

Crystallography Newsletter  
Volume 11, No. 12, December 2019

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## Visit with Us

[16th Conference of the Asian Crystallographic Association 2019 \(AsCA 2019\)](#)  
Singapore, December 17 – 20, 2019

[DESY Photon Science Users' Meeting](#)  
Hamburg, Germany, January 30 – 31, 2020

## Florida State University and Rigaku Symposium

**January 24 – 25, 2020**  
Florida State University

Florida State University and Rigaku Americas Corporation are pleased to announce that a symposium on single crystal and powder diffraction will be held on January 24 and 25 at the main FSU campus in Tallahassee, FL.

Invited speakers include:

**Angus Wilkinson**  
Georgia Institute of Technology

**Shengqian Ma**  
University of South Florida

**Corey Thompson**  
Purdue University

**Weiwei Xie**  
Louisiana State University

**Susan Latturmer**  
Florida State University



## A Note to Our Readers

Dear Reader,

We will be moving to quarterly editions of the newsletter in 2020, with the next newsletter coming in March. The content will remain mostly the same as we continue to provide items of interest to our single crystal and SAXS customers. This month we have several interesting citations, the annual December spotlight on Rigaku's labs, some useful links, and a review of a thought-provoking book on science and society.

As you know, I have been advocating that parents need to treat girls like boys when it comes to science and engineering so girls will have the confidence to engage in STEM opportunities later in life. My friend Jenny Martin has published a children's book funded by Griffith University and SCANZ titled *My Aunt Is a Protein Crystal Scientist - That's Rad*. This book is a great way to get youngsters, especially girls, interested in science, in general, and crystallography, specifically. [You can get a copy from Griffith University](#).

We wish you and your family happy holidays and a prosperous new year.

Joe Ferrara

## Crystallography in the News

**October 9, 2019.** Australian researchers have determined first structure of a [planar hexagonally coordinated transition metal complex](#) using neutron and X-ray diffraction.

**October 9, 2019.** Georgina Ferry provides a [historical perspective on the discovery of the structure of DNA](#).

**October 14, 2019.** Researchers in the US and China have used scanning electron microscopy to determine the [sub-Å structures of solid state materials](#).

**October 23, 2019.** Using DLS, researchers from the Denmark, Japan and the UK determined the structure of an [antiaromatic-walled nanopore](#).

**November 15, 2019.** Researchers at the University of Massachusetts have [discovered a new allotrope of carbon](#) that is ferromagnetic to 125°C, harder than stainless steel and more conductive and reflective than aluminum.

**November 27, 2019.** Researchers in the US determine structures and gating mechanism of [human calcium homeostasis modulator 2](#).

**December 3, 2019.** Researchers at Stanford used CryoEM to determine the structure of a [40 kDa SAM-IV riboswitch RNA](#) at 3.7 Å resolution.

**December 6, 2019.** Researchers at Duke and Harvard used crystallography and CryoEM to study the targeted selection of [HIV-specific antibody mutations](#) by engineering B cell maturation.

**December 11, 2019.** As someone who spent their PhD working with Ni(0) in a glove box, including mounting crystals in capillaries, I can say that the [air stable Ni\(0\) catalyst synthesized](#) by the scientists at the Max Planck Institute is really cool.

## Workshops

**Akhilesh Tripathi**  
Rigaku Americas Corporation

**Pierre LeMagueres**  
Rigaku Americas Corporation

In addition the lectures, there will be hands-on workshops led by Pierre Le Magueres and Akhilesh Tripathi of Rigaku Americas Corporation. Registration is free but required, as places are limited.

### [Registration Information](#)

## **Rigaku User Meeting and CrysAlis<sup>Pro</sup>/Olex<sup>2</sup> Workshop**

**March 24 – 26, 2020**  
Rigaku Americas Corporation

We are pleased to announce that we will be holding a three-day user meeting and workshop at Rigaku Americas Corporation headquarters in The Woodlands, TX. The meeting will start Tuesday, March 24, 2020 and conclude Wednesday, March 25. The workshop will begin on March 25 and conclude March 26.

### [Registration Information](#)

## **Rigaku Reagents: Wizard Classic**



Rigaku Reagents' Wizard Classic screens were designed to increase the probability of producing crystals during the coarse screening crystallization trials of biological macromolecules.

Wizard Classic screens offer a large range of crystallants, buffers, and salts covering a broad range of crystallization space at pH levels from pH 4.5 to pH 10.5. They are proven to be a highly effective starting point for screening, with non-repeating formulations. Each of these screens is offered in either a 96 deep well block plate format or in 10 ml tubes.

Contact [ReagentOrders@Rigaku.com](mailto:ReagentOrders@Rigaku.com)  
For more information, visit the  
[Rigaku Reagents website.](#)

## **Survey of the Month**

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



The Chemical and Biophysical Instrumentation Center (CBIC) hosted the Rigaku Symposium on October 17th, 2019 at Yale University. As in previous years, the Yale chemistry community was present in a majority along with visitors from other Yale departments and nearby universities. This was the first workshop-focused event, with the day's program devoted to lectures and practical tutorials. The audience was comprised of a mix of faculty, postdoctoral researchers, and graduate and undergraduate students. Dr. Jeff Lengyel from the Cambridge Structural Database gave a fascinating retrospective on the CSD's history and recent developments in their suite of programs. Dr. Lengyel's presentation concluded with an in-depth tutorial of available features in Mercury, the structure visualization software. Dr. Pierre LeMagueres spoke to students about his career path and introduced new hardware from Rigaku. His presentation ended with step-by-step instructions on advanced features for users of the data processing software CrysAlis<sup>Pro</sup>. The program concluded with an evening poster session where we also celebrated the Rigaku Symposium's 10 year anniversary at Yale. We were delighted to be joined by Associate Provost Christopher Incarvito, who started the event in 2009 when he was the CBIC director.

## **Product Spotlight**

### [XtaLAB Synergy-DW](#)



## **A Multi-functional Single Crystal X-ray Diffractometer for a Wide Range of Crystallographic Applications**

One source with two high-flux wavelengths is the foundation of the revolutionary XtaLAB Synergy-DW single crystal X-ray diffractometer. It combines the increased flux of a rotating anode X-ray source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of research interests.

## **Configuration**

The XtaLAB Synergy-DW diffractometer is based on the proven, low-maintenance MicroMax-007 HF microfocus rotating anode. The target is constructed with two different X-ray source materials (Cu and Mo) and is coupled with an auto-switching dual wavelength optic. Copper or molybdenum X-ray radiation is available at the click of a button. The XtaLAB Synergy-DW offers up to 12x higher flux compared to the standard sealed tube X-ray sources and, utilizing only one generator, means overall maintenance is reduced.

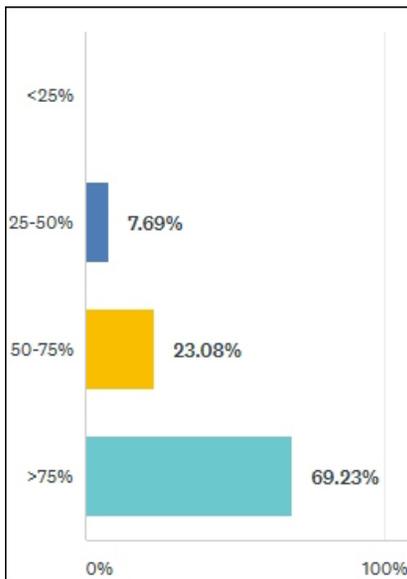


Photo by Brooke Lark on Unsplash

[Take the Survey](#)

### Last Month's Survey Results

One way to be environmentally friendly is to read and maintain journals and periodicals in digital format. Of the work-related material you read, what percent is in digital format?



### Video of the Month

Here is a link to the 29th First Annual Ig Nobel Award Ceremony. As always, the awards make you laugh then think.



[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

Rounding out the XtaLAB Synergy-DW configuration is the [fast and efficient four-circle kappa goniometer](#) which is compatible with a wide range of detectors including the HyPix-6000HE and other Hybrid Photon Counting (HPC) X-ray detectors; e.g., PILATUS and EIGER detectors.



### Benefits

- Multi-functional diffractometer to cover you wherever your research takes you
- High flux performance means you all your crystallography needs can be carried out "in-house"
- Very little downtime and easy maintenance
- No need to purchase extra software for different applications

[For more information, watch our video on the XtaLAB Synergy-DW](#)

### Lab in the Spotlight

As we have done for the last two years, I will be spotlighting our own laboratories in Frankfurt, The Woodlands and Tokyo.



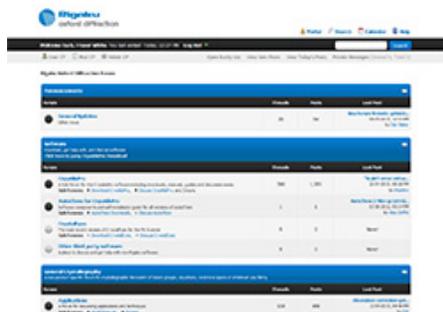
Above is the XtaLAB Synergy-S (back) and SmartLab (front) that form the core of the Rigaku Europe facility. In addition to this equipment, we have two more SmartLabs, two MiniFlexes, and two XRF tools.



Here is a panorama of the Rigaku Americas application laboratory with the FR-X and BioSAXS-2000<sup>nano</sup> with ASC-96 in the right foreground, a brand new XtaLAB Synergy-S on the left side, and MicroMax-007 HF with AFC11 and ACTOR using CrysAlis<sup>Pro</sup> for instrument control and scheduling. Not visible are the SmartLab and SmartLab SE bays, nano3DX X-ray microscope and CT Lab bay, MiniFlexes, and XRF instrument bays.

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](http://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<sup>Pro</sup> 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](http://www.Rigaku.com/subscribe)



Here is a view looking into the main entrance of the application laboratory at our Tokyo factory. In front are display cases showing some of the awards Rigaku has won. To the left is the "mini" bay with a Miniflex and XtaLAB mini. Along the corridors, you will find an XtaLAB Synergy-S and BioSAXS-2000<sup>nano</sup> as well as tools for GP-XRD, X-ray Microscopy, X-ray fluorescence, stress measurement, and thermogravimetric analysis.

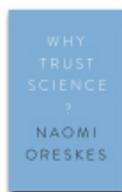
### Useful Link



#### [C&EN's Holiday Gift Guide 2019](#)

Need inspiration for holiday gifts? Leave it to C&EN's 2019 holiday gift guide. Ideas are chemistry-themed gifts for the scientists in your life.

### Book Review



#### [Why Trust Science?](#)

By Naomi Oreskes, ISBN: 9780691179001

Naomi Oreskes' *Why Trust Science?* is the book version of a series of lectures the scientist and science historian gave at Princeton University in Fall 2016. For those not fortunate enough to have attended the university's Tanner Lectures on Human Values, the book contains not only the text of Oreskes' two lectures, but the four commentaries given at the time by distinguished members of other fields. It also includes Oreskes' reply to her commentators.

Although Oreskes gave her original lectures over three years ago, the content and context of her work is as relevant as ever. One critical thing to remember when reading is that the title of her book is not *Should We Trust Science?*, but rather *Why Trust Science?*, and in this book, Oreskes details exactly that, using specific examples to illustrate a larger issue plaguing the American zeitgeist as the second decade of the twenty-first century comes to a close.

Oreskes answers her titular question eloquently in the first chapter, "Why Trust Science?: Perspectives from the History and Philosophy of Science." Her second chapter, "Science Gone Awry," is where things get interesting. It implicitly addresses the question of "should we trust science?" since, as Oreskes demonstrates, sometimes science does get it wrong. Her examples—the Limited Energy Theory, rejection of Continental Drift, eugenics, the link between hormonal birth control and depression, and dental floss—illustrate an important point. Sometimes, science gets the facts wrong, plain and simple. And sometimes, science gets it right, but the powers that be manipulate the perception of scientific discovery in the eyes of the general public.

One critical example Oreskes visits in the book that gets revisited by her commentators is that of climate change. A significant proportion of climate change research in the past decades has been funded by none other than the petroleum industry. Indeed, as I am writing this, oil and gas giant ExxonMobil is headed to court in New York over claims that the company misled investors regarding the planetary impact of climate change as caused by overuse of petroleum-based products and transportation. At this stage in the game, climate change denial seems futile in the face of the mounting evidence to the contrary—but thanks to decades of false information perpetuated by big oil conglomerates with a significant conflict of interest, the damage, both to popular perceptions of the problem and to the planet itself, is largely irreversible.

Oreskes does not address the Big Sugar scandal that hit the news in Fall 2016—only a few months before she gave her original lectures. But that instance—where sugar manufacturing corporations paid Harvard University researchers to downplay in published works the negative health effects of sugar consumption—further illustrates a similar point.

Science, like any discipline, can be distorted and skewed by the lens through which its

findings are viewed. Nazi scientists took Charles Darwin's theories of evolution and natural selection to a eugenics extreme. Their abuse of Darwin's survival of the fittest research was abominable—but it does not and should not detract from the heft of his original contributions to the field of evolutionary biology.

Before discounting any scientific research, or even before believing every newly published paper out there, one should consider the context of the facts being presented.

Oreskes book is highly academic, both in diction and tone—indicative of the book's origins as a series of lectures at a top university. She makes multiple references to her other published works throughout the book, including *Merchants of Doubt*, and after having read *Why Trust Science?*, I find myself inclined to give them a read.

Review by Jeanette S. Ferrara, MA



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