

Crystallography Newsletter
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In this issue:

- [A Note to Our Readers](#)
- [Crystallography in the News](#)
- [Workshops](#)
- [Webinars](#)
- [Product Spotlight](#)
- [Unipuck Kit](#)
- [Survey of the Month](#)
- [Last Issue's Survey](#)
- [Lab in the Spotlight](#)
- [Useful Link](#)
- [Videos of the Month](#)
- [Join Us on LinkedIn](#)
- [Rigaku X-ray Forum](#)
- [Book Review](#)

Rigaku Oxford Diffraction Webinar
March 31, 2020
1400 CDT

Joe Ferrara will be hosting a webinar titled "What to do when the lights go out — rethinking the homelab for structural biology research". You may register [here](#).

Rigaku Oxford Diffraction Webinar
April 9, 2020
1600 CEST, 1500 BST, 0900 CDT

Mathias Meyer will be hosting a webinar titled CrysAlis^{Pro} 40: 64-bit, Synergy, HyPix-Arc 150^o, AutoChem^{4.0}, Ewald 3D. This webinar is being presented in lieu of the in-person presentation that was to be given at a workshop after the BCA meeting at the same date and time. You may register [here](#).

Rigaku Reagents: Unipucks and Tools

Unipucks and tools are available to purchase individually or as kits. Each part of the V1-Puck has a unique serial number for identification. Custom serial numbers and puck coloring is available by request.



Unipuck Kit
SKU: 1013169
Price: \$4,075.00

[Click Here for More Information](#)

The Universal V1-Puck (unipuck) is a sample pin storage and shipping container that is compatible with many automated sample mounting systems currently in use at synchrotrons and home laboratories worldwide. The unipuck was developed in collaboration between the ALS, APS, SBC-CAT and SSRIL staff. The unipuck uses the standard AL tools for manipulation and has an outside form factor resembling the ALS pucks. There are many online resources for using unipucks, including the [following manual](#) from SSRIL and [helpful videos](#) from Diamond Light Source.

Survey of the Month

The novel coronavirus will impact climate change in a positive way by replacing face-to-face interactions with telepresence:

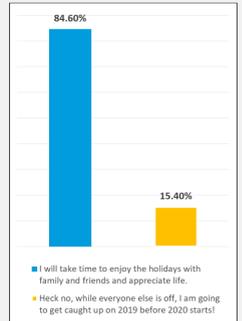


Photo by Bill Oxford on Unsplash

[Take the Survey](#)

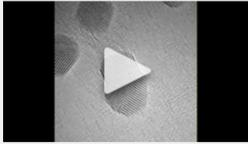
Last Issue's Survey Results

Well, it is that time of the year when people take time off and recharge, or not.



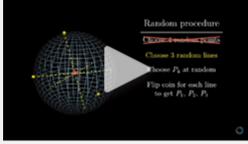
Videos of the Month

In situ formation process of a 5-fold twin from <https://doi.org/10.1126/science.aax6511>



[Watch the Video](#)

An interesting video on recasting problems to simplify them by changing perspective. The example 3Blue1Brown (a great YouTube channel) is from the 2005 Putnam Mathematical Competition



[Watch the Video](#)

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.

Rigaku X-ray Forum



www.RigakuXrayForum.com

Here 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.

We look forward to seeing you on there soon.

Subscribe to Rigaku eNewsletters



Each month, Rigaku distributes two eNewsletters: The *Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.

www.Rigaku.com/subscribe

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A Note to Our Readers

Dear Reader,

Here is the first newsletter of 2020, and a lot has happened since December 2019. The end-of-year holidays have come and gone. The novel coronavirus has spread around the globe and impacted just about everyone in profound ways. Conferences, for example, the APS and ACS national meetings, have been cancelled. Other conferences have been postponed. You'll not find us anywhere but home until mid-May. Air travel has been curtailed and people are telecommuting where possible. This month's Lab in the Spotlight, Useful Links and Survey reflects current events.

Lastly, if you are doing coronavirus research, we would very much like to hear what you are doing and if there is anything we can do to help you. If there is something we can do, by all means please let us know.

Joe Ferrara

Crystallography in the News

December 13, 2019. Researchers in the U.S. and Germany [created nitrogen vacancy color centers](#) at the very surface of the diamond anvil in a DAC as probe for stress and magnetism measurements *in situ*.

December 13, 2019. Researchers at Northwestern University, Aberdeen Proving Ground and Hong Kong Polytechnic University have developed [a series of MOFs that can be integrated into clothing to decompose organophosphate nerve agents](#). J. Am. Chem. Soc. 2019, 141, 51, 20016-20021.

December 24, 2019. Researchers in Australia used powder diffraction to determine the structure of propionitrile [to understand how it behaves in the lower reaches of Titan's atmosphere](#).

January 15, 2020. Researchers in the U.S. and Japan used X-ray crystallography to show that [β-amyloids oligomers are allosteric ligands of the α2A adrenergic receptor](#) and that preventing the activation of the receptor reduces Alzheimer's symptoms in mouse models.

January 30, 2020. Researchers from Australia, China, France, Germany, Italy, Switzerland and the U.S. [determined the structure of Trypanosoma brucei IMP dehydrogenase](#) from crystals grown in *cellulo* to identify the real cofactors of the enzyme.

February 19, 2020. Researchers in China used [cerium oxide nanowires doped with single molybdenum atoms](#) to selectively oxidize methane.

February 20, 2020. Researchers in China and Australia used powder diffraction to [study phase transitions of Prussian blue cathode models](#) as sodium ions move in and out.

February 21, 2020. Researchers in the U.S. and China used electron microscopy to observe in real time [the formation of five-fold twins among gold nanoparticles](#).

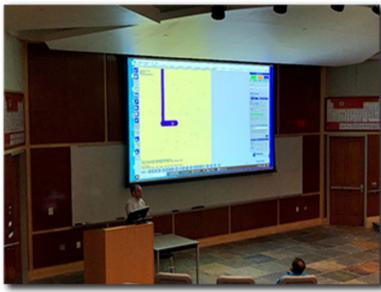
March 4, 2020. Scientists in South Korea, China and Sweden have been able to produce good crystals under conditions not normally considered viable – [while stirring in the presence of polyionic liquids](#).

And here is a paper from scientists in China [a new method for growing large, high-quality perovskite single crystals](#).

March 9, 2020. Researchers at Princeton, Cornell and Rutgers University have teased out [collective motions that produce macromolecular diffuse scattering](#) from a 3D reconstruction of reciprocal space.

Workshops

In January, we held the first Rigaku Symposium and Workshop on X-ray Crystallography, organized in collaboration with Prof. Michael Shatruk at Florida State University. More than 70 students attended, including 25 from neighboring institutions such as the University of Florida, as well as the University of South Carolina and Mississippi State University.



The afternoon of the first day was devoted to plenary lectures from researchers invited by Prof. Michael Shatruk:

- Prof. Angus Wilkinson, Georgia Institute of Technology
- Prof. Corey Thompson, Purdue University
- Prof. Weiwei Xie, Louisiana State University
- Prof. Susan Lattner, Florida State University

Two presentations were then given by Rigaku applications scientists: Dr. Akhilesh Tripathi (powder diffraction) and Dr. Pierre Le Magueres (single crystal diffraction).

On the second day, X-ray data collection and processing workshops were carried out, using the local Rigaku diffractometers at Florida State. Dr. Tripathi led the session on powder diffraction while Dr. Le Magueres did the same for single crystal diffraction.

Following a set of introductory sessions on the dual-source XtaLAB Synergy-S, recently installed at Florida State for several small groups, about 40 students gathered in a conference room for a live demonstration. Dr. Le Magueres remotely connected to the FSU diffractometer's control computer and showed all the steps of a single crystal crystallography analysis using CrysAlis^{Pro}: sample screening, pre-experiment, strategy calculation and data collection. The morning session ended with a run of manual data processing in CrysAlis^{Pro}. A similar workshop was run concurrently by Dr. Tripathi for general purpose X-ray diffraction on the SmartLab at FSU.

In the afternoon, the powder and single crystal groups were swapped so powder crystallography students could learn the basics of single crystal analysis, and vice-versa.

Pierre Le Magueres, Director of Scientific Support

Product Spotlight

[Rigaku HyPix-Arc 150^o](#)



Features

- Lowest reflection profile distortion
- Faster data collection
- Higher 2θ coverage in a single image
- All reflections measured under the same conditions
- Capture more diffracted photons per exposure

The HyPix-Arc 150^o is a unique, curved Hybrid Photon Counting (HPC) X-ray detector for single crystal diffraction applications. HyPix-Arc 150^o has the highest 2θ range at a single position available for the home lab. Collect more data in a single exposure with less reflection profile distortion: The HyPix-Arc 150^o offers 150 degrees angular coverage from edge to edge. This is more than enough to collect complete single crystal diffraction data, according to IUCr guidelines, for even Cu Kα X-ray wavelength from a single theta position. High and low angle data are measured at the same time, under the same conditions for better scaling, faster data and reduced dose time. A curved detector minimizes peak distortion by ensuring that, even at short crystal-to-detector distances, diffracted beams are closer to perpendicular than is possible with a flat geometry.

Lab in the Spotlight



February 19, 2020. Jason McLellan and coworkers at the University of Texas at Austin and the National Institute of Allergy and Infectious Diseases published the CryoEM structure of the spike protein of the novel coronavirus CoVID-19 in *Science* (DOI: 10.1126/science.abb2507). In addition to CryoEM, the [McLellan lab](#) uses X-ray crystallography to study the structural basis of host-pathogen interactions. Jason is a past (2018) winner of the American Crystallographic Association's Margaret C. Etter Early Career Award.

Useful Links

- [Worldometer's Coronavirus Live Updates](#)
Here is a link to Worldometer's coronavirus web page. There is a lot of useful info here that has tracked well with other outlets, so I believe the numbers that are being posted.
- [Cancelled Academic Events](#)
A list of cancelled academic events managed by the Center for Systems Science and Engineering at JHU
- [Crowdfight COVID-19](#)
And lastly, Crowdfight COVID-19 is an initiative from the scientific community to put all available resources at the service of the fight against COVID-19.

Book Review

[Women in their Element: Selected Women's Contributions to the Periodic System](#)
Edited By Annette Lykkes and Brigitte Van Tiggelein
ISBN: 978-981-120-768-6

Women in their Element is a delightful homage to many of the unsung heroines of the Periodic Table (and several of the sung ones as well). Each of the book's 38 chapters contains the story of a female scientist whose research contributed to our understanding of the elements as presented on The Periodic Table.

A different contributor authored each entry, and the diversity of voices and writing styles mirrors the diverse women discussed and the nature of their contributions. As the editors explain in the introduction, their goal was not to provide a comprehensive guide, as one would require much more than 500-odd pages. They chose, rather, to pay respect to as many female scientists with ties to The Periodic Table as possible. Every entry provides brief biographical information to orient the reader to the respective scientist's time and place, as well as a more detailed summary of her research and its critical role in shaping our knowledge of the elements.

Quite a few well-known names make an appearance, such as Marie Curie and Lise Meitner; however, the majority of the women are lesser known—though they certainly should not be. Because each entry is fairly succinct, the reader only gets a brief glimpse into the lives and discoveries of these women. Fortunately, each entry ends with a list of references the author used when writing it—and this list often includes other, more in-depth biographical works—allowing the reader to further pursue at their leisure.

Review by Jeanette S. Ferrara, MA