Rigaku

CRYSTALLOGRAPHY TIMES

Volume 13, No. 10, October 2021

WELCOME

We are really excited about our 3DED/MicroED workshop, which we will be holding next Wednesday and Thursday (October 27th and 28th). We have over 400 registrants already, and a great lineup of speakers. If you haven't registered yet, you can here.

This month, we are mixing up the format a little. Instead of presenting some our regular features like "Lab in the Spotlight," we are highlighting our application scientists in Europe and the US. Since the application scientists tend to stay focused on their geographic territory, we thought it would be nice to introduce all of us to all of you. Next month, we'll focus on our scientists in the Asia-Pacific region. Let us know what you think.

We have our usual "Crystallography in the News" section this month and a review by Jeanette of the newly released *The Secret of Life: Rosalind Franklin, James Watson, Francis Crick, and the Discovery of DNA's Double Helix.*

Take care,

Joe

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.

CRYSTALLOGRAPHY IN THE NEWS

June 22, 2021: Scientists in Germany have synthesized and characterized the technetium hydrides [$TcH_3(PPh_3)_4$] and [$TcH(CO)_3(PPh_3)_2$] along with a number of Tc organometallic compounds.

August 30, 2021: Researchers in Japan have enclosed an enzyme in a self-assembled nanocage that preserves the activity of the protein while preventing denaturation in harsh solvents.

September 10, 2021: Researchers from China, Germany, Switzerland and the UK have synthesized and characterized a branched ultraphosphate.

October 4, 2021: Researchers at MIT have synthesized and characterized an iron(II) complex with triphosphatetrahedrane.

October 13, 2021: Scientists in Belgium, Japan and the U.S. have determined the structures of anaplastic lymphoma kinase and the related leukocyte tyrosine kinase, which are involved in neural development, cancer and autoimmune diseases.

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 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^Pro software for single crystal data processing.

JOIN HERE

FEATURED RIGAKU SCIENTISTS

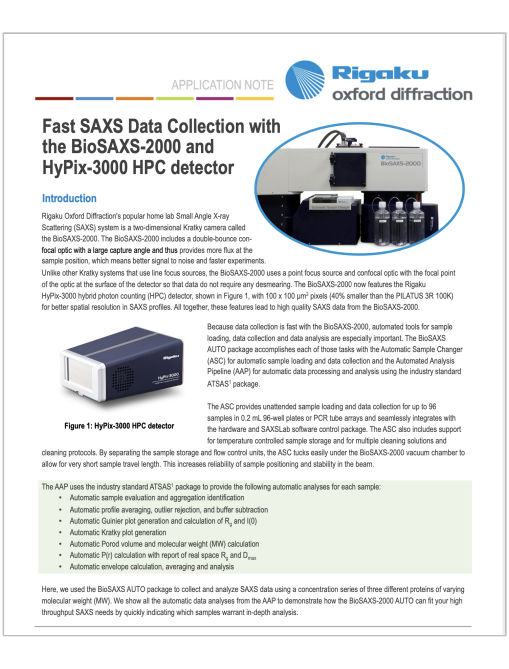
If you are like me, I always enjoy the announcements of the Nobel Prizes during October. While only a handful of scientists will ever achieve this honor, I think it is a good time to reflect on our own scientific achievements for the year. With that in mind, I would like to devote this issue of *Crystallography Times* to scientists at Rigaku who support our single crystal activities. Not only do they support our current and future customers with difficult single crystal analyses, they are also always trying to push our instruments to the limits to see what they can achieve. These efforts are shared with others in the community through application notes, as well as through Rigaku's virtual crystallographic schools, webinars, and workshops.

In this issue we highlight some of the scientists behind the single crystal activities at Rigaku in EMEA, the Americas, and ANZ.

Dr. Angela Criswell

Angela Criswell holds a Ph.D. from Rice University and has been with Rigaku for 18 years. She started in the macromolecular crystallography applications lab, focusing on X-ray techniques to study structural biology. She has gained expertise in a number of X-ray methods during her tenure at Rigaku, including small angle X-ray scattering and X-ray computed tomography. Angela likes working with customers to find the best instrumental fit for their samples while addressing their specific experimental questions.

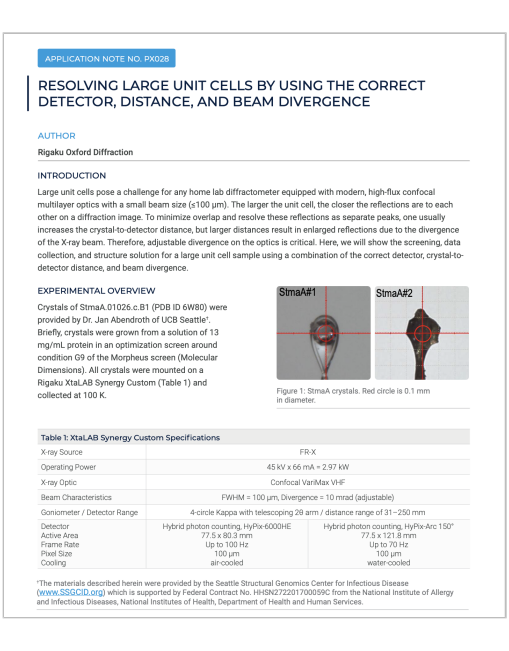
Her favorite application note is: Fast SAXS Data Collection with the BioSAXS-2000 and HyPix-3000 HPC detector.



Dr. Mark Del Campo

Mark Del Campo is a Senior Applications Scientist at Rigaku Americas Corporation with over 20-years of experience in the life sciences. For the past 10 years, he has traveled the world supporting Rigaku's macromolecular crystallography and small angle X-ray scattering customers. Mark received his Ph.D. under the supervision of Dr. James Ofengand at the University of Miami, where he worked on *E.coli* pseudouridine synthases and solved three structures deposited in the PDB. He did his postdoctoral research on fungal DEAD-box proteins and Group I and Group II introns with Dr. Alan Lambowitz at the University of Texas at Austin, where he solved eight structures deposited in the PDB. Mark was the recipient of both predoctoral and postdoctoral *Ruth L. Kirschstein* National Research Service Awards.

Mark picked the following application note as one of his favorites. "I like this app note because it illustrates how to deal with a physical property of the instrument (the divergence of the X-ray beam) when trying to collect on a sample with a large unit cell".



Dr. Joseph Ferrara

Dr. Joseph Ferrara received both his Bachelor of Science and Doctorate degrees from Case Western Reserve University in Cleveland, Ohio. His graduate research was conducted in physical organometallic chemistry and X-ray crystallography under Prof. Wiley C. Youngs. Upon completing his doctorate in 1987, he joined Molecular Structure Corporation, which became a subsidiary of Rigaku Corporation in 1996. He has spent the last 33 years developing tools for X-ray crystallography for the research community. He has also developed tools for X-ray computed tomography and X-ray photon correlation spectroscopy.

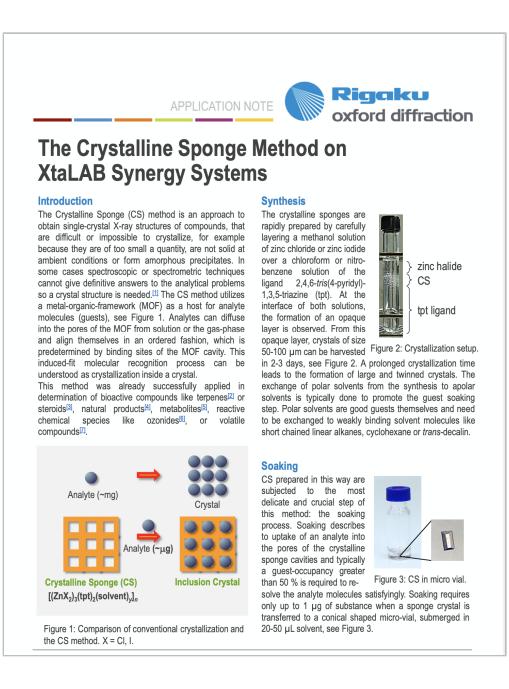
Dr. Ferrara is currently Chief Science Officer of Rigaku Americas Corp and Vice President, X-ray Research Laboratory, Rigaku Corporation. He is currently funded by the National Institute of Biomedical Imaging and Bioengineering with University College London, CreaTV MicroTech, the Center for Nanoscale Materials at Argonne National Laboratory and Sloan-Kettering Cancer Research Institute to develop a phase-based X-ray imaging system for *ex vivo* applications.
Joe's favorite (and only) application note is: PDF Analysis of Glassy Materials on a Home Laboratory Diffractometer.

Dr. Christian Göb

Dr. Christian Göb studied chemistry at the RWTH Aachen University (Germany), majoring in mesoscopic systems and catalysis. In 2018, he obtained his Ph.D. under the supervision of Prof. Dr. Iris Oppel, where he worked on the synthesis and characterization of supramolecular systems using single crystal X-ray diffraction and various spectroscopic methods. He was funded with a scholarship from the German Research Foundation (DFG) and worked in the international research training group SeleCa "Selectivity in Chemo- and Biocatalysis." This group strived for an intensive collaboration between RWTH Aachen and Osaka University (Japan). He spent three months with Prof. Dr. Yoshito Tobe at the Graduate School of Engineering Science, gaining insight into self-assembled structures at the graphite/octanoic acid interface, using scanning tunnelling microscopy and atomic force microscopy. His expertise is in application and characterization of large assemblies like molecular cages, their inclusion compounds, and polymers (molecular chains, two-dimensional networks, metal, and covalent organic frameworks).

Christian joined Rigaku Europe SE as an application scientist for single crystal diffraction in 2019 and became the application team leader of the European single crystal group in 2021. His proficiency made him contact person for the Crystalline Sponge Method, a crystallographic technique that utilizes the porous channels of MOF crystals to impose order on molecules that are otherwise difficult to crystallize due to their molecular constitution, physical properties (oils or gases) or minute amounts (nano- to microgram scale). Rigaku and Merck collaborate in the commercialization of this analytical method.

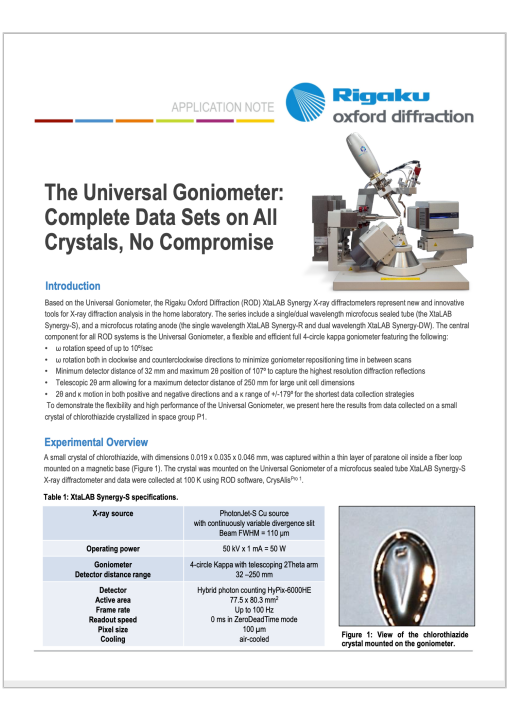
His favorite application note is: The Crystalline Sponge Method on XtaLAB Synergy Systems.



Dr. Pierre Le Maguerès

Dr. Pierre Le Maguerès obtained a Ph.D. in physical chemistry and small molecule crystallography at the University of Rennes (France) in 1995, working under Dr. LahcÃ¨ne Ouahab on the synthesis and analysis of molecular materials combining inorganic polyoxometalates and organic cation radicals based on tetrathiofulvalene derivatives. From 1996 to 2000, Dr. Le Maguerès worked as a postdoctoral researcher with renowned Prof. Jay Kochi at the University of Houston, where he pursued his work on the synthesis and X-ray characterization of air-sensitive cation radicals and charge transfer complexes. In 2000, deciding to broaden his horizons and learn protein crystallography, Dr. Le Maguerès joined the biochemistry department at the University of Houston and worked as a postdoctoral researcher with Prof. Kurt Krause on the design and X-ray characterization of potential new inhibitors for alanine racemase, a protein essential for the growth of infectious diseases such as tuberculosis.
Dr. Le Maguerès was hired in 2004 as a protein crystallographer in the Life Sciences department at Rigaku. After 14 years in protein crystallography, he shifted to a position as a small molecule crystallographer at Rigaku Americas Corporation in The Woodlands, TX. While still helping with protein crystallography if needed, Dr. Le Maguerès' duties are now centered on the analysis of small molecule samples and the development of hardware and software products at Rigaku for small molecule crystallography.

Pierre's favorite application note concerns completeness of data: "Some experienced crystallographers are suspicious about older strategy programs and therefore always collect in primitive triclinic or use their own collection strategy, which they have perfected over the years. As a result, though, they often end up collecting more data than necessary and therefore wasting machine time. This app note demonstrates how reliable the Universal Goniometer, combined with the strategy algorithm in CrysAlis^Pro, is to always collect complete data sets, including on the most difficult case of a P1 space group."

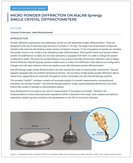


Dr. Christian Schürmann

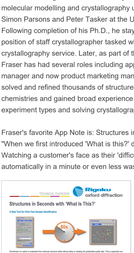
Dr. Christian "Chris" Schürmann studied Chemistry at the Georg-August University in Göttingen, where he showed interest in experimental charge-density studies from early on. He did his Bachelor thesis in the group of Birger Dittrich, calculating and testing transferrable anisotropic scattering factors (invarioms) and later joined the group of Prof. Dr. Dietmar Stalke for his Master and Ph.D. theses. Here, he did a range of experimental charge-density studies, with a focus on the experimental method and data quality. The basic idea was that charge-density refinement requires the highest data quality and subsequently yields accurate models of the charge-density distribution. In return, the accurate charge-density models can be used to assess the quality of density models from theoretical approaches, or alternatively, the overall data quality of different experimental systems. This approach was used to test the latest generation of in-house diffractometers at the time, resulting in differences mostly caused by the employed detector technology.

Chris joined Rigaku Europe SE as an application scientist for single crystal diffraction in 2019 and has cross-trained for powder diffraction applications since early 2020. He quickly learned the powder application techniques and supported his colleagues on the XRD team, especially for MiniFlex applications. Accordingly, his favorite application note combines single-crystal and powder applications by using single-crystal instruments for powder diffraction measurements from microscopic amounts of sample.

Favorite application note: Micro Powder Diffraction on XtaLAB Synergy Single Crystal Diffractometers.



Dr. Fraser White



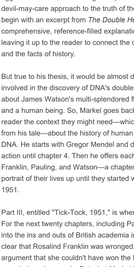
Fraser White began his career as a crystallographer with a Ph.D. in molecular modelling and crystallography under the tutelage of Professors Simon Parsons and Peter Tasker at the University of Edinburgh in 2004. Following completion of his Ph.D., he stayed at Edinburgh, accepting the position of staff crystallographer tasked with running the departmental X-ray crystallography service. Later, as part of the Rigaku Oxford Diffraction team, Fraser has had several roles including application scientist, demo lab manager and now product marketing manager. During his career Fraser has solved and refined thousands of structures for a diverse sample chemistries and gained broad experience in diffraction techniques, experiment types and solving crystallographic problems.

Fraser's favorite App Note is: Structures in Seconds with 'What is this?' "When we first introduced "What is this?" demos were really good fun. Watching a customer's face as their 'difficult' structure appeared automatically in a minute or even less was really satisfying."

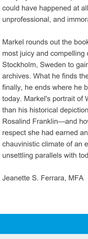
Dr. Jakub Wojciechowski

Dr. Jakub Wojciechowski obtained a Ph.D. in chemistry and structural analysis at the Technical University of Łódź in 2014, working on the charge density analysis of amino phosphonic acids and their derivatives. In 2009 he visited and worked in the group of Prof. Christian Jelsch at CRM2 in Nancy for three months, to learn and help develop the MoPro suite software for charge density refinement and analysis. From 2011 to 2018, Jakub worked as chemist, teacher, and service crystallographer at his alma mater, where he gathered in-depth experience on a wide range of diffraction systems and sample types. In early 2018 he worked at the Department of Chemistry of Middle Tennessee State University as the main crystallographer for the boron chemistry group and helped establish a regular service crystallography laboratory. He joined Rigaku in 2018 as an application scientist to support and train users in small molecule crystallography. Currently, Jakub's duties are shifting towards protein crystallography and the development of hardware and software products at Rigaku for single crystal diffraction group.

His favorite app note: Resolving large unit cells by using the correct detector, distance, and beam divergence.



BOOK REVIEW



The Secret of Life: Rosalind Franklin, James Watson, Francis Crick, and the Discovery of DNA's Double Helix
By Howard Markel
ISBN: 9781324002239

The first thing you might notice upon picking up Howard Markel's latest book, *The Secret of Life: Rosalind Franklin, James Watson, Francis Crick, and the Discovery of DNA's Double Helix* is that he gives Rosalind Franklin top billing—even though her contribution to the discovery of DNA's double helix structure was infamously excluded by the winners of the Nobel Prize. The second thing you might notice is that Maurice Wilkins—Franklin's colleague at King's College London—receives no billing at all, despite sharing the aforementioned 1962 Nobel Prize in Physiology and Medicine with James Watson and Francis Crick. Both of these critical decisions convey a great deal about the tone with which Markel approaches the convoluted and complicated academic history behind one of the most critical scientific discoveries of the 21st century.

Markel's book reads like a detailed, fleshed out script for a documentary mini-series on the discovery of DNA's double helical structure. He leans into this screenplay metaphor, titling the first chapter of the prologue "Opening Credits" and the final chapter "Closing Credits." He begins by setting the scene for the discovery of the DNA double helix back in 1953, in a passage that seems to play homage to Watson's claims about the moment as he expressed them in his wildly problematic and wholly inaccurate 1968 memoir *The Double Helix*. But Markel immediately takes a step back, making it clear this is not some kind of Watson homage sequel to *The Double Helix*, but in fact a deconstruction of its false truths. Of Watson's supposedly truthful narrative about the discovery of DNA's double helix and how it all played out, Markel makes a strong claim: "It never happened."

This three-word sentence really establishes Markel's thesis, if none of the other editorial choices gave a clear enough hint. He's taking *The Double Helix* and pulling it apart, debunking all of Watson's inaccuracies, self-aggrandizements, unflattering and questionable portraits, and overall devil-may-care approach to the truth of the narrative. Many of the chapters begin with an excerpt from *The Double Helix*, only to be followed by a comprehensive, reference-filled explanation of what really happened—leaving it up to the reader to connect the dots between Watson's "truth" and the facts of history.

But true to his thesis, it would be almost disrespectful to everyone else involved in the discovery of DNA's double helix to simply write a book about James Watson's multi-splendored flaws as a narrator, researcher, and a human being. So, Markel goes back to the beginning, giving the reader the context they might need—which Watson of course excludes from his tale—about the history of human understanding of genes and DNA. He starts with Gregor Mendel and doesn't circle back to the main action until chapter 4. Then he offers each key player—Crick, Wilkins, Franklin, Pauling, and Watson—a chapter-long biography, a character portrait of their lives up until they started working on the DNA problem in 1951.

Part III, entitled "Tick-Tock, 1951," is where things start to get interesting. For the next twenty chapters, including Parts IV and V, Markel digs deeply into the ins and outs of British academia in the early 1950s. He makes it clear that Rosalind Franklin was wronged. There is, of course, the argument that she couldn't have won the Nobel Prize because it can't be awarded posthumously. But what Markel hammers home is the delicate imbalance of political power in the academic circles in which all these players ran. Watson and Crick's discovery was critically dependent on an X-ray diffraction pattern collected by Franklin—which was distributed to them without her knowledge or consent. Certainly, Franklin had passed away by the time the prize was awarded—but whether or not the discovery could have happened at all was dependent on an altogether unethical, unprofessional, and immoral breach of academic conduct.

Markel rounds out the book with two short chapters that are perhaps the most juicy and compelling of the whole work. He describes his ventures to Stockholm, Sweden to gain access to the Nobel Prize nomination letter archives. What he finds there I'll leave for you to glean for yourself. And, finally, he ends where he began—with Watson, the only living player today. Markel's portrait of Watson today is no more flattering or endearing than his historical depiction. And Watson's reaction to any mention of Rosalind Franklin—and how he cheated her out of the recognition and respect she had earned and deserved—paints a vivid picture of the chauvinistic climate of an earlier time—and calls into question some unsettling parallels with today's.

Jeanette S. Ferrara, MFA

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