

for long-term maintenance and new developments. CCP4 libraries have been created and shaped over many years, and concentrate a vast experience of building crystallographic software. In the talk, I will give an overview of CCP4 libraries and describe their general concepts and functionality.

**Keywords:** crystallography, computations, CCP4

## MS.62.3

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### Libraries and software development at rigaku

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Software development at Rigaku relies on strategic leveraging of 3rd party software, both commercial and open source. For example, the *Computational Crystallography Toolbox* [1] is integral to our current methods development efforts. The cctbx library was especially useful in expediting the development of our new space group determination program, XPlain, in which the determination of the Patterson symmetry (Laue group + lattice centering) from an unreduced unit cell relies heavily on cctbx functions. The cctbx library was also found useful for transforming space group symbols and for associating observed absences with compatible space groups.

On the user interface side, we use Nokia's Qt software for rapid development of user interfaces to Mac/Linux/Windows compatible programs, such as our new CollectionStrategy program (a complementary part of Rigaku's HKL3000R suite), and our new reciprocal space exploration program, RSV3D.

[1] W. Ralf Grosse-Kunstleve, K. Nicholas Sauter, W. Nigel, *Moriarty and Paul D. Adams, J. Appl. Cryst.* **2002**, *35*, 126-136.

**Keywords:** software, libraries, programming

## MS.62.4

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### DiffPy - an open-source library for powder crystallography

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DiffPy is an open-source collection of applications and libraries for structure analysis from powder diffraction data. DiffPy is written in Python and C++ and has been developed as a part of DANSE, the Distributed Data Analysis for Neutron Scattering Experiments. The library is focused on nanoscale structure analysis using atomic Pair Distribution Functions (PDF), and on sequential Rietveld refinements of multiple datasets that are obtained with latest, high-throughput neutron instruments. For such studies the library provides user-friendly GUI applications PDFgui [1] and SrRietveld [2], which are intended for general, non-programmer users. The library can be also accessed at a lower level to calculate various structure quantities (e.g., PDF, bond valence sums, Rietveld refinement residuum) or to setup a specialized structure refinement that combines multiple experimental probes in a single fit (e.g., x-ray and neutron PDFs). DiffPy can be used as a library from both Python or C++ layer, where Python interface has

been designed for ease of use and the C++ layer for speed. The object-oriented design makes the library easy to extend or customize, for example the PDF calculator can be easily switched to use user-defined peak profiles, that can be implemented either in Python or C++. The DiffPy library includes the Liga algorithm for structure determination from experimental PDFs. [3] The presentation will provide an overview of the DiffPy functionality, demo several examples for accessing the library from Python and C++, and describe its usage for structure analysis of metallofullerene molecules from experimental PDF.

[1] C.L. Farrow, P. Juhas, J.W. Liu, D. Bryndin, E.S. Bozin, J. Bloch, Th. Proffen, S.J.L. Billinge, *J. Phys. Condens. Matter* **2007**, *19*, 335219. [2] P. Tian, W. Zhou, J. Liu, Y. Shang, C.L. Farrow, P. Juhas, S.J.L. Billinge, *arXiv: 1006.0435*, **2010**. [3] P. Juhas, D.M. Cherba, P.M. Duxbury, W.F. Punch, S.J.L. *Nature* **2006**, *440*, 655-658.

**Keywords:** software, diffraction, powder

## MS.62.5

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### MyTARDIS: Managing the Lifecycle of Crystallography Data

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MyTARDIS is an automated solution for cataloging, managing and assisting the sharing of data in a private and secure way. TARDIS is its counterpart that provides a central index for published data. MyTARDIS is currently deployed at the Australian Synchrotron to automatically catalogue and store a scientist's raw data. Together, MyTARDIS and TARDIS provide a complete end-to-end solution for data management, from the initial generation of the data through to its eventual publication.

As a scientist collects data at the Australian Synchrotron, it's routed to a MyTARDIS federated node hosted at the their home institution. This allows them to log in to the MyTARDIS web interface using their standard institutional log in credentials, browse their data locally and its associated metadata parameters and download all or parts of an experiment. Researchers can freely add derived data alongside their raw data via a simple dataset upload mechanism. MyTARDIS has been designed to provide researchers with the ability to regularly archive, share and preserve their data across time and has already resulted in raw and derived data being published and cited within publications in journals such as Nature.

This presentation will demonstrate the entire workflow of the MyTARDIS/TARDIS systems, from the initial collection of raw diffraction images, to its eventual publication. Additionally, new features planned and prototyped such as molecular replacement in the cloud via the MyTARDIS interface will be explained and demonstrated.

**Keywords:** data, publishing, synchrotron

## MS.63.1

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### Structural and magnetic transitions of Cd<sub>6</sub>R approximants

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Cd<sub>6</sub>R(R:rare earth elements) crystals are regarded as 1/1 approximants to the Cd<sub>5,7</sub>Yb icosahedral quasicrystal[1]. At 300K, they are *bcc* phases which are made of so-called Tsai-type clusters. A Tsai-type cluster is composed of four successive atomic shells of, from the center, Cd<sub>20</sub> dodecahedron, R<sub>12</sub> icosahedron, Cd<sub>30</sub> icosidodecahedron and Cd<sub>60</sub> rhombic triacontahedron. At the center of the cluster, there exists a disordered Cd<sub>4</sub> tetrahedron.

An occurrence of a structural phase transition has been observed in a number of the Cd<sub>6</sub>R crystals, which is attributed to orientational ordering of the central Cd<sub>4</sub> tetrahedra, resulting in various types of superstructures below *T<sub>c</sub>*. First, we will describe and classify the superstructures of Cd<sub>6</sub>R and then discuss key factors which strongly influence the transitions based on the observations.

The Cd<sub>6</sub>R crystals are also of interest in view of the magnetism since recently they are found to exhibit magnetic transitions below *T<sub>c</sub>* in a striking contrast with the cases of other 1/1 approximants. For instance, three successive magnetic transitions have been reported for R=Tb[2] and Sm[3] with different magnetic orders at the lowest temperature, i.e., antiferro- and ferrimagnetic orders at 2K, respectively. We will present magnetic properties of Cd<sub>6</sub>R(R=Nd, Sm, Gd, Tb, Dy) having the same C2/c-type superstructure below *T<sub>c</sub>* and comparison of the magnetic orders in the isostructural compounds will be made.

[1] A.P. Tsai, J.Q. Guo, E. Abe, H. Takakura, T.J. Sato, *Nature* **2000**, *408*, 537–538. [2] R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto, T. Takabatake, *Phys. Rev. B*, **2010**, *82*, 220201. [3] R. Tamura, Y. Muro, T. Hiroto, H. Yaguchi, G. Beutier, T. Takabatake, submitted.

**Keywords:** quasicrystal

### MS.63.2

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#### A dense quasicrystalline phase of hard tetrahedra

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Quasicrystals have traditionally been discovered in many binary and ternary metallic alloys. It has now become evident that aperiodic order can also be found on larger length scales in soft matter with micelles, colloids and macromolecules [1]. The experimental findings that nanoparticles can self-assemble into highly complex, ordered structures are also backed up theoretically by computer simulations [2] which, due to the larger size of the particles involved and resulting simpler particle interactions, are well suited to reproduce and study the crystallization process.

As it is now possible to synthesize nanoparticles of various shapes and interactions with high yield and high structural perfection, these particles can be seen as building blocks for assembling novel materials from bottom up with the goal of improved or unusual electrical, mechanical or other physical properties. In my presentation I focus particularly on the behavior of hard regular tetrahedra. The tetrahedral shape is highly anisotropic and therefore in its behavior distinctly different from what is known from atoms and spherical colloids.

The question of how densely tetrahedra pack has attracted much interest over the last years. In a first study, we have reported the spontaneous formation of a dodecagonal quasicrystal in Monte Carlo computer simulations [3]. A crystalline approximant of the quasicrystal with an 82-particle unit cell was compressed to a then-record packing fraction of 85.03% [3]. Very shortly after, a family of dimers packings were proposed, which were subsequently optimized to a packing fraction of 85.63% [4], the currently densest known packing of tetrahedra.

Due to its higher packing density, the dimer crystal is thermodynamically favored in the limit of infinite pressure. However, which structure is stable at finite pressures is an open question. I will discuss how we use thermodynamic integration and free energy calculations to explore the relative stability of these very different ordered phases as a function of packing density [5].

[1] S.C. Glotzer, M. Engel, *Nature* **2011**, *471*, 309-310. S. Fischer, A. Exner, K. Zielske, J. Perlich, S. Deloudi, W. Steurer, P. Lindner, S. Förster, *Proc. Nat. Acad. Sci.* **2011**, *108*, 1810-1814. [2] M. Engel, H.-R. Trebin, *Phys. Rev. Lett.* **2007**, *98*, 225505. M. Engel, *Phys. Rev. Lett.* **2011**, *106*, 095504. C.R. Iacovella, A.S. Keys, S.C. Glotzer, *arXiv:1102.5589*, **2011**. [3] A. Haji-Akbari, M. Engel, A.S. Keys, X. Zheng, R.G. Petschek, P. Palffy-Muhoray, S.C. Glotzer, *Nature* **2009**, *462*, 773-777. [4] Y. Kallus, V. Elser, S. Gravel, *Disc. Comp. Geom.* **2010**, *44*, 242-252. E.R. Chen, M. Engel, S.C. Glotzer, *Disc. Comp. Geom.* **2010**, *44*, 253-280. [5] A. Haji-Akbari, M. Engel, S.C. Glotzer, preprint **2011**.

**Keywords:** quasicrystal, nanoparticles, simulation

### MS.63.3

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#### Prediction of low-temperature phase transition in Al<sub>11</sub>Ir<sub>4</sub> compound

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The average structure of the Al<sub>11</sub>Ir<sub>4</sub> phase [1] exhibits mean occupancy of 0.5, providing 60 sites for 30 atoms in a cubic cell with 7.7Å long side. To resolve the occupancy correlations, we employ ab-initio methods and empirical pair potentials fitted to ab-initio data. Our first result is that the part of the structure plagued by many nearby low-occupancy sites is an irregular IrAl<sub>10</sub> cluster. Due to mismatch between high (icosahedral) symmetry of the cage surrounding the low-symmetric IrAl<sub>10</sub> “core”, the structure possesses configurational degrees of freedom down to low temperature. By simulated annealing in 4x4x4 supercell, we find phase transition at the temperature as low as 500 K. While the high-temperature phase has simple cubic symmetry (space group P23) in accordance with the experimentally refined structure, we predict the low-temperature phase is 2x1x1 supercell, with Pma2 space group. According to our ab-initio total energy calculations at T=0K, the low-temperature structure is stable against decomposition into competing crystalline phases.

[1] Yu. Grin, K. Peters, U. Burkhardt, K. Gotzmann, M. Ellner, *Zeitschrift für Krist.* **1997**, *212*, 439-444.

**Keywords:** phase transition, molecular dynamics simulation, atomic structure

### MS.63.4

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#### The structure of Al-Cu-Me (Me = Co, Rh, Ir) quasicrystals

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We present a real space structure refinement of three decagonal phases: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir. The structure factor, which