Microsymposia

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

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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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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

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Structure utilities hosted by the Bilbao crystallographic server Mois I. Aroyo, Emre S. Tasci, Gemma de la Flor, Danel Orobengoa, J. Manuel Perez-Mato, Departamento de Fisica de la Materia Condensada, Universidad del Pais Vasco, Bilbao (Spain). E-mail: mois.aroyo@ehu.es

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