Volume 12, No. 9, November 2020

WELCOME

Good day everyone. We've had a busy month and have a lot to show for it. First, we have almost 400 people registered for the Advanced Topics School on December 7-11. We still have plenty of room so you can register below.

REGISTER

We are introducing a new hybrid counting detector this month, the HyPix-Arc 100°, which puts the unique features of the HyPix-Arc 150° into a more compact form factor.

The researcher in the spotlight this month is Dr. Johan Turkenburg, the X-ray Facilities Manager at York University's Structural Biology Laboratory.

This month we have a special treat, an article about Claire Jones, a deaf crystallographer who attended our first Practical Crystallography School with the assistance of her palantypist (stenographer). I hope you find her life story as inspiring as I have.

Our usual sections include a few noteworthy crystallography papers, a couple of interesting videos, one about Arcimboldo and the other a TED talk about Marie Curie, and links to the Arcimboldo website and applets for teaching Braggâs law as well as other crystallographic concepts. This month, Jeanette reviews *Equity in Science*, which as the title suggests is about diversity, inclusion and representation in the scientific enterprise.

Lastly, I would ask you to take a few moments to provide feedback to us in the survey so we can make sure the newsletter is as useful to you as possible.

Be safe, be sane,

Joe

CRYSTALLOGRAPHY IN THE NEWS

August 19, 2020: Researchers in the U.S. and Germany have determined the structure of hepcidin-bound ferroportin as an important step to certain disorders of iron homeostasis.

October 23, 2020: Researchers at UC Berkeley have designed a cubane-like linker for covalent organics frameworks that holds the promise of more of the structural variance that is currently possible with MOFs.

November 13, 2020: Scientists in Australia, Europe and Japan have determined that the furin-cleaved S1 fragment of the SARS-CoV2 spike protein binds directly to cell surface NRP1. Blocking this interaction with a small-molecule inhibitor or monoclonal antibodies reduced viral infection in cell culture.

PRODUCT IN THE SPOTLIGHT

HyPix-Arc 100°

The newest addition to Rigaku's HyPix range is the HyPix-Arc 100° detector. Following the early success of the HyPix-Arc 150° detector, it was clear to us that curved detectors not only make sense, but are also highly desirable. The HyPix-Arc 100° detector takes our curved HPC concept and applies it to a smaller, agile form factor. Build redundancy faster, get better data. Itâs that simple. The HyPix-Arc 100° detector provides an extra 17º of diffraction coverage compared to the HyPix 6000, which you can use to increase data collection speed or redundancy. The curvature means that reflections have less incidence angle variation, which improves data quality.

Rigaku's Family of HyPix Direct X-ray Detection Detectors

The Large Hadron Collider demanded a new detector technology that would allow subatomic particles to be measured without electronic noise. The result was hybrid photon counting (HPC) technology. By separating the electronics from the photodiode substrate, it was possible to create an area detector which is extremely fast, yet sensitive. These new detectors are able to digitally count events while eliminating noise sources such as readout noise and dark current allowing them to successfully detect extremely difficult-to-detect particles such as the Higg's boson.

Rigaku adopted the HPC detector technology for its HyPix brand of detectors due to HPC's unique, beneficial characteristics. HPC detectors directly count X-ray photons as they strike the detector and eliminate the need for an intermediate conversion of X-rays to light and subsequent integration of signal. The elimination of the X-ray-to-light conversion means that an HPC detector does not suffer from peak broadening and thus the detector can be positioned closer to the sample relative to a phosphor-based detector. The physical size of a detector face does not tell the true story of how much data can be measured. It also depends on the crystal-to-detector distance. Without peak broadening due to scintillator blooming, HPC detectors can be positioned much closer to the detector leading to a larger apparent aperture size. When the aperture is curved, it creates an even larger capture angle in the horizontal direction and far surpasses flat detectors of competing technology.

HyPix-Arc 100°

With all of the benefits of HPC technology, collect at 100 Hz without noise and measure the best data your sample has to offer, with a better capture angle due to the curved aperture.

RESEARCHER IN THE SPOTLIGHT

Dr. Johan Turkenburg

Dr. Johan Turkenburg is the X-ray Facilities Manager at York Universityâs Structural Biology Laboratory (YSBL). His main interest is the application of crystallographic and cryo-EM techniques to structural studies of biological macromolecules.

He is responsible for the in-house X-ray data collection facilities and coordinates all aspects of the application for beam time at synchrotron facilities and of synchrotron data collection. He provides crystallographic expertise to many of the research groups within the YSBL, and installs, tests and makes available crystallographic software.

More recently, he has also taken on responsibility for the cryo-EM facilities in YSBL. This currently involves sample preparation, grid screening and computing requirements, both software and hardware.

York University's biological chemistry research, including structural and chemical biology, has its epicenter in the York Structural Biology Laboratory (YSBL). Work focuses on the fundamental chemical bases for biological and biochemical processes, the use of small molecules to probe cellular biology, software and methods development and on the exploitation of enzymes in bio-catalysis.

Protein structural research was established at York in 1976 with the arrival of Eleanor and Guy Dodson. Rod Hubbard and Keith Wilson were appointed in 1983 as lecturers and together this team began the build-up of research into the development and application of the methods of protein structural analysis.

The pre-eminence of York for protein crystallography was recognized through the election of both Guy Dodson (1994) and Eleanor Dodson (2002) as FRS. Gideon Davies, who came to York full time in 1996 and became a professor in 2001, was elected as FRS in 2010.

In 2019 the YSBL was awarded the Queenâs Anniversary Prize for its pioneering work in protein molecule research.

THE RIGAKU SCHOOL FOR PRACTICAL CRYSTALLOGRAPHY MAKES A DIFFERENCE

The Rigaku School for Practical Crystallography offers scientists the opportunity to gain, revise or enhance the basic foundations of single crystal X-ray diffraction (XRD) techniques. The courses cover small molecule crystallography, as well as topics in macromolecular crystallography and powder diffraction.

The mission of the school is to expand the knowledge base of the crystallographic community and promote continued learning to as many people as possible. In keeping with this, the Rigaku School strives to accommodate and encourage the participation of people with disabilities. Recent sessions were offered online because of lockdowns resulting from the COVID-19 outbreak.

In the June session, Rigaku was pleased to welcome Dr. Claire Jones, a deaf scientist, who received her Ph.D. in Chemistry from Newcastle University and was a postdoctoral research associate at The University of Manchester (she has now moved-on to the Université de Rennes, France). Claire's Ph.D. involved the design of a set of hybrid ligands and the synthesis of lanthanide complexes of these ligands. At Manchester she worked on developing molecular organometallic photoresists for extreme ultraviolet lithography (EUVL). Currently at Université de Rennes she uses XRD as one method to characterize the metal coordination environment when photoswitchable ligands connecting two single molecular magnets (SMMs) are switched on and off. She focuses on how photoswitching of the ligands affects the magnetic properties of the complexes.

Claire decided to become a scientist at a very young age. Although her first inclination was to join the police force, her hearing loss precluded that. It was a school chemistry teacher, Mr. Brown, who encouraged her and helped her get a Nuffield Research placement, whereby a student can work in a university research group over the summer. Claire noted in hindsight that the Nuffield bursary scheme can play a significant role in helping people to determine how they feel about working in a laboratory environment. It was during this summer method project, at the University of East Anglia, that she first used crystallography.

While attending the Crystallography School, Claire was able to access her courses online via Zoom. To participate in the sessions, she was aided by a remote support worker, Laura Harrison, funded by Access to Work (AtW), a U.K. government-funded program that can help workplaces to support people with disabilities. Ms. Harrison, a palantypist, provides real-time speech-to-text reporting, delivering live streaming of text for Jones to read.

Claire tried to get a palantypist as an undergraduate, but her attempts were not successful. She experienced barriers when people erroneously assumed that her ability to speak indicated that she must also be able to hear.

Being an undergrad was actually the hardest part of her university career, Dr. Jones says now: participating and benefitting from lectures, in particular, was not always easy. "Blackboard lectures have no subtitles."

She was finally given access to a palantypist as a Ph.D. student, however, and has since found Palantype to be increasingly necessary for talks and conferences, as well as helping her to manage interactions with new or unfamiliar people (*e.g.* Skype interviews).

Claire notes that the shift to online collaboration and learning during the pandemic, while being challenging for many, has improved things for her in some regards. For example, the now-common experience of having a microphone turned off during a Zoom meeting has the useful side effect of simulating her daily life, making people more aware of the need to hear and be heard.

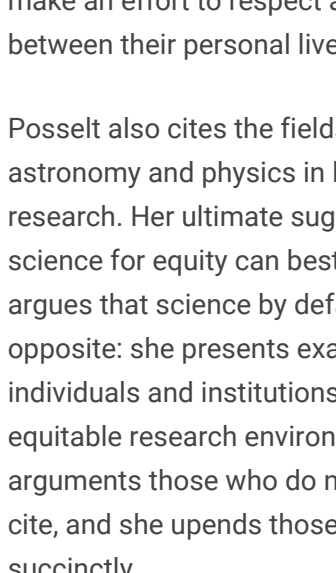
The recent online Rigaku School for Practical Crystallography was enlightening not only from a clinical standpoint–"it was good reminder of everything and it went into areas other schools did not." Most usefully, however, it offered a tailored learning experience and was receptive to feedback.

So what advice would she give to younger scientists with disabilities? Dr. Jones points out that support systems for different disabilities vary significantly among countries. She states that people have to network and take opportunities to educate others, and that the key to success is perseverance. Sometimes it will be necessary to bend rules or confront university politicians, but eventually this will earn respect.

The same is true, Dr. Jones says, for being a woman in science. There are more women in science now than ever before, yet she would still like to see a cultural change in the way early career colleagues of both sexes are treated. There are also still sometimes difficulties in collaboration for both women and those with disabilities and she has been faced with both sets. "I think people at the post-doc level are prepared to collaborate," she says, "but this does not necessarily mean that their bosses are."

Dr. Jones looks forward to realizing change as a new generation comes to prominence, although she anticipates having to fight for it.

BOOK REVIEW



Equity in Science: Representation, Culture, and the Dynamics of Change in Graduate Education
By Julie R. Posselt
IBSN: 9781503612716

Julie R. Posselt's *Equity in Science* takes a hard look at equity in the sciences through the lens of graduate education. As Posselt explains in her Preface, she chooses to focus her investigation on equity in graduate science education, as graduate studies tend to more directly feed into academia. Lack of equity, representation and diversity in graduate programs leads directly to a lack of equity, representation and diversity in post-graduate academia, such as research fellowships and professorships.

Posselt starts by presenting equity work as a research science and outlines her methodology for studying it. She positions herself, a straight, cis-gendered, female, white social scientist, as someone who has not been subjected to a significant number of the biases that she studies. She does however clarify that she has been subjected to sexual harassment and explains that the same principle applies to other forms of discrimination—it fundamentally creates an inequitable work environment for everyone.

She then moves forward with her argument and presents the various aspects of her research, detailing the means by which institutions must manage the complexity involved in changing their patterns of behavior. Posselt cites geoscience as an example of a scientific discipline with a tremendous amount of field work--a research situation in which the environment by definition is typically not as rigid or enclosed, and in which the line between personal and professional can easily be blurred. She details the hazardous implications of a "roll with it" mentality in such situations, explicating that authority figures have a responsibility to engage with their graduate students and familiarize themselves with their studentsâ varying comfort levels and make an effort to respect and understand their perspectives regarding the line between their personal lives and professional work.

Posselt also cites the fields of chemistry, psychology, applied physics, astronomy and physics in her various case studies of equity in graduate research. Her ultimate suggestion for success maintains that retooling science for equity can best be done via cultural translation. Posselt in no way argues that science by default must be an inequitable field. Quite the opposite: she presents examples of specific failures and successes by individuals and institutions to provide their graduate students with an equitable research environment. Posselt also provides a list of unfounded arguments those who do not wish to put in the effort to effect change often cite, and she upends those arguments and counters them sufficiently and succinctly.

Posselt's book reads like a dissertation and is not written in such a way that indicates she intends for her audience to be non-scientifically inclined. This book is a presentation of research written by an research academic for fellow research academics and scientists to provide them with an outline of where things stand, what things can and need to be improved, and how to improve them with regards to equity in graduate sciences. Posselt's goal, presumably, would be that a focus on establishing genuine equity in graduate scientific studies across representational groups would not only trickle down to undergraduate scientific studies but also flow upstream into tenured professorial roles.

Jeanette S. Ferrara, MFA

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.

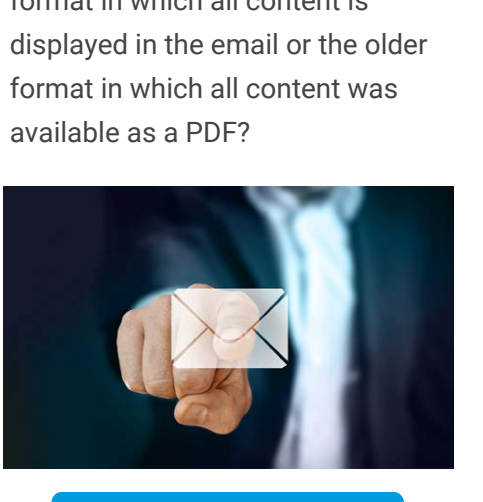
RIGAKU REAGENTS

Rigaku Reagents has extended its sales channels and is collaborating with SWISSCI to provide Rigaku Reagents' products to the European marketplace. SWISSCI is now a distributor of the popular Wizard crystallization screens manufactured by Rigaku Reagents: Unipuck Tools, stock solutions and plates.

SHOP HERE

SURVEY OF THE MONTH

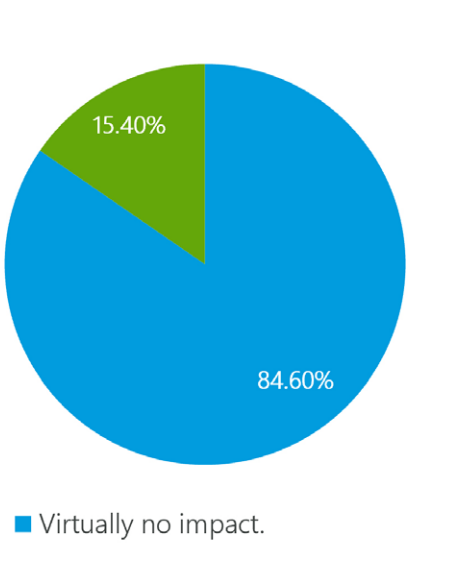
We have used the new format for the newsletter for the last two months. We would like some feedback. Do you prefer the new format in which all content is displayed in the email or the older format in which all content was available as a PDF?



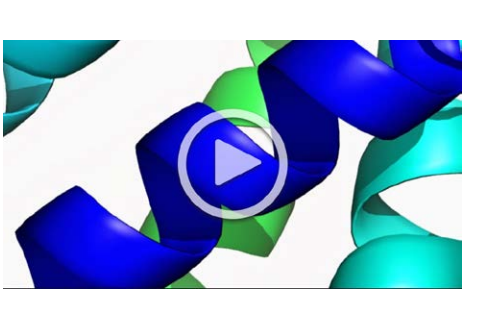
TAKE THE SURVEY

LAST ISSUE'S SURVEY RESULTS

COVID-19 cases are again rising around the world in what appears to be a second wave. How will this impact your current work regimen?



VIDEOS OF THE MONTH



ArcimboldoTeam

Welcome to the official YouTube channel for the ArcimboldoTeam tutorial videos. ARCIMBOLDO constitutes a general method for macromolecular structure solution, based on a combination of location of model fragments like small α-helices with PHASER and density modification with SHELXE. Other programs and methods are developed within our group, and content related to those will also be available.

The Genius of Marie Curie

Marie Skłodowska Curie's revolutionary research laid the groundwork for our understanding of physics and chemistry, blazing trails in oncology, technology, medicine and nuclear physics, to name a few. But what did she actually do? Shohini Ghose expounds on some of Marie Skłodowska Curie's most revolutionary discoveries.Â

USEFUL LINKS

ACRIMBOLDO

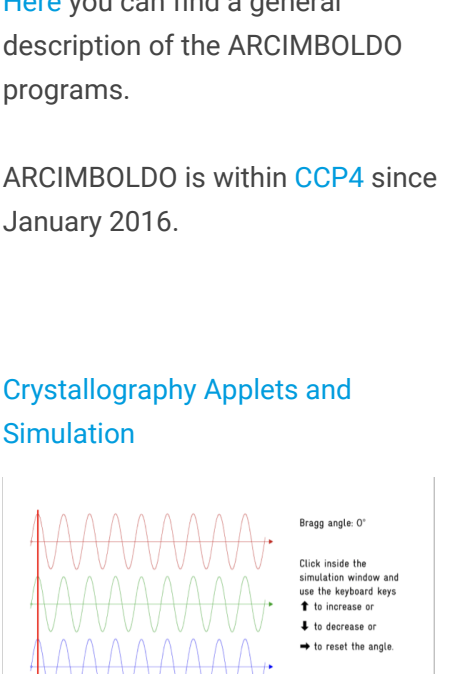
Crystallographic Ab Initio protein solution below atomic resolution

Ab Initio macromolecular phasing has been traditionally limited to small proteins at atomic resolution (1.2 Å or better unless heavy atoms are present). ARCIMBOLDO constitutes a general method for 2 Å data, based on combination of location of model fragments like small α-helices with PHASER and density modification with SHELXE, distributed over a grid of computers.

Here you can find a general description of the ARCIMBOLDO programs.

ARCIMBOLDO is within CCP4 since January 2016.

Crystallography Applets and Simulation



This web page is dedicated to the teaching of crystallography and was developed at the EPFL in Lausanne (Switzerland).

It was first developed by Wes Hardaker and further extended by Nicolas Schoeni under the responsibility of Prof. G. Chapuis.

All the applets were updated in 2016 by Nicolas Casademont et Maria Sisto.

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.

JOIN HERE

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 Diffractionâs CrysAlis^{Pro} software for single crystal data processing.

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