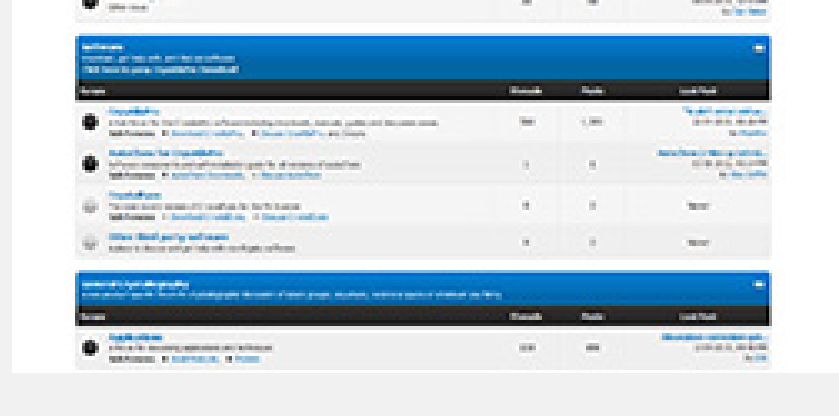


Crystallography Newsletter
Volume 9, No. 7, July 2017[Subscribe](#)**In this issue:**

- [Join ROD on LinkedIn](#)
- [Crystallography in the news](#)
- [Rigaku X-ray forum](#)
- [Survey of the month](#)
- [Last month's survey](#)
- [Product spotlight](#)
- [Video of the month](#)
- [Lab in the spotlight](#)
- [Useful links](#)
- [Upcoming events](#)
- [Recent crystallographic papers](#)
- [Book review](#)

Join ROD on LinkedIn

The [Rigaku Oxford Diffraction 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.

Rigaku Oxford Diffraction invites all users of Rigaku equipment to join us on our X-ray forumwww.rigakuxrayforum.com

Here 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.

We look forward to seeing you on there soon.

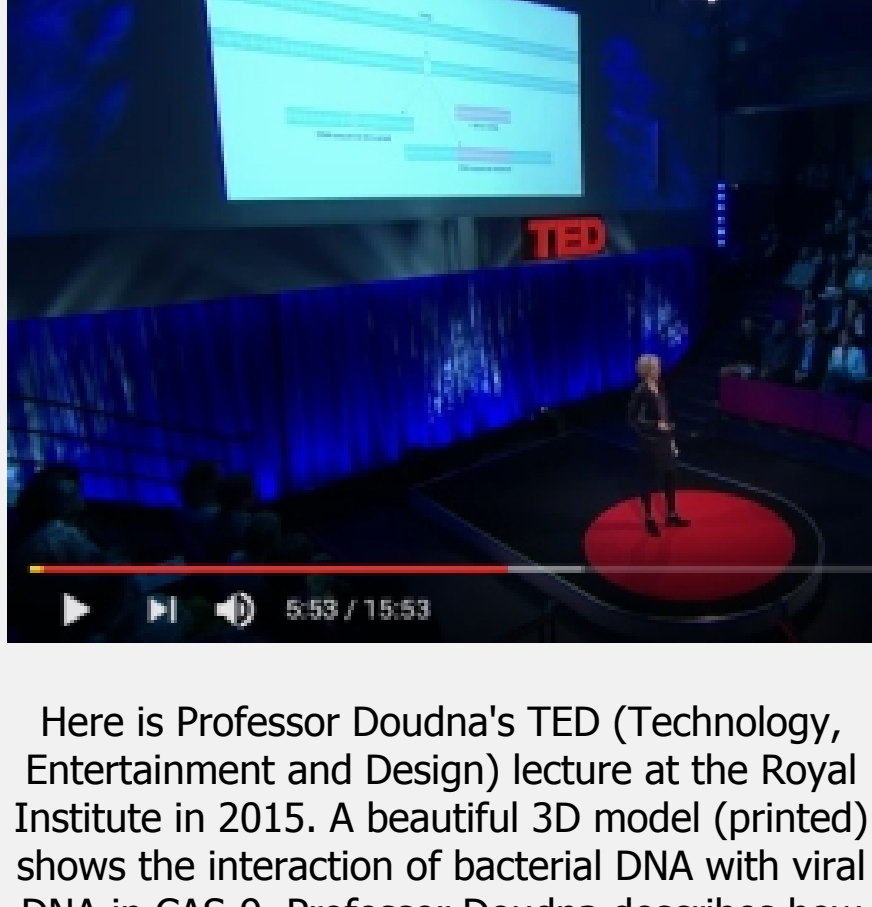
Survey of the month**July 17 SCX Survey****Will you be attending IUCr in Hyderabad?**

- ☐ Still haven't decided
- ☐ Yes
- ☐ No
- ☐ I would if I had the funding

Take the Survey**Last month's survey**

What is the first thing you do in the morning?

Grab my smartphone, connect to the lab and check on the status of an experiment	8%
Grab my smartphone and check the news	16%
Get a cup of coffee	64%
Take a couple of aspirin	8%
I don't get up in the morning	4%

Video of the month**How CRISPR lets us edit our DNA by Jennifer Doudna**

Here is Professor Doudna's TED (Technology, Entertainment and Design) lecture at the Royal Institute in 2015. A beautiful 3D model (printed) shows the interaction of bacterial DNA with viral DNA in CAS-9. Professor Doudna describes how this method can be used to insert genes into any DNA sequence and goes onto look into the ethical issues of this method of genetic modification.

Watch the Video**Upcoming events**

[Denver X-ray Conference 2017](#)

July 31 – August 4, 2017 in Big Sky, MT

[PPXRD-15](#)

August 18 – 20, 2017 in Hyderabad

[International Union of Crystallography](#)

August 21 – 28, 2017 in Hyderabad

[See full list >](#)

**Crystallography in the news**

July 1, 2017. The [2018 Croonian Medal and Lecture](#) is awarded to Professor Jennifer Doudna ForMemRS for her outstanding structural and functional studies of RNA and ribonucleoproteins and for elucidating the molecular mechanism of the CRISPR-Cas9 system and developing it for genetic engineering.

July 5, 2017. A novel method to improve the high-yield, high-purity, high-activity [purification of complex proteins](#) by 10- to 500-fold has been developed at the University of Alabama at Birmingham. Dmitry Vassilyev, professor of biochemistry and molecular genetics, said that this new method offers a number of crucial advantages to both researchers and the pharmaceutical industry.

July 5, 2017. Dublin City University has today formally named six buildings after renowned public figures. Dame Kathleen Lonsdale (1903-71), a crystallographer born in Newbridge, County Kildare, was at the vanguard of establishing crystallography science. The [Lonsdale Building](#), which houses the Schools of Chemical Sciences and Biotechnology, has been named in her honour.

July 5, 2017. By taking a series of near-atomic resolution snapshots, Cornell University and Harvard Medical School scientists have [observed step-by-step how bacteria defend against foreign invaders](#) such as bacteriophage, a virus that infects bacteria.

July 6, 2017. Researchers from the University of Copenhagen (Denmark), led by the Spanish researcher Guillermo Montoya, have [discovered how Cpf1, a new molecular scissors, unzips and cleaves DNA](#).

July 10, 2017. A team led by Washington University in St. Louis has unraveled the structure of a protein that allows [respiratory syncytial virus \(RSV\) to elude the immune system](#). This structure could be a target for researchers developing vaccines or treatments for RSV infection.

July 10, 2017. Marijuana receptor caught in the act: [High-resolution X-ray structures of a cannabinoid receptor](#) with activating agents help reveal how it works.

July 11, 2017. A new algorithmic framework called [multi-tiered iterative phasing \(M-TIP\)](#) utilizes advanced mathematical techniques to determine 3-D molecular structure of important nanoobjects like proteins and viruses from very sparse sets of noisy, single-particle data.

July 18, 2017. Bordeaux Acquisition, a majority-owned subsidiary of AIM-traded scientific instrument-focussed [Judges Scientific, acquired 100% of the issued share capital in Crystallon](#) on Tuesday, which itself is the holding company of Oxford Cryosystems.

Product spotlight: XtaLAB Synergy-R

The XtaLAB Synergy-R is the most powerful small molecule diffractometer available. It includes a high-flux, low-maintenance microfocus rotating anode, the PhotonJet-R, with a high-precision kappa goniometer and Rigaku's own Hybrid Photon Counting detector (HPC) the HyPix-6000HE. The PhotonJet-R X-ray source is comprised of a Micromax-007 HF rotating anode and a newly designed optic. It is available with either Cu or Mo anodes.



For labs with high-throughput requirement, increasing the flux will reduce data collection time and thus increase the number of samples that can be studied in your laboratory. For extremely small samples, additional flux will extend the minimum size limits for crystals that you can study.

Benefits include:

- Fast workflow due to complete integration of software and hardware
- Excels at the most challenging applications, e.g. MOFs or incommensurate structures
- Extremely high performance due to bright source, noise-free detector and fast goniometer speeds
- Provides unparalleled throughput
- Compact design to fit in your laboratory

Features include:

- True shutterless data collection
- Noise-free HPC detector for better measurement of weak data
- 4-circle kappa goniometer with high accuracy and speed

[For more about XtaLAB Synergy-R.](#)

Lab in the spotlight**Dr. Luca Jovine**

Karolinska Institutet
Department of Biosciences and Nutrition
Center for Innovative Medicine
Hälsövägen 7, SE-141 83 Huddinge, Sweden

By marking the very beginning of a new individual, egg-sperm interaction at fertilization is a crucial step in the life cycle of all sexual organisms. Human sperm was first visualized at the end of the 17th century, and scanning electron microscopy pictures taken in the 1960's captured the collective imagination by offering low resolution glimpses of the encounter between human gametes. However, the molecular details underlying the species-restricted embrace between germ cells remained until recently completely obscure. The ultimate aim of the Jovine laboratory is to use structural biology to provide a definitive answer to this fundamental biological problem with important evolutionary implications.

The Jovine lab focuses on the zona pellucida (ZP), a thick, specialized extracellular matrix that surrounds mammalian eggs and plays essential roles in oogenesis, fertilization and pre-implantation development. Depending on the species, the ZP contains 3 or 4 glycoprotein subunits (denominated ZP1-4) that assemble into micrometer-long filaments using a conserved polymerization module of ~260 amino acids, the so-called ZP domain. Additional regions contained within individual ZP subunits are responsible for their specific functions in the fertilization process. For example, ZP3 and ZP2 have long been suggested to mediate interaction with sperm. At the same time, the polymerization and receptor activities of ZP subunits are intimately connected to each other, not only because their supramolecular arrangement ensures that enough receptor molecules are concurrently presented to the head of sperm, but also because post-fertilization changes in the overall structure of the ZP have an important role in the block to polyspermy. This interplay between structure and function is further highlighted by the observation that mice lacking ZP3 or ZP2 do not have a ZP and are completely infertile, and that alterations of the structure of the ZP as well as mutations of the ZP1 gene are implicated in human infertility.

The structures of ZP3 and Juno were the first to be reported of vertebrate proteins that are both essential for fertilization and directly involved in the interaction between gametes. Similarly, our structures of VRL/lysin complexes provided the first atomic-resolution information on how sperm recognizes the egg coat at the beginning of fertilization. To gain further insights into the molecular basis of this fundamental process, the Jovine lab is now targeting additional complexes between key egg-sperm recognition proteins, as well as trying to understand how structural alterations of ZP module polymers translate into human disease at the molecular level. The Jovine lab relies on a comprehensive range of techniques that include DNA cloning, protein production in both prokaryotic and eukaryotic systems (with a very strong focus on mammalian cell expression), protein purification, biochemical characterization and 3D structure determination by X-ray crystallography. In collaboration with several other groups, the Jovine lab is also performing functional and electron microscopy studies.

Useful links

Here are links to two servers that analyze diffraction anisotropy in order to provide for better scaling of data and ultimately refinement of useful data.

[The Diffraction Anisotropy Server from the UCLA-DOE Lab](#)

[The STARANISO Server from Global Phasing Limited](#)

Selected recent crystallographic papers

Science of crystal structures: highlights in crystallography. Helliwell, John R. *Crystallography Reviews*. Jul2017, Vol. 23 Issue 3, p231-236. 6p. DOI: [10.1080/0889311X.2017.1295039](#).

A view inside the nature of protein crystals. Oswald, R.; Pietzsch, M.; Ulrich, J. *Journal of Crystal Growth*. Jul2017, Vol. 469, p176-179. 4p. DOI: [10.1016/j.jcrysgro.2016.09.059](#).

Understanding Structure: A Computer-Based Macromolecular Biochemistry Lab Activity. McLaughlin, Kristie J. *Journal of Chemical Education*. Jul2017, Vol. 94 Issue 7, p903-906. 4p. DOI: [10.1021/acs.jchemeduc.6b00464](#).

A Database of Transition-Metal-Coordinated Peptide Cross-Sections: Selective Interaction with Specific Amino Acid Residues. Dilger, Jonathan; Glover, Matthew; Clemmer, David. *Journal of the American Society for Mass Spectrometry*. Jul2017, Vol. 28 Issue 7, p1293-1303. 11p. DOI: [10.1007/s13361-016-1592-9](#).

Using crystallography, topology and graph set analysis for the description of the hydrogen bond network of triamterene: a rational approach to solid form selection. Hughes, David S.; Delori, Amit; Rehman, Abida; Jones, William. *Chemistry Central Journal*. 7/13/2017, Vol. 11 Issue 1, p1-19. 19p. DOI: [10.1186/s13065-017-0293-1](#).

Mapping-Out Catalytic Processes in a Metal-Organic Framework with Single-Crystal X-ray Crystallography. Burgun, Alexandre; Coghlan, Campbell J.; Huang, David M.; Chen, Wenqian; Horike, Satoshi; Kitagawa, Susumu; Alvino, Jason F.; Metha, Gregory F.; Sumbly, Christopher J.; Doonan, Christian J. *Angewandte Chemie International Edition*. 7/10/2017, Vol. 56 Issue 29, p8412-8416. 5p. DOI: [10.1002/anie.201611254](#).

A novel tubular hydrogen-bond pattern in a new diazaphosphole oxide: a combination of X-ray crystallography and theoretical study of hydrogen bonds. Sabbaghi, Fahimeh; Pourayoubi, Mehrdad; Farhadipour, Abolghasem; Ghorbani, Nazila; Andreev, Pavel V. *Acta Crystallographica: Section C, Structural Chemistry*. Jul2017, Vol. 73 Issue 7, p508-516. 8p. DOI: [10.1107/S205322961700794X](#).

Unusual saccharin-N₂O (carbonyl) coordination in mixed-ligand copper(II) complexes: Synthesis, X-ray crystallography and biological activity. Mokhtaruddin, Nur Shuhada Mohd; Yusof, Enis Nadia Md; Ravoo, Tahira B.S.A.; Tiekin, Edward R.T.; Veerakumarasivam, Abhi; Tahir, Mohamed Ibrahim Mohamed. *Journal of Molecular Structure*. Jul2017, Vol. 1139, p1-9. 9p. DOI: [10.1016/j.molstruc.2017.03.037](#).

Effect of ligands on crystallography, morphology and photo-catalytic ability of ZnS nanostructures. Kaur, Balwinder; Singh, Karamjit; Malik, Ashok Kumar. *Dyes & Pigments*. Jul2017, Vol. 142, p153-160. 8p. DOI: [10.1016/j.dyepig.2017.03.013](#).

The uniqueness of subunit α of mycobacterial F-ATP synthases: An evolutionary variant for niche adaptation. Ragunathan, Priya; Sielaff, Hendrik; Sundararaman, Lavanya; Blukovic, Goran; Subramanian Manimekalai, Malathy Sony; Singh, Dhirendra; Kundu, Subhashri; Wohland, Thorsten; Fransch, Wayne; Dick, Thomas; Grüber, Gerhard. *Journal of Biological Chemistry*. 7/7/2017, Vol. 292 Issue 27, p11262-11279. 18p. DOI: [10.1074/jbc.M117.784959](#).

When defects turn into virtues: The curious case of zirconium-based metal-organic frameworks. Taddei, Marco. *Coordination Chemistry Reviews*. Jul2017, Vol. 343, p1-24. 24p. DOI: [10.1016/j.ccr.2017.04.010](#).

The multidrug-resistance transporter MdfA from *Escherichia coli*: crystallization and X-ray diffraction analysis. Nagarathinam, Kumar; Jaenecke, Frank; Nakada-Nakura, Yoshiko; Hotta, Yunhon; Liu, Kehong; Iwata, So; Stubbs, Milton T.; Nomura, Norimichi; Tanabe, Mikio. *Acta Crystallographica: Section F, Structural Biology Communications*. Jul2017, Vol. 73 Issue 7, p423-430. 7p. DOI: [10.1107/S2053230X17008500](#).

Analytical techniques for the study of polyphenol-protein interactions. Poklar Urih, Nata?a. *Critical Reviews in Food Science & Nutrition*. 2017, Vol. 57 Issue 10, p2144-2161. 18p. DOI: [10.1080/10408398.2015.1052040](#).

Ultra-high-resolution structure and charge-density analysis of high-potential iron-sulfur protein. Takeda, Kazuki; Miki, Kunio. *FEBS Journal*. Jul2017, Vol. 284 Issue 14, p2163-2166. 4p. DOI: [10.1111/febs.14036](#).

Amino-functionalized MIL-101(Fe) metal-organic framework as a viable fluorescent probe for nitroaromatic compounds. Karthik, Peramaiah; Pandikumar, Alagarsamy; Preeyanghaa, Mani; Kowsalya, Mariyappan; Neppolian, Bernadshaw. *Microchimica Acta*. Jul2017, Vol. 184 Issue 7, p2265-2273. 9p. DOI: [10.1007/s00604-017-2215-2](#).

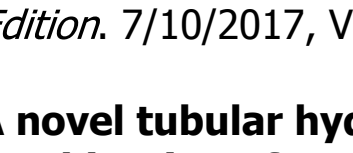
X-ray diffraction, spectroscopic and DFT studies on nickel(II)-triphenylphosphine complexes of 2-hydroxyacetophenone thiosemicarbazones. Kilic-Cikla, Isin; Güveli, Sükrüye; Bal-Demirci, Tülay; Aygün, Muhittin; Ülküseven, Bahri; Yavuz, Metin. *Polyhedron*. Jul2017, Vol. 130, p1-12. 12p. DOI: [10.1016/j.poly.2017.03.059](#).

Tetrakis [N-(2-pyridyl) sulfonamide] di palladium: synthesis, X-ray diffraction, antibacterial properties and as a novel binuclear Pd-complex for coupling reactions. Mehdiipour, Ebrahim; Shafieyoon, Parvaneh; Salavarzi, Maryam; Amani, Vahid. *Journal of the Iranian Chemical Society*. Jul2017, Vol. 14 Issue 7, p1575-1582. 8p. DOI: [10.1007/s13738-017-1098-9](#).

Book review

Back in January the *IA* podcast did a special on dystopian novels because of the surge in sales of books in that genre since November 2017. *1984* was at the top of the list, but because I have read it once a decade since high school I didn't reread it this year. I picked up two of the novels on the list, *It Can't Happen Here* and *A Handmaid's Tale*, and also found a Great Course titled *Great Utopian and Dystopian Works of Literature*.

***Great Utopian and Dystopian Works of Literature*, Pamela Bedore, Ph.D., The Great Courses, Chantilly, VA, 2017.**



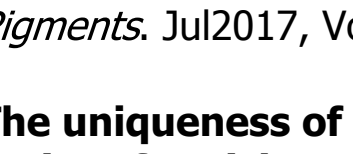
Professor Bedore is an English professor at the University of Connecticut. She is the recipient of an Excellence in Teaching Award and when you listen to the course you will understand why. I wish my English teachers in college had been as animated as she is. The course begins with an analysis of Thomas More's *Utopia*. The next few lectures cover the classics by Voltaire, Swift, Hawthorne, Alcott, Butler and Bellamy. For me, things began to get interesting with the analysis of H.G. Wells' *The Time Machine*. Here is where I realized one being's utopia is another's dystopia, a fact Bedore points out in a later lecture. The mid-20th century classics are included for analysis: Huxley's *Brave New World*, Orwell's *1984*, one of my favorites, Dick's *Minority Report*, and Burgess' *A Clockwork Orange*. Here Bedore begins the analysis of movie versions of the studied novels. More recent classics are also studied: Atwood's *A Handmaid's Tale*, Collins' *The Hunger Games* trilogy and McCarthy's *The Road*. I found this a fascinating and rewarding series of lectures and highly recommend it as a diversion from current events.

***It Can't Happen Here*, Sinclair Lewis, Signet Classics, New York, 1935-2014, 416 pp, ISBN: 978-0451465641.**

The novel is set in the 1930s and is based on the premise that Franklin Delano Roosevelt loses the 1936 election to a fictional character, Buzz Windrip, modeled on Huey Long (who was assassinated just before the election). Dystopia arises from Windrip's destruction of American democracy and imposition of totalitarian rule through a paramilitary force created from unemployed workers. The hero is Doremus Jessup, a journalist, who fights Windrip throughout the novel. I don't want to spoil the ending, but I really enjoyed the book.

***A Handmaid's Tale*, Margaret Atwood, Houghton Mifflin Harcourt, New York, 1986, 320 pp, ISBN: 978-0385490818.**

The novel is a first person narrative provided by the protagonist, a woman renamed Offred, who has been forced to become a handmaid (surrogate for infertile wives) in an America that has become a theocracy called Gilead based on the Old Testament. Since women have been relegated to subservient tasks throughout the society, Offred manages to write the account. You will find out in the last chapter how she provides any more information will spoil the ending. Hulu has produced a miniseries based on the novel, which has received a lot of positive press, at least in the periodicals I read; however, I always recommend reading the book before seeing any screen adaptations.



Review by Joseph Ferrara
Deputy Director, X-ray Research Laboratory, Rigaku

