CRYSTALLOGRAPHY TIMES

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WELCOME

I'd like to begin this month's newsletter by congratulating the winners of the Ed Stevens Award for Excellence in Small Molecule Crystallographic Research: Chris Gianopoulos of the University of Toledo and Florian Kleemiß of the University of Regensburg, and the winner of the Ward Smith Award for Excellence in Macromolecular Crystallographic Research, Stephanie Bester of the University of Colorado Anschutz Medical Campus.

For those of you in time zones earlier than CDT, you still have time to register for the complete High-Pressure Crystallography workshop starting today. If you receive this newsletter in the CDT zone or later, you can still register and attend, but you will be a little late to the workshop.

The ACA Virtual Annual Meeting, Denver X-ray Conference, and the IUCr Hybrid Triennial Congress are fast approaching. I hope you will be able to attend at least one if not all of them. We are participating in all three conferences and will have virtual booths at all three, so please stop by and chat.

In this issue, we highlight PDF and total scattering, high-pressure crystallography, and Gloria Borgstahl and her laboratory at the University of Nebraska Medical Center.

Lastly, I review a book on Julia, MIT's (not so) new computer language.

All the best,

Joe

RIGAKU CRYSTALLOGRAPHIC AWARDS

Earlier this year, Rigaku announced the creation of awards honoring two of our crystallographic colleagues who passed away last year. The Ed Stevens Award for Excellence in Small Molecule Crystallographic Research and the Ward Smith Award for Excellence in Macromolecular Crystallographic Research.

We are pleased to announce the winners of these awards.

The Excellence in Macromolecular Crystallographic Research award goes to **Stephanie Bester**. Ph.D., currently a postdoctoral fellow in the lab of Mamuka Kvaratskhelia, Ph.D., Interdisciplinary Professor of Medicine Division of Infectious Diseases, University of Colorado School of Medicine. During graduate school, her research was focused on utilizing X-ray crystallography to study human acetylcholinesterase (hAChE), the nerve agents that inhibit it, and the therapeutic agents for treating nerve agent exposure. Currently, she is assessing the structural and mechanistic basis for viral resistance to GS- 6207, as well as utilizing structure-based drug design to develop new CA inhibitors.

Dr. Stephanie Bester

The Excellence in Small Molecule Crystallographic Research award will be shared by two excellent candidates: **Dr. Florian KleemiÃ**, UniversitÃ¤t Regensburg and **Chris Gianopoulos**, The University of Toledo. **Florian's** work on NoSpherA2 and the application of Quantum Crystallography in the context of medicinal chemistry and rational drug design based on small molecule diffraction data led to design and prediction of the silicon analogous of ibuprofen, called Sila-Ibuprofen, which in fact proved to show similar IC50 values as expected from the modelling based on the X-ray derived properties. **Chris's** work has involved charge density measurements of heavy-element systems at helium temperatures. This work has demonstrated that it is possible to collect highly accurate diffraction data at helium temperatures and that meaningful experimental charge density distributions for actinide-containing compounds can be reconstructed by means of multipole modeling with a modified Hansen-Coppens approach.

Dr. Florian KleemiÃ

Dr. Chris Gianopoulos

CRYSTALLOGRAPHY IN THE NEWS

February 13, 2020: Brent L. Nannenga, the ACA's 2022 Margaret C. Etter Early Career Award winner, has published a short review of microED (electron diffraction) and development in Structural Dynamics.

June 28, 2021: Researchers at Emory University and UC Anschutz Medical Campus have isolated and characterized a compound from the European chestnut that reduces the toxicity of MRSA.

July 1, 2021: Researchers in the UK have determined the structure of nucleic acid-bound DNA-binding domain of interferon regulatory factor 4 using very long wavelength SAD phasing methods.

July 2, 2021: Researchers in Germany and Switzerland have determined the crystal structure of an ethane-activating enzyme, an essential step towards understanding anaerobic ethane activation.

July 15, 2021: Two papers describe the use of different AI algorithms to accurately predict protein folding: one from DeepMind and Seoul National University and one from a multinational collaboration of structural biologists.

July 16, 2021: If only all crystals behaved this way: Researchers in India report on self-healing piezoelectric crystals.

WHAT CAN YOU DO WITH YOUR SYNERGY?

Calibrating the XtalLAB Synergy-S for Pair Distribution Function (PDF) Analysis

Pair Distribution Function (PDF) Analysis has become a versatile tool for understanding the structure, and ultimately properties, of materials. The most popular tool for the refinement of structures using PDF data is PDFgui. In order to bootstrap refinement of a structure using PDFgui, it is important to have reasonable starting values for the lattice parameters, and the parameters Q_{damp} and Q_{broad}. The unit cell parameters can be determined using whole powder pattern fitting (WPPF) but Q_{broad} and Q_{damp} must be determined for your experimental setup.

Observed versus calculated G(r) function. Observed data are blue circles, calculated data is the red line and the residual is the green curve.

In this application note, we have shown the process by which one can calibrate an XtalLAB Synergy system for PDF data. It is important to remember that the calibration data should be collected under the same conditions as you might collect the data on an unknown; that is, using the same wavelength, sample-to-detector distance, etc.

READ THE APPLICATION NOTE

RESEARCHER IN THE SPOTLIGHT

Professor Gloria Borgstahl
EPPLEY INSTITUTE FOR RESEARCH IN CANCER AND ALLIED DISEASES
University of Nebraska Medical Center

Dr. Borgstahl has been primarily interested in the structural biology of macromolecules essential to life. Survival and normal growth of cells rely on the basic processes of cell mobility, protection against oxidative damage, and DNA metabolism. The entire genome must be replicated reliably every cell cycle and any defect must be corrected. Borgstahl performs basic research on the protein-DNA and protein-protein interactions that govern DNA metabolic processes. Specific current studies include examination of the effects of posttranslational modification on protein-protein-DNA complexes, their binding and DNA repair activity. The laboratory is also using high-throughput screening techniques to find small molecule inhibitors as a potential breast, ovarian and pancreatic cancer treatments. A second focus is on neutron crystallography of MnSOD which is a NADA project involving crystal growth at the International Space Station. Another project includes innovative research in cellular motility that will provide new tools to macromolecular crystallographers for structure determination from modulated crystals employing the four-dimensional superspace approach, and will also provide unique structural information for the actin filament.

BOOK REVIEW

Think Julia: How to Think Like a Computer Scientist
Ben Lauwens and Allen B. Downey. O'Reilly Media, Inc., 2019. 298 pages
ISBN-13: 978-1492045038

I will be the first to admit I missed the boat on Python as a coding language. So, when a colleague mentioned this new language from MIT called Julia that was very efficient and fast, I decided to look into it. I was pleasantly surprised at the compactness of the download and the wealth of information available online. You can see this in the useful links and videos listed above. I generally look to O'Reilly for books on computer science and related topics, so I picked up *Think Julia*.

The book first elucidates some fundamental programming concepts as well as how to install and run Julia. The book progresses through more complex and abstract concepts: variables, expressions and statements, functions, conditionals and recursion, iteration, strings and arrays, dictionaries, tuples, files, structures and objects, structures and functions, multiple dispatch, subtyping, and debugging. The authors also provide details on syntax and the utilities in the base Julia distribution. Interspersed throughout the text are case studies diving deep into particular problems. Each chapter ends with hints for debugging, a glossary, and a set of exercises.

I do have one minor complaint: the book was written with the Julia 1.0 base in mind, and some features of the package associated with the book did not work with the current distribution, 1.6. Nevertheless. I found the book an easy and enlightening read, and Julia a lot of fun.

RIGAKU TOPIQ WEBINARS

Rigaku has developed a series of 20–30 minute webinars that cover a broad range of topics in the fields of X-ray diffraction, X-ray fluorescence and X-ray imaging. You can register here and also watch recordings if you cannot attend live sessions.

UPCOMING EVENTS

This workshop is primarily geared towards crystallographers with little or no experience in high-pressure crystallography and who are interested in learning how to get started. Presentations are intended to be practical and educational and include reviews of diamond anvil cells (DACs) and accessories from two DAC manufacturers, sample preparation under pressure in DACs, sample mounting/centering on a Rigaku diffractometer and data collection, and data processing and correction. The workshop will be held on July 21-22, 2021 at 8:00 AM CDT.
Read More >

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RIGAKU REAGENTS

Crystals of Fab 47e, a functionally sufated anti-gp 120 human antibody, crystallized with PS reagent 56

Discover more protein crystallization kits with Wizard Precipitant Synergy. The Wizard Precipitant Synergy protein crystallization screen targets all types of soluble protein and protein complexes. Tests have shown that this screen can triple the number of unique crystals when compared with other screens. Each unique formulation is made available in three different concentrations to increase the coverage of crystallization space. ***These related formulations are positioned in neighboring wells or tubes to simplify the analysis of crystallization behavior.*** Think smarter, not harder than the previous 64-well formats and it enables high-throughput crystallization, using 2 x 96 + 192 well formats in non-crystallization plates, for initial protein crystallization screening and crystallization optimization.

Wizard Precipitant Synergy Tubes: 1009539
Tubes, Wizard Precipitant Synergy – Rigaku Reagents

Wizard Precipitant Synergy Block: 1009552
Block, Wizard Precipitant Synergy Set – Rigaku Reagents

VIDEO OF THE MONTH

Introduction to Pair Distribution Function

A video tutorial from MoZEES (Research Centre for Mobility Zero Emission Energy Systems) and Institutt for Energiteknikk (IFE). While Bragg diffraction is well known for providing average structure information, synchrotron or neutron sources enable wider and better access to local structure information hidden in the scattering space by calculating the pair distribution function. Highly suitable for studying amorphous materials!

USEFUL LINKS

High-Pressure Crystallography
The Parsons Group
The University of Edinburgh

Crystallography and Properties of Metal Organic Framework (MOF) Compounds
Winnie K. Wong-Ng, Craig M. Brown
NIST

JOIN US ON LINKEDIN

Our LinkedIn group shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or *Rigaku Journal* issue. We also hope that you will share information about your own research and laboratory groups.

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RIGAKU X-RAY FORUM

At rigakuxrayforum.com you can find discussions about software, general crystallography issues and more. It's also the place to download the latest version of Rigaku Oxford Diffraction's CrysAlis^{Pro} software for single crystal data processing.

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