workshop was held on the Saturday before the ACA annual national meeting in downtown Chicago and was planned as an all-day event at the convention site. Judy Flippen-Anderson (Research Collaboratory for Structural Bioinformatics, RCSB) and Bernard Santarsiero organized the event with help from the RCSB, the

Cambridge Crystallographic Data Centre (CCDC) and several session speakers. Along with the American Institute of Physics and other scientific organizations, the ACA has been interested in outreach for K-12 pre-college students for decades. First, it provides a venue to encourage students to learn more about science, mathematics and engineering, to demonstrate both the utility and enthusiasm that scientists have about their chosen profession, and potentially to foster interest in a career in science, mathematics and engineering for pre-college students. Second, it promotes the goal of establishing a scientifically literate population by extension of university faculty beyond the traditional university boundaries. This is especially important in a secondary effort to expand diversity in the scientific communities.

The workshop, entitled 'X-rays, Crystals, Molecules, and YOU!', was focused on examining the structure of molecules, large or small, using X-ray diffraction, and provided a framework on how to dissect large protein structures into smaller simpler units: atoms, chemical groups and amino acids. Much of the workshop used a simple PC with internet access, which enabled visualization of a protein structure as a three-dimensional model. We took advantage of the structural information from the RCSB Protein Data Bank (PDB) and the CCDC small-molecule database. Even for students at the pre-college level, it was relatively easy to talk about X-ray diffraction and, in particular, crystallography as a science that provides us with a tool to 'see' molecules and understand how they function. Once they understand how proteins function, we can explore how to change a protein – generate a mutant – and see if it functions differently, or we can explore how a mutant does not work as well as the native protein. The results from a crystallography experiment or measurement are the structure of a molecule and its shape, and any K-12 student can look at and then compare the shapes of these various objects. Thus, with this knowledge about molecules and shapes, one can explore the fundamentals of pharmaceutical drug discovery through a discussion of a simple 'lock-and-key' model, in which the student can compare the shape of a binding site with the shape of a substrate or inhibitor. Much of this can now be extended to the study involving materials science, nanotechnology, self-assembled materials, surfaces and large extended molecular arrays

Katherine Kantardjieff (Cal State Fullerton) began the morning session with a discussion of crystallography and how we use X-ray diffraction to see molecules (Fig. 4). Karen Lipscomb (CCDC) followed by talking about the small-molecule database, how small-molecule structural information can be retrieved, and how small molecules can be used as building blocks to construct larger molecular assemblies, like proteins, and take on characteristic shapes. David Goodsell (The Scripps Research Institute) presented an overview of the PDB and showed how structural information can be retrieved and visualized. One can look at small helix-turn-helix structures, or the larger multidomain, heteromultimeric structures, like a virus. Tim Herman (Milwaukee School of Engineering) talked about scientific inquiry and model building. Tommie Hata (The Pingry School) talked about 'SMART Teams:

Students Modeling a Research Topic.' The morning session provided a strong cohesive framework to understand why we use crystallography and X-ray diffraction, how and why we store structural information, and then how it can be used to approach a specific scientific inquiry (Fig. 5).

Following lunch and an open discussion with the session speakers, the afternoon session started with Alex McPherson (University of California, Irvine) and a laboratory exercise on growing protein crystals. Lysozyme can be easily and rapidly crystallized, and McPherson brought materials so that attendees could grow and view protein crystals within the allotted hour. Given time, one could include a session on symmetry to explore regular objects and delineate differences between these objects. In addition to protein crystals, rock samples can also be used to demonstrate the relationship between microscopic packing and regularity – ‘atomic building blocks’ – and macroscopic faces and edges. The afternoon session finished up with teams doing model building and using the databases with help from the session organizers. Since the opening reception for the ACA meeting started that evening, attendees were invited to that reception. The ACA reception included presentations by vendors of various scientific equipment and poster presentations. Since a majority of the posters included representations of protein structures and a discussion of structure and function, it provided real examples of this type of research in parallel to the workshop.

One type of outreach program that has been under general discussion in several scientific organizations is choosing a single day or week across the country to encourage scientists, engineers and mathematicians to plan a visit to their local secondary or high school. Visitors would talk about their career and perhaps bring materials to allow students to carry out some kind of experiment, analysis or discussion. With tens of thousands of scientists engaged in this sort of exercise each year, it would have a tremendous impact to foster greater interest in a scientific career.

One major problem with the workshop was getting students and teachers to attend on a free Saturday during the summer. It might have had greater success if the workshop had been held during the normal school academic year. In 2010, the USNCCr and the ACA hosted a workshop on crystallography education for high school teachers. The workshop was designed to supply teachers with lesson and experiment plans that could be taken back to their schools, and provided professional development through the College of Education at the University of Illinois at Chicago. The workshop organizers were also in contact with the Director of the K-12 Science Program in the Chicago Public Schools system, who helped advertise the event on their teachers' listserv.

Topics focused on visual concepts that are easy to comprehend and retain. Diffraction basics can be explained by simple wave pictures combined with visible light gratings. Constructive and destructive interference as well as Bragg's law can be derived using simple geometric constructions. The different patterns observed for the gratings can be related back to the shapes of the unit cells that result in the seven crystal systems.

The seven crystal systems can be introduced with drawings, models and where appropriate mineral crystals. Different atomic packing efficiencies can be understood through hands-on comparison of the weight of equal volumes of different materials. This experiment can focus on significant differences in packing (*e.g.* polymer, inorganic salt, metal) or on more subtle differences (*e.g.* face-centered cubic and body-centered cubic metals), depending on the level desired in the classroom.

The importance of crystallography for understanding the function of the human body and diseases can be emphasized through visual representations involving DNA, proteins, viruses and complexes. The relationship between crystallography and designed active site inhibitors used for treating diseases can be emphasized. While it is not possible to teach high school students how to solve a protein crystal structure,

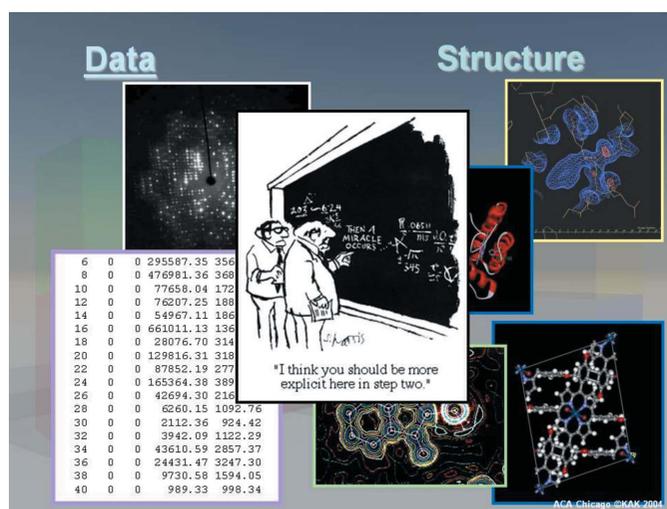


Figure 4 'Crystallography Nuts and Bolts.' Slide taken from a presentation given by Katherine Kantardjieff at the 'X-rays, Crystals, Molecules, and YOU!' ACA workshop, 2004.



Figure 5 'X-rays, Crystals, Molecules, and YOU!' Teachers and students participate in the 'X-rays, Crystals, Molecules, and YOU!' ACA workshop, 2004.

emphasizing that crystallography is crucial in providing the three-dimensional visual model of these macromolecular structures should instill in students an appreciation for the usefulness of crystallography and a desire to learn more in the future.

3.2. NSF-sponsored workshops in chemical sciences

To promote crystallographic science, the Keck Center for Molecular Structure (CMoS) in the California State University has been engaged for 13 years in organizing and hosting professional development workshops and summer schools for faculty, graduate students, postdoctoral fellows, community college instructors and high school teachers. Sponsored by the National Science Foundation and following the guidelines of the USNCCr, these workshops and summer schools aim to provide working knowledge and hands-on experience to users of crystallographic information. The goals of the workshops and summer schools are twofold: to instruct participants in the use of X-ray diffraction to answer structural problems in their own research; and to prepare current and future faculty and secondary science teachers to competently and enthusiastically teach crystallography. One such workshop, 'Mysteries of Water', was specifically intended to inform secondary chemistry and biology teachers in Orange County, CA, about crystallography. This 2006 workshop, an outreach component of a Chemistry Research Center grant to Kenneth Janda at the University of California Irvine, supplied secondary teachers with educational materials, and provided them with practical experience in growing crystals and in structure determination (Fig. 6).

4. Consortia

4.1. CAL-PRISSM

The Partnership for Remote Instruments to Study the Structure of Matter (CAL-PRISSM) is a California

e-consortium currently supported by The Boeing Company (Kantardjieff *et al.*, 2007). The effort is led by Katherine Kantardjieff, Director of the Keck Center for Molecular Structure (CMoS), an X-ray diffraction core facility for the California State University Program for Education and Research in Biotechnology (CSUPERB) located at California State Polytechnic University Pomona. CAL-PRISSM members include several predominantly undergraduate institutions, community colleges and high schools. CMoS pioneered the use of remote instrumentation access for education and training at predominantly undergraduate institutions, first placing its instruments online in 1997. CAL-PRISSM's remotely enabled instruments include remote access to diffractometers at CMoS and the Stanford Synchrotron Radiation Laboratory; nuclear magnetic resonance and electron paramagnetic resonance spectrometers at Cal State Fullerton; atomic force and environmental scanning electron microscopes, as well as an inductively coupled plasma mass spectrometer, at Cal State Long Beach's Institute for Integrated Research in Materials, Environments and Society; a visible/near infrared spectrometer, circular dichroism spectropolarimeter and computer cluster at Cal Poly Pomona's Center for Macromolecular Modeling and Materials Design; and nuclear magnetic resonance spectrometer at Cal State Stanislaus. A cohort of 13 CAL-PRISSM high school classroom teachers from seven high schools is led by Julie Karjala, a science instructor at Newport Harbor High School, Newport Beach, CA, and curator of web resources for high school teachers.

By harnessing the power of end-to-end cyberinfrastructure and building on existing programs and expertise, CAL-PRISSM is providing students, college/university faculty and secondary classrooms with real-time remote access and control of specialized scientific instruments from remote locations, together with real-time discourse. CAL-PRISSM aims to promote cross-disciplinary collaboration between researchers using these technologies, and to improve educa-



Figure 6
'Mysteries of Water.' Secondary chemistry and biology teachers participate in the NSF-sponsored 'Mysteries of Water' workshop, held at the University of California Irvine in 2006.



Figure 7
CAL-PRISSM. Secondary biology, chemistry, earth science and physics teachers work with university faculty to develop teaching materials for the high school curriculum that incorporate remote-enabled instruments and conform to California Science Content Standards.

tional quality and student opportunities at the undergraduate and secondary levels in learning about and researching the structure of matter. Its members design, deploy and assess learning units and simulations that address California State University Programmatic Student Learning Outcomes and the California Science Content Standards with regard to various aspects of the structure of matter (Fig. 7).

5. Concluding remarks

In 1948, Paul Ewald eloquently described our rich and interdisciplinary science of crystallography (Ewald, 1948): 'It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features.' It is with this perspective that we strive to educate secondary science teachers and their students. In addition to developing competence and confidence to teach, we hope to develop an understanding and appreciation that the bounty of knowledge gained from structures determined by the methods of crystallography is a key underpinning of modern science and technology.

We would first like to thank Wally Cordes for his dedication and enthusiasm, and for spear-heading inspiring and entertaining symposia on teaching crystallography at annual ACA meetings. Many thanks to past and present members of the United States National Committee for Crystallography Education Subcommittee, the American Crystallography Association Continuing Education Committee and the International Union of Crystallography Commission on Crystallographic Teaching for continuing to raise awareness about the

importance of crystallographic science. We thank those who have helped support our efforts to enhance coverage of crystallography in secondary education: The W. M. Keck Foundation, the National Science Foundation, the National Aeronautics and Space Administration, The Boeing Company, and iLinc Communications. We extend our gratitude to Dr Alex McPherson and Greg Jenkins for their guidance and participation in the space workshops. We also thank the Alabama Space Grant Consortium, NASA, for their support in this program at UAHuntsville. Finally, we thank all our workshop and consortia participants, teachers and students for sharing our enthusiasm and ideas.

References

- Barnes, C. L., Snell, E. H. & Kundrot, C. E. (2002). *Acta Cryst.* **D58**, 751–760.
- Ewald, P. (1948). *Acta Cryst.* **1**, 1–2.
- Kantardjieff, K. A., Rogers, H., Miller, S. A., Monteyne, K., Nelson, P. R., Corcoran, T. C., Sharma, S., Fultz, M., Mason, A. Z. & Karjala, K. (2007). *CAL-PRISSM: Partnership for Remote Instruments to Study the Structure of Matter*. Program Abstracts, American Chemical Society Western Regional Meeting, San Diego, CA, USA.
- Kantardjieff, K. A., Vasquez, C., Castro, P., Warfel, N. M., Rho, B.-S., Lakin, T., Kim, C.-Y., Segelke, B. W., Terwilliger, T. C. & Rupp, B. (2005). *Acta Cryst.* **D61**, 355–364.
- Law, K.-S., Acey, R. A., Eckenrod, B., Stedman, R., Kantardjieff, K. A., Smith, C. R., Benton, D. A. & Nakayama, K. (2007). *Biochem. Biophys. Res. Commun.* **355**, 371–378.
- Lorber, B., Théobald-Dietrich, A., Charron, C., Sauter, C., Ng, J. D., Zhu, D.-W. & Giegé, R. (2002). *Acta Cryst.* **D58**, 1674–1680.
- Ng, J. D. (2002). *Ann. N. Y. Acad. Sci.* **974**, 598–609.
- Ng, J. D., Lorber, B., Giegé, R., Koszelak, S., Day, J., Greenwood, A. & McPherson, A. (1997). *Acta Cryst.* **D53**, 724–733.
- Szocs, L. & Kantardjieff, K. A. (2009). *Computational Studies on Enantiomeric Preference by Sporobolomyces salmonicolor Carbonyl Reductase Mutants*. Program Abstracts, 21st Annual CSUPERB Symposium, San Jose, CA, USA.