complicated, like determining the electron density of states from the band structure, instructors tend to skip the long tedious calculations needed since there is not enough time for this during lectures. The online student presentations have no such limitation and can explain how to do a long calculation step-by-step. This can be a valuable resource for those trying to perform similar calculations but for whom the scientific literature is still to difficult to digest. Students teach at the right level for their fellow students to understand. The production of a collection of long and detailed calculations that go into more detail than the lectures but are written in a style that is accessible to students was an unexpected outcome of this experiment. An important factor for the success of this model is the sheer volume of material produced. The students produce much more material than a single instructor could. The students are also more likely to try new approaches. Not all material that the students produce is useful but the less useful material gets displaced by other student projects as the students continuously try to improve the course. The students of our solid state physics course have created some wonderful material that has enriched the course. The biggest challenge for the instructor is managing the influx of material that is produced.

Keywords: education, solid-state physics

MS.97.2

WebCSD: bringing the Cambridge Structural Database to undergraduate teaching

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The Cambridge Structural Database (CSD) represents a vast and ever growing compendium of accurate 3D structures that has massive chemical diversity across organic and metal-organic compounds. For these reasons, the CSD is finding increasing application in chemical education.

WebCSD is a web-based search engine for interrogating the CSD and displaying CSD information content. Requiring just a standard web-browser, and without the need for any local software installations, WebCSD is designed for use in classroom and computational teaching laboratory environments. This ease of access makes the online version of the CSD the ideal platform for furthering students' understanding of 3D chemistry, and introducing them to the 3D realities of the chemical world.

This talk will showcase examples of how WebCSD is currently being used to enhance student learning across the entire span of the chemistry curriculum. We will also introduce a teaching subset of more than 500 CSD structures created specifically to illustrate key chemical concepts, and a number of teaching modules that make use of this subset in a teaching environment.

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Keywords: database, teaching

MS.97.3

Remote access to SSRL crystallography beamlines: Tools for education and training

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For the last six years, the Structural Molecular Biology (SMB) group at the Stanford Synchrotron Radiation Lightsource (SSRL) has provided general users of the facility fully remote access to their macromolecular crystallography beam lines. This was made possible by implementing fully automated beam lines with a flexible control system and an intuitive user interface (Blu-Ice) [1], and by the development of the robust and efficient Stanford Automated Mounting (SAM) robotic sample changing system [2]. The ability to control a synchrotron beam line remotely from the comfort of the home laboratory has set a new paradigm for the collection of high-quality X-ray diffraction data [3] and has fostered new collaborative research whereby a number of remote users from different institutions can be connected at the same time to the SSRL beam lines. The use of remote access has revolutionized the way in which scientists interact with synchrotron beam lines and collect diffraction data, providing a true high-throughput crystal screening and collection system at a significantly reduced cost to researchers. Moreover, it has also triggered a shift in the way crystallography students are introduced to synchrotron data collection and are trained in the best methods to collect high quality data and make the best possible use of these facilities. SSRL provides expert crystallographic and engineering staff, state-of-the-art crystallography beam lines and X-ray detector technology, and a number of accessibility tools to facilitate data collection and in-house "remote training". The use of these facilities at SSRL for education, training, outreach and collaborative research [4] is strongly encouraged.

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Keywords: synchrotron, remote access, education

MS.97.4

Structure utilities hosted by the Bilbao crystallographic server

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The experimental procedures (such as scattering and powder diffraction) and computational methods (such as ab-initio calculations and Monte-Carlo simulations) reveal the information on the lattice parameters and the atomic positions but since there is no unique way to describe a structure, in order to correctly classify and further compare it with other similar types of structures, it is necessary, in general, to take the equivalent descriptions into account. For the determination of a compatible orientation and/or origin shift, it is thus necessary to specify the transformation between different settings, followed by a systematic comparison of the corresponding descriptions.

Various tools are offered by the Bilbao Crystallographic Server for such purposes (http://www.cryst.ehu.es) [1]. CELLTRAN and TRANSTRU transform unit cell parameters or atomic coordinates into

another setting while SETSTRU converts alternative settings structure description to a standard setting and vice versa. EQUIVSTRU applies the space-group normalizers to derive the equivalent descriptions of the same structure.

The structure utilities are not restricted only to transformations: for a given pair of structure descriptions, STRAIN is used to calculate the linear and finite strain tensors as well as the degree of the lattice deformation and COMPSTRU tries to find the normalizer transformation that best matches the transformation between different descriptions. The program is also helpful for the recognition of identical or nearly identical atomic arrangements of different compounds which is essential for the crystal-structure classification problem. WPASSIGN identifies the Wyckoff positions to which the occupied atomic orbits of a structure belong.

The structures can be visualized in an interactive 3D environment via the VISUALIZE tool, using the Jmol script [2].

Where applicable, the tools support the CIF file format both for input and output, making it easy to exchange information between various related software packages.

[1] M.I. Aroyo, J.M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, H. Wondratschek. *Z. Kristallog.* **2006**, *221*, 15-27. [2] *Jmol: an open-source Java viewer for chemical structures in 3D.* http://www.jmol.org .

Keywords: crystal-structure description, structural similarity, Bilbao crystallographic server

MS.97.5

Jpowder: a Web/Java based program for the display of powder diffraction data

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Jpowder [1,2] is a Java/Web based program which purposes are:
• Display and inspect powder diffraction data quickly and efficiently
• Use it to create web based crystallographic teaching content by allowing users to create interactive plots of data in addition to static plots [3]

Jpowder is written in Java and uses its associated JavaWeb Start and Java applet technologies. Java Web Start provides the ability to launch fully featured Java applications with a single click and without the need to go through operating system installation procedures. Based on the same code-base, a version of Jpowder has been exposed in the form of a Java applet – a self-contained Java component that can be embedded within a standard HTML web page. This means a user may initially use Jpowder to highlight regions of interest in datasets and then save such data not just as static images, such as jpgs, but also as 'Jpowder-applet format' files. These can subsequently be used as teaching material allowing students not only to learn from static images but also from interacting with the images directly.

[1] A.J. Markvardsen, K. Puphaiboon, M. Arjeneh, K. Shankland, H.L. Guest, T.A.N. Griffin, D.R. Badham, D.W. Flannery, *J. Appl. Cryst.* **2010**, *43*, 1532-1534. [2] http://www.jpowder.org [3] Details on how to use this feature see http://www.jpowder.org/JpowderApplet.html

Keywords: teaching, powder, Web

MS.98.1

Solving the incommensurately modulated structure in profilin: actin crystals

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Cellular motility, critical for neuronal development, cellular immunity, and intracellular bacterial locomotion, etc., is regulated through cytoplasmic actin/profilin interactions. In these interactions, profilin sequesters actin monomers for delivery to actin filament assembly sites. Detailed structural information on monomeric actin has been provided by X-ray crystallography, but it is not known how actin is delivered by profilin to the end of a growing actin filament. To study the structural rearrangements of actin and the associated changes in protein-protein interactions in filament formation, profilin:actin (PA) crystals provide an excellent model because they retain the dynamic nature of actin. Twenty five years ago it was found that when PA crystals were exposed to conditions known to promote actin filament formation, they transformed into a modulated state characterized by unusual off-lattice satellite reflections. The satellites are caused by the formation of an actin superstructure within the crystal. Methods for solving such modulated crystal structures are known to aperiodic small-molecule crystallographers, yet macromolecular crystallographers have not yet solved one. Several crystals of macromolecular complexes have modulations and cannot be solved. The biologically-important, modulated PA crystals will be solved as a first case and bring the 25 year old mystery of what is happening in these crystals to a close. The crystallographic tools we are developing for this PA case will provide the platform needed to tackle similar, rare, but important, structural conundrums.

These PA crystals contain an incommensurate modulation in one direction, a so-called (3+1) dimensional modulation. We can reproducibly produce isomorphously modulated crystals of PA and collect complete cryocooled data to 2 Å resolution. These data can be indexed with the q vector approach and the main and satellite reflections integrated using EVAL15 software. We have reindexed these data with an approximate super cell and solved a superstructure approximation of the modulated structure. Routes for solving the incommensurate crystal structure using the full super space theory will be discussed.

Keywords: aperiodic, incommensurate, protein

MS.98.2

Soft Quasicrystals Thermodynamic stability of complex structures

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There is growing interest in recent years in the ability to grow quasicrystals and other complex structures, whose building blocks are on a mesoscopic scale of tens to thousands of nanometers. These range from artificially constructed metamaterials, such as photonic quasicrystals, to self-assembled soft-matter quasicrystals [1-3]. In addition to having promising applications, especially in the optical domain, these materials give us the opportunity to study quasicrystals in ways that were impossible before. As time permits, I will discuss a few aspects of our ongoing work on these systems, ranging from our recent explanation of the stability of quasicrystals composed of soft isotropic