

Volume 16, No. 1, January 2024 INTRODUCTION

Crystallographic Service's instruments after famous female the presentation of a certificate to Elspeth.

The UK National Electron Diffraction Facility grand opening was held on January 16, 2024. In keeping with the tradition of naming the UK National

Kathleen Lonsdale, the recently installed XtaLAB Synergy-ED was named Els after Elspeth Garman. This was celebrated at the grand opening with

crystallographers, Ada Yonath, Rosalind Franklin, Dorothy Hodgkin and

Left to right, front row: Simon Coles (Professor of Structural Chemistry and director of the

UK NCS and NEDF) Andrew Hector (Head of the School of Chemistry), Mark Benson,

illustrious career of Damian Kucharczyk, the visionary founder of KUMA

on a well-deserved retirement, leaving an indelible mark on the world of

Throughout his remarkable journey, Damian has not only pioneered the

field but has also played a pivotal role in shaping the next generation of

expertise in the art of crystallography to the innovative instruments he

crystallographers. Countless individuals, both past and present, owe their

Adrian Jones presenting Damian with a retirement gift of a signed group photo of the

As Damian transitions into this new chapter of life, we extend our heartfelt

legacy that will endure in the annals of crystallography. Moreover, Damian

leaves behind a strong team poised to continue his ground-breaking work,

Rigaku. May this well-earned respite be a time of reflection and enjoyment for Damian, who has undeniably enriched the scientific community with his

This month we highlight the XtaLAB Synergy-S, Mark Del Campo provides the Tip of the Month and Jeanette reviews: Not Just for the Boys: Why We

TOPIQ | High-pressure Crystallography on

the Rigaku XtaLAB Synergy-S Diffractometer

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A RIGAKU WEBINAR

High-pressure Crystallography on the Rigaku XtaLAB Synergy-S Diffractometer

In this Webinar, the process of conducting a high-pressure crystallographic

pressure crystallography provides a tool for researchers to effect changes in

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experiment on the XtaLAB Synergy-S will be explained and software

features in CrysAlisPro relevant to the technique will be covered. High-

the structure of matter and ultimately understand the phenomena such

ensuring that the torch of innovation and discovery remains brightly lit in

wishes for a retirement filled with joy, fulfillment and the satisfaction of a

Diffraction in 1993. After decades of dedicated service, Damian embarked

Elspeth Garman (Oxford University Emerita) and Hiroyuki Kanda.

crystallography.

meticulously designed.

Rigaku Polska Team.

passion and contributions.

Need More Women in Science

Joe Ferrara and Mark Benson

changes can induce.

Time Zone Converter

Wednesday, March 7, 2024 at 09:00 CST

TOPIQ | Pump-multiprobe

A RIGAKU WEBINAR

Synergy-R system

XtaLAB Synergy-R system >

LAURE VENDIER

Time Zone Converter

Presenter

Atlanta).

Wednesday, January 31, 2024 at 09:00 CST

Dr. Lauren Hatcher, Cardiff University

Photocrystallography on the XtaLAB

Pump-multiprobe Photocrystallography on the XtaLAB Synergy-R system

In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pump-

Read more about TOPIQ | Pump-multiprobe Photocrystallography on the

REGISTER NOW

Laure Vendier (INSA Toulouse engineer, physics engineering option, 1994), obtained her PhD in 1997 in the field of materials for electronics (thesis cosupervised by the INSA Toulouse and the Georgia Institute of Technology in

She was recruited at the CNRS in 1998 for an engineering position at

CEMES within the X-ray diffraction department, and joined the LCC in 2003

Her main interests are crystallography on small molecules, more specifically the determination of molecular architecture by X-ray diffraction, on sensitive crystals, but also structural studies on powders and nanomaterials by X-ray

RESEARCHER IN THE SPOTLIGHT:

to take responsibility for the laboratory's XRD platform.

probe Photocrystallography data down to a time-resolution of 10 ms, producing full, 3D structures at regular time-points to create 3D molecular

Be safe,

Last month marked a momentous occasion as we celebrated the

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 and electron diffraction, X-ray fluorescence and X-ray imaging. You can watch recordings of our past sessions here. **UPCOMING WEBINAR: TOPIQ | Pump-multiprobe**

09:00 CST

Photocrystallography on the **XtaLAB Synergy-R system** Wednesday, January 31, 2024 at Presenter: Dr. Lauren Hatcher, **Cardiff University** In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pumpprobe Photocrystallography data down to a time-resolution of 10 ms, producing full, 3D structures at regular time-points to create 3D

molecular movies. Register now> **TOPIQ | High-pressure** Crystallography on the Rigaku **XtaLAB Synergy-S** Diffractometer Wednesday, March 7, 2024 at 09:00 CST In this Webinar, the process of conducting a high-pressure crystallographic experiment on the XtaLAB Synergy-S will be explained and software features in CrysAlis^{Pro} relevant to the technique will be covered. Highpressure crystallography provides

a tool for researchers to effect changes in the structure of matter and ultimately understand the phenomena such changes can

induce.

Register now> **UPCOMING EVENTS:** Pittcon 2024, February 24- 28, 2024, San Diego, CA ACS Spring 2024, March 17- 21, 2024, New Orleans, LA 32nd Annual Meeting of the German Crystallographic Society (DGK), March 18-21, 2024, Bayreuth, DE.

BCA Spring Meeting, March 25-28, 2024, Leeds, UK. 2024 ACA Summer Course in Chemical Crystallography at Purdue University from June 23-30, 2024.

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updates on how they use these

laboratories. You can also catch

up on the latest newsletter or

Rigaku Journal issue. We also

techniques in their own

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

CrysAlis^{Pro} software for single

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Rigaku Oxford Diffraction's

crystal data processing.

diffraction. Recently she had the opportunity to train and develop studies under high pressure by XRD on single crystal. **TECHNIQUE IN THE SPOTLIGHT:** HIGH-PRESSURE CRYSTALLOGRAPHY High-pressure crystallography has been conducted for many decades now,

diffract from the sample inside.

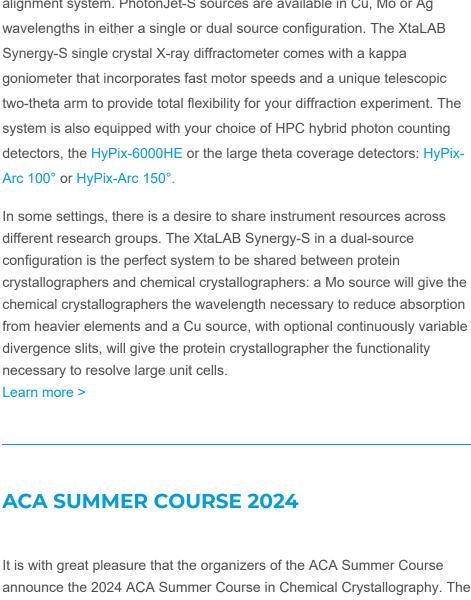
magnetism or polymerization, among others. Understanding these structural changes can lead to an understanding of how to control the effects in a desirable and useful way. Conducting high-pressure experiments allows researchers to observe

with the origins of the modern method in approx. the 1970s. The method uses a device called a Diamond Anvil Cell (DAC) to isotropically compress a sample to pressures of up to 100 GPa whilst allowing X-rays to reach and

The application of pressure can bring structural changes, typically through the modification of intermolecular interactions, which in turn may bring about

effects such as phase changes, amorphization, superconductivity,

XtaLAB Synergy-S



course will be held at Purdue University from June 23-30, 2024. For more

details, please check the web page at https://acasummercourse.net/

TIP OF THE MONTH Tip of the Month: Beam Slit (Divergence) Control By Mark Del Campo When using Cu radiation with a Rigaku VHF optic on a XtaLAB Synergy-S, -R, or -DW, diffraction spots can overlap in certain situations. For example, if a crystal is pseudo-merohedrally twinned then the spots from multiple

down list, followed by a left-click on Beam slit.

START/STOP

🛑 CRYO)(🕞 X-RAY)

CAM)

lattices may overlap. Also, if a crystal has one or more large unit cell

dimension (>120 Å) then the spots on that long edge may overlap. In both cases, the beam divergence should be reduced using the Beam Slit Control in CrysAlis^{Pro} to move the beam slit into the X-ray beam. First, make sure the detector is at the appropriate starting distance based on the unit cell's largest primitive dimension (i.e., for a Rigaku HyPix detector use a distance in mm equal to the longest cell edge divided by 3). Then, access the Beam Slit Control by a right-mouse-click on the X-RAY button to open a drop-

> Generator options Display generator state

Devices connection manager

Beam slit

determination of beam-sensitive nanocrystalline materials.

Relative intensity 100 Figure 3. Beam Slit - Set Values Dialog. For a XtaLAB Synergy-DW, the DW Beam Slit Controller interface is a little different in appearance, but similar in function. First, click on Init Beam Slit Control to connect to the slit and establish control. Then, click on the right button to change to the scale desired for changing the slit. The options are mR (divergence), % intensity, or mm position of the slit. Then, enter a numerical value in the box that is within the range displayed and click on

Set value to move the slit. Finally, click on Exit and disconnect.

4.00

39

3.03

DW Beam Slit Control (Optics: VHF 450mm) (1.0.2)

Beam Sit status Beam Sit Cu: 4.00mR

mR:

Int. [%]:

Pos. [mm]

appropriate slit setting for a given crystal.

BEAM SLIT - set values dialog (1.0.1) Mode operation Service

Motor position

Divergence

0

9.0

CRYSALIS

Range: 10.00 - 0.10 mR

<10.00:0.10>

<100:0>

Figure 4. The XtaLAB Synergy-DW Beam Slit Controller interface.

Be patient and remember that it may take several rounds of changing the beam divergence followed by a pre-experiment (screening) to establish an

displayed at the top of the image display in CrysAlis^{Pro}. And when opening any data set in a data processing instance of CrysAlis^{Pro}, the slit setting

Finally, note that the current slit position of the instrument is always

used for the data can be viewed under the Data Collection executive summary on the right side of the GUI. LM: 40.00 mA: 30.00 Temps 10000 K Sample light on, Beam slift positions 9 step(s), divergences 7.1mR, intensitys 74% Figure 5. The current slit position of the instrument is always displayed at the top of the image display in CrysAlis^{Pro}. B **Data Collection** Edit runs

Review: Not Just for the Boys: Why We Need More Women in Science By Athene Donald ISBN 9780192893406 Athene Donald's Not Just for the Boys: Why We Need More Women in Science is a concise but compelling read for anyone and everyone. It's a book for women who have pursued a career in science, regardless of where they are in that career. It's also a book for men in the same

have an interest in science or math. Indeed, although Donald is writing about the importance of women in science and detailing the historical, present, and future impediments that can keep them from reaching their desired position in their respective fields, much of Donald's argument can be applied to any field in which men outnumber women. As a Professor Emerita of Experimental Physics at the University of Cambridge, Donald certainly has her own breadth of experience navigating science and academia as a woman. And while she does draw on that experience, much of Not Just for the Boys includes numerous anecdotes and personal stories from women across scientific disciplines, as well as explanations of research findings from studies designed to determine if gender gaps really do exist in the sciences, both at the professional and student level (spoiler alert: they do). Donald begins with a chapter entitled "What's the Problem?" in which she outlines and addresses the issues at hand—namely, after decades of initiatives to increase the number of women in science and the fact that the population of the world is roughly 50% women, women do not account for 50% of scientists. She then proceeds to delve into the issue as deeply

as she can in a book of a little over 200 pages, starting with how scientists are perceived in society (mostly as men) and how that impacts young women's perceptions of what they can be. She also digs into what can keep young women from pursuing roles in scientific careers even if they have a proven interest, and what obstacles women can face once they've already made their career in the sciences. At the end of the day, it's still a man's world, and science is no exception. Donald argues that science, like any field, benefits from the diversity of those pursuing it. She acknowledges that, as a white woman, she still garners certain privileges not afforded to colleagues of color, particularly women of color. But Donald also acknowledges that as a white woman, she is not the right person to be writing a book about intersectionality in the sciences. While Donald's book will certainly resonate for any woman in the sciences, if you're looking for a read about women of color in the sciences, Jasmine Brown's Twice as Hard is an excellent choice.

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9009 New Trails Drive, The Woodlands, TX 77381, United States

3-dimensional structural changes at pressure, and is a valuable tool in materials science, pharmaceutical research and much more. Modern instrumentation has made high-pressure structural research more accessible than ever before, with advances in software and hardware reducing the entry barrier for new researchers. If you are interested in this technique and would like to know more, please join us for our webinar in March. PRODUCT IN THE SPOTLIGHT **XtaLAB Synergy-S**

With your success utmost in our minds, we have developed the XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction. Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, accurate data in an intelligent fashion. The system is based around the PhotonJet-S series of microfocus X-ray sources that optionally incorporate continuously variable divergence slits. These third-generation sources have been designed to maximize X-ray photons at the sample by using a combination of new optics, new longer-life tubes and an improved alignment system. PhotonJet-S sources are available in Cu, Mo or Ag wavelengths in either a single or dual source configuration. The XtaLAB Synergy-S single crystal X-ray diffractometer comes with a kappa goniometer that incorporates fast motor speeds and a unique telescopic two-theta arm to provide total flexibility for your diffraction experiment. The system is also equipped with your choice of HPC hybrid photon counting detectors, the HyPix-6000HE or the large theta coverage detectors: HyPix-Arc 100° or HyPix-Arc 150°. In some settings, there is a desire to share instrument resources across different research groups. The XtaLAB Synergy-S in a dual-source

Applications for the course opened on January 1, 2024. For international attendees requiring a visa to enter the United States: There have been increasingly long processing periods in recent years to obtain a B1 visa. If you are planning to apply for the course, please contact us as soon as possible. Should you have any questions, please email info@acasummercourse.net The Organizers Allen Oliver (University of Notre Dame), aoliver2@nd.edu Matthias Zeller (Purdue University), zeller4@purdue.edu Christos Malliakas (Northwestern), c-malliakas@northwestern.edu Charlotte Stern (Northwestern), c-stern@northwestern.edu Nathaniel Barker (Northwestern), nathaniel.barker@northwestern.edu **CRYSTALLOGRAPHY IN THE NEWS** November 16, 2023 Researchers from China have synthesized and characterized a triplet Fe

compound with a weak Fe-C triple bond that provides some unique

Scientists from Israel and the US used X-ray crystallography and cryo-EM to determine how Gabija proteins assemble into a supramolecular complex

Scientists from France and the UK have determined the structure of the glutamate receptor GluD1 with GABA bound. This receptor is present at

Scientists from Canada and Spain used NMR and X-ray crystallography to study shuttling of planar guests in a molecular box 22 Å long x 7 Å wide.

Researchers from China have synthesized and characterized a stable rhodium-coordinated carbene with a $\sigma^0\pi^2$ electronic configuration.

Scientists from Canada, Germany and Sweden report the use of serial STEM data collection provided high-resolution data for ab initio structure

synthetic properties. November 22, 2023

December 7, 2023

January 3, 2024

January 4, 2024

January 9, 2024

that degrades phage DNA in bacteria.

both excitatory and inhibitory synapses.

Figure 1. Access the Beam Slit Control. For a XtaLAB Synergy-S or -R, this opens a Beam Slit Controller interface that shows the current motor position of the slit and the approximate divergence and relative beam intensity. Click on the Set button to open the settings. Then, click and drag the slider to the right to choose a reduction in beam divergence and click **OK** to move the slit. XtaLAB Synergy Beam Slit Controller (1.0.2) IS system cabinet 2.0.0.61 Final_rev941_PC82 Motor position Divergence 9.0 100 Status Set values Motor fault O Motor target position Motor pos invalid O Six encoder fault O \ Status: Device connected. Figure 2. The XtaLAB Beam Slit Controller interface.

Cu

STATUS

STATISTICS
Frames/Runs: 1940/7, done: 1940/7
scan width: 0.20, distance: 33.00
Overflows: 0
Pixel min: -1, max: 21682, max cps: 47151
Exposure time min: 0.60, max: 0.60
Dose time 19m 24s
Total time 20m 21s
HyPix readouts: 44620
HyPix readouts: 44620
Typix readouts: 44620
HyPix readouts: 44620
Typix readouts: 44620
Typix readouts: 44620
Typix readouts: 44620 40.0/40.0,mA: 30.000/30.000 (min/max) n slit: 7.1mR divergence, 71% intensit Figure 6. The slit setting used for the data can be viewed under the Data Collection executive summary on the right side of the GUI. **BOOK REVIEW** ATHENE DONALD

position. It's a book for anyone who has a young girl or young woman in their life with an interest in science and math. But it's also a book for anyone who has a young girl or young woman in their life who doesn't

Review by Jeanette S. Ferrara, MFA