CRYSTALLOGRAPHY TIMES

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WELCOME

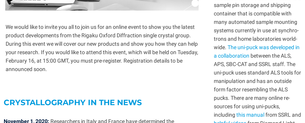
Good day, everyone. I think 2021 is off to a good start. The coronavirus vaccines are now being deployed. I've talked to a number of people who received either the Pfizer/BioNTech or Moderna vaccine. This is good news and a step toward getting back to normal.

This month, our product in the spotlight is the XtaLab Synergy-S, our most popular single crystal X-ray diffractometer. Our researcher in the spotlight is Michael Shatruk from Florida State University.

As usual, we highlight a few noteworthy crystallography papers. This month, we feature a video illustrating how an anti-TB drug stops ATP synthase and another of Jennifer Doudna's Nobel Lecture. The useful links include a calendar of celestial events from the *New York Times*, the Crystallographic Open Database and a hypertext book of crystallographic space group diagrams and tables. Jeanette reviews *Editing Humanity*, a book about CRISPR.

Joe

UPCOMING EVENT



We would like to invite you to join us for an online event to show you the latest product developments from the Rigaku Oxford Diffraction single crystal group. During this event we will cover our new products and show you how they can help your research. If you would like to attend this event, which will be held on Tuesday, February 16, at 15:00 GMT, you must pre-register. Registration details to be announced soon.

CRYSTALLOGRAPHY IN THE NEWS

November 1, 2020: Researchers in Italy and France have determined the structure of kalophilite, a rare mineral form of $KAlSiO_4$, after a century of attempts, using a number of diffraction, imaging and spectroscopic techniques.

December 14, 2020: Researchers in the U.K. synthesized and characterized a molecular endiess (T_4) knot, a knot with seven crossings in a 258-atom-long closed loop.

January 1, 2021: Researchers in the U.S. determined the crystal structures of 11 vitamin K epoxide reductases to understand the structural basis of antagonizing the vitamin K catalytic cycle for anticoagulation.

January 7, 2021: Researchers in Japan have determined the crystal structure of death-associated protein kinase 1 in complex with the dietary compound resveratrol, a possible route to development of Alzheimer's disease inhibitors.

January 8, 2021: Researchers in Australia and China report the structure of the antibody 1G5.3 and flavivirus nonstructural protein 1, a step in development of vaccines for diseases caused by the dengue and Zika viruses.

January 14, 2021: Researchers from Australia, Finland, France, Sweden and the U.S. have used serial crystallography to learn how proteins use conformational dynamics to stabilize the charge-separation steps of electron-transfer reactions using an XFEL and a photosynthetic reaction center.

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-S

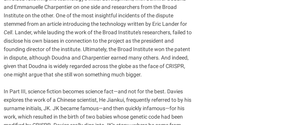
The XtaLAB Synergy-S is Rigaku's most popular single-crystal X-ray diffractometer. Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S provides fast, accurate data in an intelligent fashion. The system 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-6000HE or the large theta coverage detectors: HyPix-Arc 100° 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.

RESEARCHER IN THE SPOTLIGHT

Professor Michael Shatruk
Cottrell Family Professor, Chemistry
Florida State University

The Shatruk group works in a broadly defined area of advanced functional materials. Their current, more specific research interests include photo-switchable molecular materials, intermetallic materials for magnetic refrigeration and electric vehicles, and low-dimensional magnetic materials such as spin-frustrated 2D magnets and nanomagnets. The disciplinary focus of their work lies within inorganic materials chemistry, with strong interdisciplinary crossover to physical and organic chemistry, as well as to condensed matter physics and machine learning. The students and postdocs obtain diverse training in inorganic and organic synthesis, X-ray and neutron scattering methods, magnetic and electrical property measurements, optical, infrared, NMR, and EPR spectroscopy, as well as computational approaches to elucidation and discovery of new functional materials.



BOOK REVIEW

Editing Humanity: The CRISPR Revolution and the New Era of Genome Editing
By Kevin Davies
ISBN: 978-1-64313-308-9

Kevin Davies' *Editing Humanity* is fresh and riveting. Indeed, as the author acknowledges himself, much of the technology he describes has been developed in less than a decade. Davies' book takes a deep dive into CRISPR, the history of gene editing and genetic manipulation, and the ethical and moral implications of this work.

While the narrative feels largely non-linear, Davies weaves in and out of the more recent history of CRISPR development, providing his readers with flashback historical context when necessary and quick but detailed biographical sketches of key players. Davies also inserts himself into the narrative where relevant, explicitly highlighting the characters he's describing based on up-close and personal experience versus that of research and reporting from a distance. The resultant effect is a narrative with a very human voice, telling a very human story about a technology that has the ability to challenge all our preconceived notions about humanity and what it truly means to be human on a genetic level. It also provides the work with a unique level of journalistic integrity. If at any point while reading you have concerns that Davies has any biases, he very clearly articulates where they may lie. You don't get the sense he is hiding anything or has ulterior motives in his writing.

Davies starts, like all good authors do, with a prologue outlining his ultimate goals in writing the book. The result is a seemingly comprehensive history of CRISPR technology, complete with all the requisite contextualization to make it comprehensible to someone who isn't a geneticist.

Part I introduces the CRISPR technology itself—what it is, how it works and why we should care about the ramifications of where and when it is used. Of the book's four parts, Part I is probably the most technical, although Davies does an admiral job of walking readers through the biomechanics behind the system.

Part II is where things start to get—for lack of a better, more scientific word—quite juicy. Davies provides a neutral account of the CRISPR patent drama that unfolded following the technology's initial development, with Jennifer Doudna and Emmanuelle Charpentier on one side and researchers from the Broad Institute on the other. One of the most insightful incidents of the dispute stemmed from an article introducing the technology written by Eric Lander for Cell. Lander, while lauding the work of the Broad Institute's researchers, failed to disclose his own biases in connection to the project as the president and founding director of the institute. Ultimately, the Broad Institute won the patent in dispute, although Doudna and Charpentier earned many others. And indeed, given that Doudna is widely regarded across the globe as the face of CRISPR, one might argue that she still won something much bigger.

In Part III, science fiction becomes science fact—and not for the best. Davies explores the work of a Chinese scientist, He Jiankui, frequently referred to by his surname initials, JK. JK became famous—and then quickly infamous—for his work, which resulted in the birth of two babies whose genetic code had been modified by CRISPR. Davies really digs into JK's story—where he came from, what his background was, what motivated him, and of course, where he ended up. Perhaps the most interesting takeaway from this section was the number of researchers and colleagues JK consulted with who encouraged or supported his workjust were not implicated to the extent he was (i.e., no prison time).

CRISPR is cutting-edge technology, but the morality and ethics of it, as Davies makes clear, is heavy stuff. Part IV explores the many possible applications of CRISPR technology beyond human genome editing, such as improving agricultural products and oyster, or even organ growing and harvesting for transplant. Despite some of the more terrifying possibilities Davies outlines throughout the book, he ends on a hopeful note. CRISPR is not inherently an evil technology. How we choose to use it as a society will be telling. As one superheros uncle once said: "With great power comes great responsibility."

Though much of its subject matter is historical, the book itself feels firmly rooted in the present, thanks to the references to the current COVID-19 pandemic and frequent callouts to popular culture *Rampage* and *Frankenstein* were the standouts. Davies makes numerous references to conferences that should have happened or talks and events he had hoped to attend while researching his book that were cancelled as a result of the pandemic. These references to current cultural events and influences serve to further enrich the humanizing tone Davies has mastered as well in his work. He brings the high caliber work of esteemed scientists around the globe to a level that can be understood by those without the technical research background to conduct the scientific work themselves.

Review by 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.

RIGAKU REAGENTS

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

Uni-puck Kit
SKU: 1013169
Price: $4,075.00

The Universal VT-Puck (uni-puck) 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 uni-puck was developed in a collaboration between the ALS, APS, SBC-CAT and SSRL staff. The uni-puck uses standard ALS tools for manipulation and has an outside form factor resembling the ALS pucks. There are many online resources for using uni-pucks, including this manual from SSRL and helpful videos from Diamond Light Source.

SHOP HERE

SURVEY OF THE MONTH

Which of the following statements best describes your COVID-19 life?

TAKE THE SURVEY

LAST ISSUE'S SURVEY RESULTS

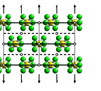
Do you plan on being vaccinated for COVID-19 when a vaccine is made available to you?

VIDEOS OF THE MONTH

Hit Movie Reveals How A Tuberculosis Drug Halts ATP Synthesis

Structural data revealing how an anti-tuberculosis drug works could aid efforts to improve therapeutic options for the disease. The findings also uncover aspects of how the drug's target, the ATP synthase enzyme, operates.

Valerie Mizrahi, Clifton E. Barry III⅄



Nobel Lecture: Jennifer Doudna, Nobel Prize in Chemistry 2020

Jennifer Doudna delivered her Nobel Lecture on December 8, 2020. She was introduced by Professor Claes Gustafsson, Chairman of the Nobel Committee for Chemistry.

USEFUL LINKS

Here is a link from the *New York Times* that will allow you to sync your calendar with the solar system.

Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding biopolymers.

Including data and software from CrystalEye, developed by Nick Day at the department of Chemistry, the University of Cambridge under supervision of Peter Murray-Rust. All data on this site have been placed in the public domain by the contributors.

A Hypertext Book of Crystallographic Space Group Diagrams and Tables

Birkbeck College, University of London.

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. Itás also the place to download the latest version of Rigaku Oxford Diffractionás CrysAlisPro™ software for single crystal data processing.

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