

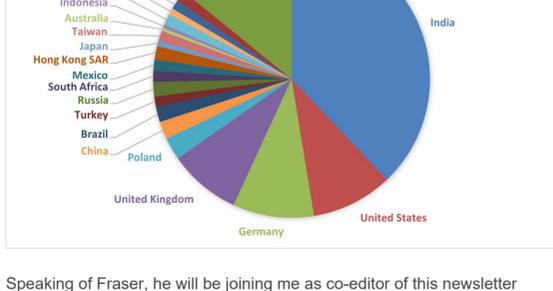


CRYSTALLOGRAPHY TIMES

Volume 14, No. 2, February 2022

WELCOME

Just after the January newsletter posted, we completed the Rigaku School for Practical Crystallography. For this edition of the school, the number of students peaked at more than 500 and most who took the exam passed. I had planned some swag for whoever scored 100 on the exam, but, alas, the high score was 96. The pie chart below shows the distribution of students who attended by country. I'd like to offer special thanks to all the instructors: Mathias Meyer, Bernhard Spingler, Pierre Le Maguerès, Christian Göb, Chris Schürmann, Horst Puschmann, Fraser White and Jakub Wojciechowski. I'd like to thank Fraser, who coded all the backend automation and Amanda Cochran, who handled Zoom Webinar.



Speaking of Fraser, he will be joining me as co-editor of this newsletter going forward. Fraser will be handling the spotlight items, videos, useful links and other items with me.

This month I am pleased to report that we will attend many conferences and workshops this spring and summer in person. The first is the German Society for Crystallography (DGK) Annual Meeting in München, Germany. The other meetings we'll be attending in person are listed to the right.

In other good news, researchers at McMaster University have developed an [inhaled COVID vaccine](#) that shows promising efficacy.

Joe

LABORATORY IN THE SPOTLIGHT

Professor Neil Champness
University of Birmingham



Professor Champness is currently at the School of Chemistry, University of Birmingham, where he holds the Norman Haworth Chair. Prior to taking up this position in 2021, he spent some years in the chemistry department at the University of Nottingham, where he took up his first academic position in 1995 and held the Chair of Chemical Nanoscience starting in 2004.

Professor Champness is an active author, having published over 280 research papers in addition to review papers and book chapters. He is interested in the fields of supramolecular chemistry, metal-organic frameworks, mechanically interlocked molecules and surface self-assembly.

In a recent *Nature Communications* paper, Professor Champness and coauthors were able to determine the structure of samples of only approx. 100 nm thickness using Rigaku's XtaLAB Synergy-ED.

You can read the full paper here: [Pearce, N., Reynolds, K.E.A., Kayal, S. et al. Selective photoinduced charge separation in peryleneimide-pillar\[5\]arene rotaxanes. *Nat Commun* 13, 415 \(2022\)](#)

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-S

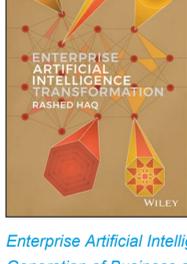


The XtaLAB Synergy-S is Rigaku's most popular single crystal X-ray diffractometer. Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, accurate data in an intelligent fashion. The system 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 Hybrid Photon Counting (HPC) detectors, the HyPix-Arc 100° (pictured), the HyPix-6000HE or HyPix-Arc 150°.

The Synergy-S will improve your ability to investigate small samples because the solid-state pixel array technology of the HyPix X-ray detectors means that X-ray photons are counted instantaneously as they arrive at the detector. There is no conversion to visible light by a scintillator so the energy of the photon can be assessed at moment of detection leading to essentially noise-free images. Noise-free images mean you can count longer for weakly diffracting crystals without a loss in data quality arising from detector noise. Most of our customers tell us that the HyPix detector has been a game changer for their productivity by speeding up data collection times and reducing the size of crystals that can be measured.

[Read More >](#)

BOOK REVIEW



[Enterprise Artificial Intelligence Transformation: A Playbook for the Next Generation of Business and Technology Leaders](#)

By Rashed Haq

ISBN: 978-1-119-66593-9

Rashed Haq's *Enterprise Artificial Intelligence Transformation: A Playbook for the Next Generation of Business and Technology Leaders* is an excellent guide to the critical importance of developing AI infrastructures from a business leadership standpoint. Haq is the Vice President of Robotics at Cruise, a leading company in the self-driving vehicle industry.

Prior to that, he was the Global Head of AI & Data and Group Vice President at Publicis Sapient. He's been at the forefront of AI innovations in data and analytics from a business perspective for over two decades.

The book begins with a foreword by Steve Guggenheimer, the Corporate Vice President for AI at Microsoft. Guggenheimer describes the number of patterns emerging in AI development across industries, from virtual customer service agents to autonomous systems, such as self-driving cars. The intent of the book is made quite clear: this isn't meant for an AI systems expert who wants to learn more about their field. This is intended for anyone in the business world today faced with the economic and social challenges of maintaining massive data infrastructures and allowing them to adapt and evolve in real-time.

In the prologue, aptly titled "A Guide to This Book," Haq lays out his roadmap and clearly indicates where the reader is going to start with this self-titled playbook, and where they are going to end up. In the event a reader feels a certain later section might better apply to their immediate needs than an earlier one, Haq makes it very easy for them to jump around and explore each self-encapsulated chapter in the manner that is most productive for their business needs.

Part I, A Brief Introduction to Artificial Intelligence is just that. Haq walks the reader through a brief history of AI, how the concept came to be and was developed to fruition. He explains exactly what AI is, how it works and, perhaps most importantly, the critical applications of AI in any modern business.

Part II, Artificial Intelligence in the Enterprise delves more deeply into these applications and the role AI can play in any business model to improve data collection, storage, and analysis. Haq walks through the role of AI in specific fields, such as finance and healthcare, and explains not only what the current AI possibilities are today but what the potential gaps are that future AI developments may be able to bridge.

Part III, Building Your Enterprise AI Capability is where the "playbook" part of the title really comes into play. Haq provides the reader with a seemingly step-by-step guide to AI-related strategy and lifecycle development that can be applied to any business in any industry.

Part IV, Delving Deeper into AI Architecture and Modeling is a hands-on dive into AI specifics and how to build them. Haq walks the reader through a specific example of AI platform development and how to structure effective AI modeling processes.

Part V, Looking Ahead is the briefest section of the book. Here, Haq outlines some of the challenges and considerations that need to be considered by any business employing AI infrastructures and models in order to ultimately protect the people the AI is designed to help.

Unlike many books of this nature that are either written in an extremely technical fashion by a leading academic or written in true layman's terms by a journalist, *Enterprise Artificial Intelligence Transformations* falls somewhere in the middle of that spectrum. That said, it's incredibly well-written, easy to understand, and conceptually clear. Haq takes a subject that inherently can be and often is very confusing and challenging to wrap one's brain around unless you are active in the field and makes it digestible for anyone with a desire to improve the data-driven strategy in their business.

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.

VISIT US AT:

Conferences:

[DGK Annual Meeting](#), München, Germany, March 14-17.

[ACS Spring 2022 Experience](#), San Diego, CA, March 20-24.

[38th BCA Spring Meeting](#), Leeds, UK, April 11-14.

[2022 MRS Spring Meeting and Exhibit](#), Honolulu, Hawai'i, May 8-13.

[5th International School on Aperiodic Crystals](#), Kutna Hora, Czechia, May 23-27.

[Canadian Chemistry Conference and Exhibition 2022](#), Calgary, Canada, June 13-17.

[ACA The Structural Science Society Annual Meeting](#), Portland, OR, July 29-August 3.

[33rd European Crystallographic Meeting](#), Versailles, France, August 23-27.

[44th International Conference on Coordination Chemistry](#), Rimini, Italy, August 28-September 2.

[MOF2022](#), Dresden, Germany, September 4-7.

Workshops:

[Pair Distribution Function \(PDF\) Workshop](#), April 6-7, Zoom Webinar.

[Canadian Chemical Crystallography Workshop](#), Calgary, Canada, June 9-12.

[72nd ACA Annual Meeting](#), West Lafayette, IN, June 12-18.

CRYSTALLOGRAPHY IN THE NEWS

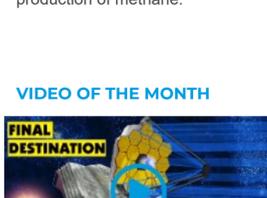
January 13, 2022: Researchers in the UK and US have synthesized and characterized [ultrahard magnetic materials](#) from mixed-valence dlanthanide complexes with metal-metal bonding.

January 28, 2022: Researchers in China have determined the structure of the [human serotonin 2A receptor with psilocin, LSD, serotonin and lisuride](#) and developed putative non-hallucinogenic psychedelic drug candidates.

February 2, 2022: Scientists in the US report the structure of a [B₁₂-dependent radical S-adenosylmethionine methylase](#) required for the synthesis of the C6 side chain needed for biosynthesis of the broad spectrum carbapenems.

Later in the same issue, scientists from France and Japan report the structure of a different [B₁₂-dependent radical S-adenosylmethionine methylase](#) to understand bacterial production of methane.

VIDEO OF THE MONTH



BIG NEWS: James Webb Space Telescope Arrives At Final Destination!

Home, home on Lagrange. Here is a video about the arrival of the [James Webb Space Telescope](#) at its home at L2.

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 [CrysAlisPro](#) software for single crystal data processing.

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