CRYSTALLOGRAPHY TIMES

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WELCOME

It is now summer and we are heading to a normal existence one day at a time. It seems Czechia is opening up and travel to IUCr might be possible. We just completed the Advanced Topics Rigaku School and I hope to talk about it at IUCr. We still have an Asia-Pacific Users' Meeting, a webinar on the SAXS Geometry and a High-Pressure Crystallography Workshop coming up.

Rigaku has announced two awards in order to honor two esteemed crystallographers we lost in 2020, Ed Stevens and Ward Smith. These awards are open to graduate students or postdoctoral fellows who have exhibited excellence in their crystallographic-related research and meet the criteria of either of the two awards as described below. The deadline for submission is June 30, 2021.

In this issue we highlight the XtaLAB Synergy-ED, the first commercial electron diffractometer, and the laboratory of Tamir Gonen at UCLA. This month's roundup of useful links and videos focuses on MicroED.

Lastly, I review *Noise: A Flaw in Human Judgment* by Kahneman, Sibony and Sunstein, and suggest we start a book club. I'd like to hear your thoughts on this.

All the best,

Joe

RIGAKU CRYSTALLOGRAPHIC AWARDS

The Ed Stevens Award for Excellence in Small Molecule Crystallographic Research

Ed Stevens was an early pioneer in charge density analysis, or what is now known as "quantum crystallography." He was a highly productive researcher throughout his career and helped develop many aspects of the science, including appropriate treatment of thermal diffuse scattering, accurate data collection at liquid helium temperature, error estimation of charge density maps, measurement of diffraction intensities at absolute scale, treating anharmonic motion, and the use of scattering factors based on wave functions, to name a few.

The winner of this award will be someone who has demonstrated an ability to push the envelope in the field of small molecule crystallography to further our understanding of structural science.

The Ward Smith Award for Excellence in Macromolecular Crystallographic Research

Ward Smith spent most of his career in industry. He started at Monsanto in St. Louis working as a structural biologist, then moved to Agouron Pharmaceuticals in San Diego at the beginning of structure-based drug design. He then joined SmithKline Beecham in Philadelphia. He ended his career as a program director for the National Institute of General Medical Sciences (NIGMS) where, among other things, he managed the Protein Structure Initiative and the NIH-sponsored synchrotron beamline facilities.

The winner of this award will be someone who has demonstrated an ability to perform ground-breaking research utilizing macromolecular crystallography to enhance the future of mankind.

The winner of each award will receive a plaque and a cash gift of $1,000. Graduate students or postdoctoral fellows may apply here.

CRYSTALLOGRAPHY IN THE NEWS

April 29, 2017: Researchers in Germany have synthesized and characterized a room-temperature stable diazaborane that displays nucleophilic at both C and N sites.

May 05, 2021: Researchers in South Korea and the U.S. have determined the structure of the BRAF/KD-belvarafenib complex, a step in understanding BRAFV600-mutant melanoma.

May 05, 2021: Researchers in Germany have discovered a covalent crosslink between a cysteine and a lysine residue resulting in a NOS bridge in a transaldolase enzyme.

May 26, 2021: Researchers from Austria, Switzerland and the U.S. have produced perovskite-type superlattices from lead halide perovskite nanocubes.

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-ED
The World's First Dedicated Electron Diffractometer

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: Rigakuʼs high-speed, high-sensitivity photon-counting detector (HyPix-ED) and one of the all-inert instrument control and single crystal analysis software platform (CrysAlis^{Pro} for ED), and JEOLʼs 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 with a fully eucentric goniometer that exist in the cell membrane work together to help cells maintain homeostasis. With that question in mind, they study membrane proteins that are involved in nutrient, ion and water uptake, waste removal, signaling and maintenance.

LEARN MORE

RESEARCHER IN THE SPOTLIGHT

Tamir Gonen
Professor of Biological Chemistry and Physiology, David Geffen Medical School, UCLA

Tamir Gonen's laboratory studies the structures of membrane proteins. Based on structure, they try to understand function and what goes wrong in disease. They focus primarily on proteins in the blood-brain barrier. The long-standing question in their laboratory is how the thousands of membrane channels and transporters that exist in the cell membrane work together to help cells maintain homeostasis. With that question in mind, they study membrane proteins that are involved in nutrient, ion and water uptake, waste removal, signaling and maintenance.

The Gonen laboratory is multidisciplinary. Over the last decade they have employed structural biology techniques such as electron cryo-microscopy (cryo EM), X-ray crystallography, NMR, molecular dynamics simulations, and used membrane biochemistry and biophysics to understand the function of the proteins of interest. Within electron microscopy they have published papers using electron tomography, single particle reconstructions and electron crystallography, however their specialty lies in electron diffraction.

Part of their laboratory is also devoted to method development in cryo EM. In recent years they have developed two important methods in electron diffraction, namely the fragment-based phase extension and MicroED.

BOOK REVIEW

Noise: A Flaw in Human Judgment
by Daniel Kahneman, Olivier Sibony and Cass R Sunstein, Little, Brown Spark, New York, © 2021, 464 pp,
ISBN: 978-031645140

Jeanette has been swamped with work, so you'll have to suffer through one of my reviews. I picked this book up because the title caught my attention and I really enjoyed *Thinking, Fast and Slow* by the first author. When I think of noise I think of the noise in linear systems, specifically X-ray instrumentation, the leaf blowers on Zoom calls or pops and clicks on vinyl albums. I never thought of human judgement as being noisy. Biased, yes, but not noisy. In this book you will learn we are very noisy, indeed.

The authors start with a basic description of the error model for human decision making using bias and noise, then describe a number of everyday phenomena that are noisy: insurance premiums, medicine, child custody, breasts, asylum decisions, personnel decisions, bail decisions, forensic science and patents. The authors use studies of the various phenomena to illustrate their points throughout the book.

The first part of the book is devoted to understanding the difference between bias and noise, and introduces the concept of a *noise audit* (how to properly execute one is described in detail in Appendix A). In Part 2, the authors analyze human judgment and separate noise in decision making (pattern noise) into two parts: level noise and occasion noise. The former is the noise in decisions between individuals and the latter the noise in decisions for a given individual at different times. Part 3 delves into ways to standardize decision making to minimize noise. Part 4 considers human psychology, the sources of noise in decisions and why humans filter noise so well. Part 5 looks at improving judgement and reducing error through a concept dubbed "decision hygiene." Part 6 addresses the issue of dealing with noise when you can't eliminate it.

Appendix B provides a checklist to reduce bias in decision making and Appendix C addresses predictions and reminds of the Bayesian analysis without the math.

I enjoyed this book so much I thought I would throw out an idea: let's start a book club where we could get together on Zoom and discuss this book. If you are interested email me at joseph.ferrara@rigaku.com.

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 of webinars you cannot attend live sessions.

UPCOMING EVENTS

In this 75-minute workshop we will introduce the concept of diffuse scattering, show how to measure it, and how to analyze it using a fast method based on the three-dimensional difference pair distribution function. We will start from the basics and do not expect from participants any prior knowledge in diffuse scattering or disorder modeling.
Read More »

Presenter: Dr. Arkadiy Simonov
Date/time (CDT): Tuesday, June 29, 2021 - 09:00 AM

REGISTER

We would like to invite you to join us for our single crystal users' meeting, held online via Zoom on June 30–July 1, 2021. The meeting will take place at 2:00–5:00 PM JST on both days to allow our users from the Asia Pacific region to attend.
Read More »

REGISTER

This workshop is primarily geared towards crystallographers with little or no experience in high-pressure crystallography and who are interested in learning how to get started. Presentations are intended to be practical and educational and will include reviews of diamond anvil cells (DACs) and accessories from two DAC manufacturers, sample preparation under pressure in DACs, sample mounting/centering on a Rigaku diffractometer and data collection, and data processing and correction. The workshop will be held on July 21–22, 2021 at 8:00 AM CDT.
Read More »

REGISTER

RIGAKU REAGENTS

Unipuck Kit

Unipucks and tools are available to purchase individually or as kits. Each part of the V1-Puck has a unique serial number for identification. Custom serial numbers and puck coloring is available by request.

Unipuck Kit
SKU 1013169
Price: $4,075.00

The Universal V1-Puck (unipuck) 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 unipuck was developed in collaboration between the ALS, APS, SSC-CAT and SSRL staff. The unipuck uses the standard AL base for manufacturing and has an outside form factor resembling the ALS pucks. There are many online resources for using unipucks, including the manual from SSRL and helpful videos from Diamond Light Source.

SHOP HERE

VIDEOS OF THE MONTH

MicroED: An update from the Rigaku JEOL collaboration

A recording of a special webinar on MicroED showing the latest progress from our collaboration with JEOL.

MicroED Structure Determination of Protein Crystals by Fragment-Based Molecular Replacement

Jennifer Mian, UCLA
COFM Study Weekend,
Nottingham, Jan 10, 2019

Micro-electron diffraction (MicroED), a cryo-electron diffraction method, has proven successful in determining the atomic structures of macromolecules using both direct methods and molecular replacement (MR) phasing protocols. For atomic resolution data (~1 Å) the atomicity constraint holds, and an ab initio solution is attainable. At lower resolutions, a known homologous structure can be used as a probe to retrieve the phases by MR. Here, we present success in structure determination of amyloidogenic peptides by MicroED using both molecular replacement and direct methods phasing.

USEFUL LINKS

Laboratory of Molecular Electron Microscopy – Tamir Gonen

A useful website for learning about MicroED, containing raw datasets for download and a good list of relevant papers, reviews, and book chapters.

The Nan Ed Project

The Nan ED Project - Electron Nanocrystallography, is an Innovative Training Network, Marie Skłodowska-Curie Actions, project funded by EU (grant agreement n. 956099) aimed to train a new generation of electron crystallographers thereby paving the way for future development and establishment of the method more broadly in the academic community and within the industry.

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

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