MS.96.4

Iron vacancy superstructure and room temperature antiferromagnetic order in superconducting XFe$_2$Se$_2$ (X=K, Cs, Rb)


Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen (Switzerland).

Laboratory of Neutron and X-ray Structural Research, Swiss-Norwegian Beam Lines at ESRF, BP220, 38043 Grenoble, (France).

We report a combined neutron and synchrotron X-ray diffraction study of the PrMn$_2$Ge$_2$Si$_x$ system, through which we gain new insights into the magnetic and structural origins of the curious behaviour of these compounds. Phase separation (both structural and magnetic) is clearly seen over a certain range of concentration and temperature, prompting us to propose a two-phase structural model driven by changes in the Mn-Mn exchange energy. Our evidence suggests that the phase separation derives from variations in local strain originating at the shared crystallographic sites. Our interpretation brings into question whether random atomic substitutions could produce such remarkable magnetoelectronic phenomena or whether site-specific local atomic order prevails in the family of mixed 122 compounds. A tendency towards site ordering also raises the possibility of a miscibility gap.

Keywords: magnetism, ternary compounds, diffraction

MS.97.1

Harnessing students to advance e-learning

Roland Resel, Peter Hadley, Institute of Solid State Physics, Graz University of Technology, Graz (Austria). E-mail: p.hadley@tugraz.ac.at

Science is typically advanced by teams which make small improvements to the state-of-the-art. Teamwork is important because the collective knowledge and skill set of the team is greater than that of any individual in the team. We have been experimenting with applying a similar model to e-learning development. In a solid state physics course that consists of lectures and a weekly exercise session, the students were asked to evaluate the e-learning components of the course and propose ways to improve it. They implemented their ideas in small teams. Collectively, a class of university students usually have produced simulations in Java and Javascript, written lecture notes, Matlab template files, solutions to exam questions, and videos. Having the same material presented in a written document and in a video file can be useful because different students learn better form different media. Some of this material is in English and some is in German (the local language). We strive to have all important material available in both languages so that both local and international students do not experience a language barrier. When a topic is intrinsically
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 too 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

Gary M. Battle, CCDC, 12 Union Road, Cambridge, (UK). E-mail: battle@ccdc.cam.ac.uk

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.


Keywords: database, teaching

MS.97.3

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

Clyde Smith, Stanford Synchrotron Radiation Lightsource, Menlo Park CA, (USA), and the Department of Chemistry, Stanford University, Stanford CA, (USA). E-mail: csmit@slac.stanford.edu

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.

Keywords: synchrotron, remote access, education

MS.97.4

Structure utilities hosted by the Bilbao crystallographic server

Mois I. Aroyo, Emre S. Tasci, Gemma de la Flor, Danel Orobonoga, J. Manuel Perez-Mato, Departamento de Física de la Materia Condensada, Universidad del País 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