



Volume 14, No. 6, June 2022

## WELCOME

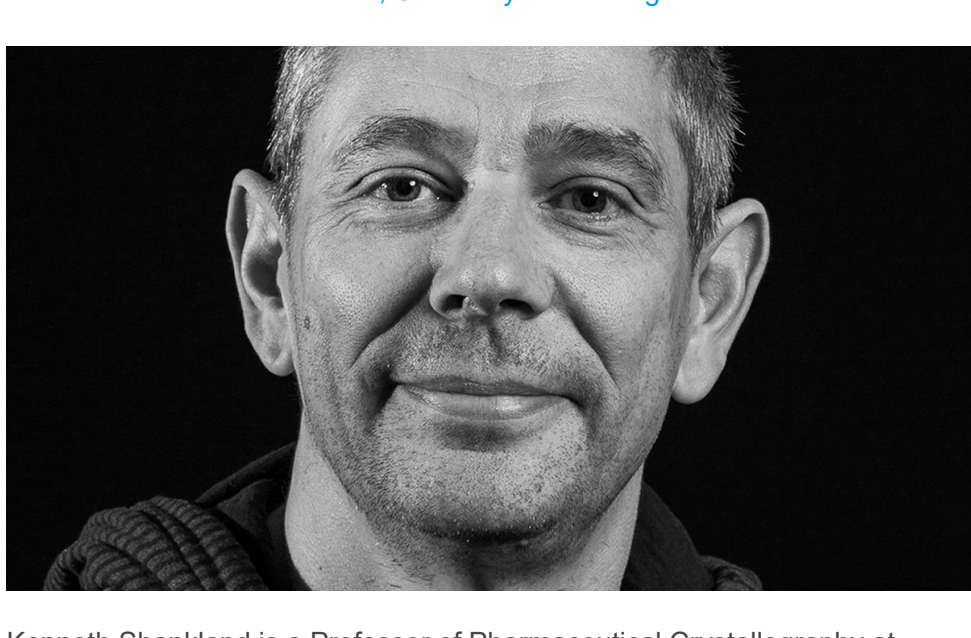
I just returned from the Canadian Chemical Crystallography Workshop at the University of Calgary. This is the first in-person CCCW since 2019. I provided my usual lecture on Fourier transforms and crystallography, while Eric Reinheimer gave a demonstration of the XtaLAB mini II and detwinning in CrysAlis<sup>Pro</sup>. This is great teaching workshop and I look forward to 2023 in Vancouver. By the way, Calgary was wonderful: cool nights and long, pleasant days. I look forward to the IUCr Congress, which will be held there in August of 2026.

As I write this Pierre Le Maguerès and Eric are teaching at the ACA Summer Course, which has been deferred until it could be held in person. We sent a XtaLAB Synergy-S to Purdue for this school, and it has been performing admirably.

This month, we highlight the work of Kenneth Shankland using DASH and microdiffraction methods. Starting on May 24, we now offer a crystal structure determination service, with data collection and scientific support on a XtaLAB Synergy-ED. We highlight this service and the XtaLAB Synergy-ED this month. Jeanette reviews *The Dawn of Everything: A New History of Humanity*. Lastly, we have compiled a list of interesting articles for your perusal and present a list of charities helping Ukraine.

## RESEARCHER IN THE SPOTLIGHT

Professor Kenneth Shankland, University of Reading



Kenneth Shankland is a Professor of Pharmaceutical Crystallography at the University of Reading. Hailing originally from Scotland and having trained as a pharmacist, he completed his first postdoctoral position in crystallography with Prof. Chris Gilmore at the University of Glasgow in 1993. He then spent 15 years working in the Data Analysis Group of the ISIS neutron scattering facility. Over his career, Kenneth has been heavily involved in crystallographic software development, principally collaborating with Prof. Bill David on the *DASH* software package for crystal structure determination from powder diffraction (SDPD) data. Marketed by the CCDC for over 20 years, *DASH* is now freely available as an open-source package (<https://github.com/CCDC-OpenSource>).

Kenneth has recently been involved with innovative work driven by his colleague Dr. Elena Kabova (principal author) with Dr. Charles Blundell (CTO, [C4X Discovery](#)) and the X-ray crystallography team at the University of Manchester's Department of Chemistry (Drs. Inigo Vitorica-Yrezabal and George Whitehead). They have used a single crystal instrument (the FR-X at Manchester) to collect SDPD-quality powder data from a wide range of pharmaceutical compounds and then solve their crystal structures to a high level of accuracy using *DASH*. This new approach is called SDPD-SX and the paper is available at the following link [Kabova et al CrystEngComm, 2022, Advance Article](#).

## PRODUCT IN THE SPOTLIGHT

Single Crystal Electron Diffraction Service

Rigaku is excited to announce that they are providing access to their state-of-the-art electron diffraction technology for crystallography projects in pharmaceutical, organic and inorganic chemistry, materials science and even mineralogy. Researchers from industry and academia will now be able to utilize the world's first turnkey electron diffractometer, the Rigaku [XtaLAB Synergy-ED](#), without the expense of having to buy one. The new program provides access to instrumentation and software—as well as in-house expertise—to assist with your projects.

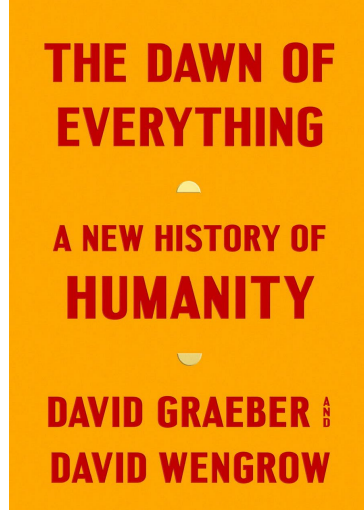
Electron diffraction is a rapidly emerging single-crystal technique for elucidating atomic structures of pharmaceuticals, catalysts, biominerals, nanomaterials and many other materials, with crystal grain sizes below 1  $\mu\text{m}$ . It requires only minute amounts of sample material and is compatible with extremely radiation-sensitive crystals. For such systems, electron diffraction goes far beyond the limits of X-ray diffraction and has been shown to succeed where even synchrotrons can't.

Rigaku will provide a comprehensive crystal structure determination service with scientific support from experienced application scientists that provides full access to everything you could possibly need, including the strictest confidentiality. Besides a refined atomic model, clients will receive all raw data generated and full access to all the software required for data processing and solution. Rigaku's widely trusted and user-friendly [CrysAlis<sup>Pro</sup>](#) and AutoChem packages will be immediately familiar to users of Rigaku's single-crystal diffractometers, providing an effortless transition.



The XtaLAB Synergy-ED is a new and fully integrated electron diffractometer, creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures. The XtaLAB Synergy-ED is the result of an innovative collaboration to synergistically combine our core technologies: Rigaku's high-speed, high-sensitivity photon-counting detector (HyPix-ED) and state-of-the-art instrumentivity control and single crystal analysis software platform (CrysAlis<sup>Pro</sup> for ED), and JEOL's long-term expertise and market leadership in designing and producing transmission electron microscopes. The key feature of this product is that it provides researchers an integrated platform enabling easy access to electron crystallography. The XtaLAB Synergy-ED is a system any X-ray crystallographer will find intuitive to operate without having to become an expert in electron microscopy.

## BOOK REVIEW



[The Dawn of Everything: A New History of Humanity](#)

By David Graeber and David Wengrow

ISBN: 9780374157357

David Graeber and David Wengrow's *The Dawn of Everything: A New History of Humanity* is a delightful foray into re-envisioning the scholarly approach to human history from a fresh and intriguing perspective that combines their respective practices of anthropology and archaeology respectively. They take the traditionally Eurocentric approach to the topic and turn it on its head and inside out at the same time, resulting in an absolute must-read work.

The book is not short; clocking in at 525 pages, it is quite a lift, literally. But Graeber and Wengrow's effortless prose style and easily digestible format for information delivery makes those pages fly by in a flash.

There are twelve chapters, each with a seemingly normal title and a wickedly cheeky subtitle. Chapter 4, titled "Free People, the Origin of Cultures, and the Advent of Private Property: (Not necessarily in that order)" is a prime example. Each chapter is divided into subsections, also with informative and interesting titles guaranteed to grab your attention (they are in all caps, to be fair) such as IN WHICH WE FIRST CONSIDER AN EXAMPLE OF STRANGER-KINGS IN THE MAYA LOWLANDS AND THEIR AFFILIATION WITH TEOTIHUACAN or ON HOW THE COLLAPSE OF THE MISSISSIPPIAN WORLD AND REJECTION OF ITS LEGACY OPENED THE WAY TO NEW FORMS OF INDIGENOUS POLITICS AROUND THE TIME OF EUROPEAN INVASION. It's easy, when reading a book of this length about a topic as broad as human history, to get a bit bogged down in the details and start to drift, but Graeber and Wengrow do an excellent job of making sure the reader stays engaged by keeping everything clear, concise, and critically interesting.

A book about the history of humanity certainly doesn't seem like it's guaranteed to be entertaining, but somehow Graeber and Wengrow manage to make it so. A good example of a chuckle-worthy moment came on page 13, when they take issue with Steven Pinker's approach to human history in his numerous works:

*Since, like Hobbes, Pinker is concerned with the origins of the state, his key point of transition is not the rise of farming but the emergence of the scholarly "Archaeologists," he writes, "tell us that humans lived in a state of anarchy until the emergence of civilization some five thousand years ago, when sedentary farmers first coalesced into cities and states and developed the first governments." What follows is, to put it bluntly, a modern psychologist making it up as he goes along. You might hope that a passionate advocate of science would approach the topic scientifically, through a broad appraisal of the evidence - but this is precisely the approach to human prehistory that Pinker seems to find uninteresting.*

If you are a huge fan of Steven Pinker and his work, you should most certainly read *The Dawn of Everything*, because you are guaranteed to need an updated perspective on human history. And if you, like myself, are not a fan of Steven Pinker, be assured you will enjoy it, perhaps even more than I did.

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:

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

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

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

[8<sup>th</sup> International Conference on Metal-Organic Frameworks and Open Framework Compounds](#), Dresden, Germany, September 4-7.

[The Pittsburgh Diffraction Conference](#), Lemont, IL, October 2-4.

[73<sup>rd</sup> Southeastern Regional ACS Meeting \(SERMACS 2022\)](#), San Juan, Puerto Rico, October 19-22.

## CRYSTALLOGRAPHY IN THE NEWS

**March 14, 2022:** Researchers from the UK analyzed 93,978 PDB entries using a new metric,  $B_{\text{net}}$ , to determine the extent of damage to previously deposited structures.

**April 21, 2022:** Researchers from Germany and US noted a change in the isotope distribution in zircon crystals about 3.8 billion years ago, suggesting this is when plate tectonics began.

**May 3, 2022:** Researchers from France, Germany and Sweden have synthesized and characterized a chiral lanthanum metal-organic framework with gated  $\text{CO}_2$  sorption and concerted framework flexibility.

**May 11, 2022:** Scientists in the US used X-ray crystallography to augment the cryo-EM structure of the plant immunity protein apo NPR1 and determined there is a zinc-finger protein at the core of its functionality.

**June 9, 2022:** Researchers from China and Sweden have visualized the entire range of noncovalent interactions in nanocrystalline MOF SCM-34 using single crystal electron diffraction.

## USEFUL LINKS

Here links to organizations helping Ukrainians survive the ongoing war in their homeland:

- [Help Humanitarian Efforts in Ukraine](#)
- [Donate to Children of Ukraine](#)
- [Nova Ukraine](#)
- [Razom for Ukraine](#)
- [World Central Kitchen](#)
- [Global Giving](#)
- [International Committee of the Red Cross](#)

## 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](http://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 CrysAlis<sup>Pro</sup> software for single crystal data processing.

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