ACA RefleXions

American Crystallographic Association Structure Matters

Number 1 **Spring 2018**

Judith Flippen-Anderson
1941-2018

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Lisa Keefe
2018 ACA President

2018 ACA Award Winners to Be Honored in Toronto

Jason McLellan
Etter Early Career Award

Frank Hawthorne
Buerger Award

Simon Billinge
Warren Award

Gautam Desiraju
ACA Living History

Nobel Laureate John Polanyi
Keynote Lecturer in Toronto

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President's Column

Lisa Keefe

Structure is what bonds us. As I pen this inaugural President's Column, I reflect back to over thirty years ago when I was introduced to the ACA and attended my first annual meeting. I was captivated by the intensity and passion that crystallographers shared in the pursuit of elucidating molecular structure. I was hooked. Over the years, ACA continued to educate and inspire, serving as a nourishing oasis for sharing results, learning new strategies, and meeting with colleagues. It is a privilege to now serve the ACA in this exciting time of growth in technology and exploration of unchartered scientific areas.

Integral to ACA's success is the staff at the headquarters in Buffalo. We wish Marcia Colquhoun much happiness in her retirement and thank her for the many years of service to ACA. Welcome to Kristin Stevens in her role as the new Director of Administrative Services. Kristin, along with Kristina Vitale, maintain ACA operations critical to successful meetings and membership services. We are grateful to Bill Duax (CEO) for continuing to offer his wisdom and guidance to all facets of ACA. The staff at ACA headquarters provide both vital support and continuity to ACA council who, in the face of annual changes of officers, bears many responsibilities in the stewardship of ACA.

In introducing the new council members, I express much gratitude to my predecessor, Amy Sarjeant, for her strong leadership and steadfast commitment to ACA, and am grateful that she will serve this upcoming year as Past President and continue to offer advice to council. A sincere thank you to Tom Terwilliger for his thoughtful insight and guidance, as he leaves his position of Past President. A warm welcome to Joe Ferrara (Vice President) as he starts the first year of his term. Continuing their service on council, I am much appreciative to Sue Byram (Treasurer), Diana Tomchick (Secretary), Tomislav Friscic (Canadian Representative), George Lountos (YSIG Representative), Hanna Dabkowska (IUCr Representative), and Narasinga Rao (CFO); it's a talented team.

ACA's objective, as stated in the By-laws, is "to promote the study of the arrangement of the atoms in matter, its causes, its nature and its consequences, and of the tools and methods used in such studies." We are in the midst of an evolution in tools and methods to garner structural information from ever more challenging molecules and complexes. We witnessed the birth of the CryoEM SIG, breathtaking advances in XFELs, and the propulsion of synchrotron radiation to a readily available source for both routine data collection and cutting-edge experiments. Complementing this growth and development is the ACA—our forum for further development, both scientifically and professionally. ACA Council is tackling a number of endeavors aimed at growing meaningfulness, strengthening relevance, and ensuring long-term sustainability. These include enriching the annual meeting experience, enhancing membership services, preserving fiscal stability, and establishing opportunities for rewarding participation, starting with the 68th Annual Meeting this summer in Toronto.

Register early and reserve your lodging for this year's meeting, July 20-24, in Toronto. Working with the SIGs, the program co-chairs, Gerald Audette and Tiffany Kinnibrugh, have organized an extraordinary scientific program. View details on the meeting website. The keynote address will be presented by John Polanyi, the 1986 Nobel Laureate in Chemistry. The Buerger Award will be presented to Frank Hawthorne (University of Manitoba) for his systematic studies of the crystal chemistry of major mineral groups. The Warren Award will be presented to Simon Billinge (Columbia University and Brookhaven National Laboratory) for his groundbreaking work in characterizing structures of nanomaterials. The Etter Early Career Award will be presented to Jason McLellan (Dartmouth College) for his extensive work on the respiratory syncytial virus (RSV) F glycoprotein and pursuing a structure-based approach to the rational design of interventions for viruses. The Transactions Symposium, Shining a Light on Structure-Based Drug Discovery, will bring together researchers with interests in a broad spectrum of disciplines, including protein crystallography, cryo-EM, small molecule crystallography, and technology innovation and development, with the aim of exploring new methods to tackle challenging projects. Engage in the rich scientific program and inspiring discussions; join us at the ACA Annual Meeting in Toronto.

How can ACA best serve you? Let us know; contact a coucil member, the RefleXions editors, or ACA headquarters. It is evident that we share a strong passion for structure. Structure is what bonds ACA members. Let's strengthen those bonds and work together to ensure the vitality of ACA—for our lifetime and for future generations. I look forward to meeting you in Toronto.

Lisa Keefe

It is with much saddness that we report that Judith Flippen-Anderson, a past president of the ACA, passed away on March 31, 2018 in Annandale, Virginia, at the age of 76. Judy was a graduate of Northeastern University and Arizona State University, and worked for more than thirty years at the Naval Research Laboratory as an X-Ray Crystallographer. She also worked as Corporate Secretary of the Board of Directors at the American Institute of Physics, a researcher at the Protein Data Bank at Rutgers University, and was serving as Co-Editor of the ACA RefleXions.

Memories of Judy

Helen Berman:

Judy was a force. She had so many aspects to her being that it is difficult to highlight just a few. I first met her at an ACA meeting in the early 70's. We had a lot in common; we were both small molecule crystallographers; we were both raised in Jewish households in the Northeast and we both had defining regional accents that we never quite lost. I was struck by her enormous energy and spirit and it was clear even back then that Judy was going to make a difference in the world.

Fast forward to the 80's when we were both on Council. We definitely made the most of our friendship and worked hard to come up with better ways of running the organization. This involved strategic brainstorming as well as actually doing the work necessary to implement the ideas. The most fun was working with her on the Philadelphia ACA meeting where we managed to hire a Benjamin Franklin impersonator who attended the banquet at the Franklin Institute and where Judy gave a most remarkable and memorable past presidents speech. She was also the Editor of the newsletter that evolved into a wonderful and colorful account of the ACA activities. Unlike most past presidents Judy managed to find a way to stay involved so she could help move the ACA to new places. The most remarkable of these accomplishments was to help establish an ACA journal-Structural Dynamics.

All the work that Judy did for the ACA was in addition to her successful career at NRL that resulted in more than 500 structures in the CSD. When she retired from NRL, she came to work for the RCSB PDB where she played many important roles and from which she retired only two years ago.

On a personal front, I always looked forward to my many trips to Washington where I would stay with Judy and Paul and enjoy memorable meals in the many restaurants they enjoyed. I had the privilege of hearing about her daughter Chenoa and husband Emilio who are very successful professors at the University of Pennsylvania. And of course, she was so proud and happy to be bubbe to two beautiful grandchildren.

In 2003, we decided to do a road trip across America when I turned 60. We had many adventures as we explored the vast stretches of the Midwest, ate barbeque, drove on scary roads in the Rockies, hiked in Utah, and gambled in Las Vegas. It was so much fun for both of us and I feel lucky to have experienced it. I will always miss Judy with her intellect, her wit, her warmth, her expansive laugh, her Boston accent and her fantastic earrings. I feel lucky to have been part of her circle.

Naval Research Laboratory 1984, outside the NRL front gate Back: Pete D'Antonio, Judy Flippen-Anderson, Cliff George, Janet Smith, Steve Brenner, Richard Gilardi, Isabella Karle, Jerome Karle. Front: John Konnert, Lynn Graham, Al Lowrey, Wayne Hendrickson. Photo courtesy Judy Flippen-Anderson.

Connie Rajnak:

I knew Judy from ACA meetings ever since I started going to ACA meetings, but didn't know her well until my sabbatical in DC in 1985, when we really bonded. In 1985-86 I spent a sabbatical at NRL. Every day Judy and I would sit at the lunch table with Isabella and Jerome Karle, Cliff George, Richard Gilardi, Peter D'Antonio, Jeff Deschamps, Steve Brenner, Mary Ann Perrozo, and occasionally, John Konnert. We would talk about all kinds of things - including politics and current news. During my time at NRL, I went to dinner with Judy and Paul either at an ethnic restaurant or at their house. They have a lovely home in Annandale, Virginia which had a 'bubble' jutting out from their dining room about 3 ft. and they grew all kinds of desert plants

(sun during the day, outside feel at night). Their living room featured a big thing that was a part of the NRL computer which Paul replaced - it was to remember how they met. Judy and Paul complemented each other so well. Paul loved to cook and garden and Judy loved to eat. I well remember the visit to your house when you both had a good laugh when I tasted one of your hot chilis. Paul was a perfectionist in all things and KNEW about computers. They both loved art. Judy contributed by sharing her friends (95% of the people she knew). They both loved Chenoa and when she married Emilio and they had children they both loved them all.

Photo in 1985 showing party at Keith Ward's house in celebration of Jerome Karle winning the Nobel Prize.
Back row: Keith Ward, Doug Collins and his wife, Isabella Karle, Jerome Karle, Pete D'Antonio, Janet Smith, Cliff George, Al Lowrey, Richard Gilardi.
Front row: Diane Ward, Judy Flippen-Anderson, Steve Sheriff, John Konnert.
Photo courtesy Judy Flippen-Anderson.

One day I was leaving NRL with Judy and we were talking and descending the semi-circular steps and I just fell flat on my face on the pavement. The next day Judy brought a camera and took a picture of my face with the resulting black eye. She then emailed it to Dave Duchamp saying 'This is what I'm going to do to you if you don't send those programs! (My original sabbatical proposal involved crystallizing a peptide 5 or 6 amino acids in length. I had brought several, but they were taking longer to crystallize than I had expected and I wanted to fill in by installing Dave's CRYM suite of programs on the NRL computer, Dave had previously agreed to this, but had not yet sent that suite of programs.

And then there were the ACA Newsletter/ACA RefleXions days. I was an Editor from the time I took over from Jenny Glusker, and I was the first to send it to Buffalo for printing and sending to ACA members. It was first called the ACA Newsletter - we came later to call it ACA RefleXions. I don't remember who came up with that classy name, it certainly wasn't me. I decided that there should be 4 issues per year, Spring, Summer, Fall, and Winter, and then decided it was taking too much time away from my real job at The Upjohn Company, so I recruited Judy to edit two of the issues. Jenny had, as I remember, 6 issues, sent by email by her secretary to all ACA members.

Judy was President of the ACA long before I was, but she understood from that experience why I would need a break as Co-Editor for the duration of my time on Council.

Sue Byram:

It won't be the same at ACA without Judy. Colleagues of all ages are already sadly sharing this sentiment. I knew Judy first as the 'go-to' person at Naval Research Laboratory, the person to get things done at the Nobel Prize-winning Laboratory for the Structure of Matter. We had fun together at ACA meetings from the 70's onwards. The group of women in crystallography was rather smaller than today and we all enjoyed getting together. I recall Judy at one memorable party held in my hotel just across the line from an alcohol-free ('dry') location where the ACA meeting was located. We were still laughing at the ACA Philadelphia meeting in 2015, where Judy sparred with 'Rocky'.

Judy welcomed everybody to ACA, kept us on track with timely submissions to ACA RefleXions and the IUCr newsletter (which she edited during Bill Duax' tenure as IUCr president), and encouraged more than a few crystallographic volunteers. I will miss her laugh and her warmth a lot.

Photo courtesy Angie Zwicker, Bruker AXS

Michael James:

Judy was an extraordinary person. She took on many projects during the time that I knew her and did all of them exceptionally well. Throughout her lifetime, she dedicated a tremendous amount of time and energy to the American Crystallographic Association. She served as President of the ACA in 1991 and

brought about many new additions and changes to its operation. For example, she was instrumental in establishing the Canadian Representative as a member of the ACA Council. Our friendship began at one of the ACA meetings in the early 1970s and has continued until now. I will miss her greatly.

Following her graduate studies at the University of Arizona, she travelled to Washington DC and eventually got a position at the US Naval Research Laboratory as a Crystallographer. Many of her early crystal structure studies were done with Isabella Karle and were determined by the newly developed "direct methods" of the symbolic addition procedure being developed by Jerome Karle.

It was always a pleasure to attend the annual (in the early days the meetings were held twice a year!) meetings of the ACA. It was a chance to meet up with old friends and especially with Judy. It always seemed that the excitement of the meeting revolved around her. Her strong interests were in convincing the young people at the meeting for the first time how important it was to make friends that would last a lifetime. Indeed it was true and through Judy I met many of the important crystallographers at the ACA meetings and through them developed collaborations and research colleagues that have lasted a lifetime. Judy was an inspiration to me and helped, perhaps unknowingly, to develop my career.

Judy loved to travel. Quite recently her husband Paul and Judy took the "Rocky Mountaineer" a train and bus trip that travels through the Canadian Rocky Mountains. It starts by train from scenic Vancouver in British Columbia and finishes with a bus trip from Jasper, Lake Louise and Banff. Needless to say both Paul and Judy were thrilled by the trip. "Imagine we walked on the Columbia Ice Fields Glacier," she wrote to me in an email after they returned home. Knowing Judy, she and Paul made many new friends from Australia, New Zealand, Europe, Canada and the USA. In her email Judy extolled the unimaginable scenery and the great enjoyment that she and Paul both had on that trip.

I will miss Judy at future ACA meetings. I was so looking forward to see her at the coming Toronto meeting. Judy always worked very hard for the ACA. It pleases me that there are many young crystallographers that are members now and they will keep the spirit that Judy established alive in the ACA.

Tom Koetzle:

Judy was a treasured colleague and a dear friend, and I miss her terribly. I will especially remember the past four years working alongside Judy as co-editors of RefleXions, and I have many fond memories from our long-standing friendship of decades. Judy was truly a 'force of nature'. She had an impressive career as a small-molecule crystallographer for thirty-five years at the Naval Research Laboratory and, following her retirement from NRL, worked with the RCSB Protein Data Bank. Through her many contributions to ACA over the years, Judy had an incalculable influence on the operations and development of the Association. In recent years, she threw herself into championing the inception and growth of Structural Dynamics, ACA's flagship journal published jointly with AIP. She was very proud of the journal's success, and it will be an important part of Judy's rich legacy.

In addition to our love of crystallography, Judy and I had in common our strong associations to the greater Boston area. I just loved Judy's New England accent — it did so remind me of my own student years in Cambridge, Mass.

The ACA community has suffered a great loss. We shall surely miss Judy's wisdom and wit. Our annual meetings will not be the same without Judy, her incredible energy, and her willingness to volunteer for any task large or small!

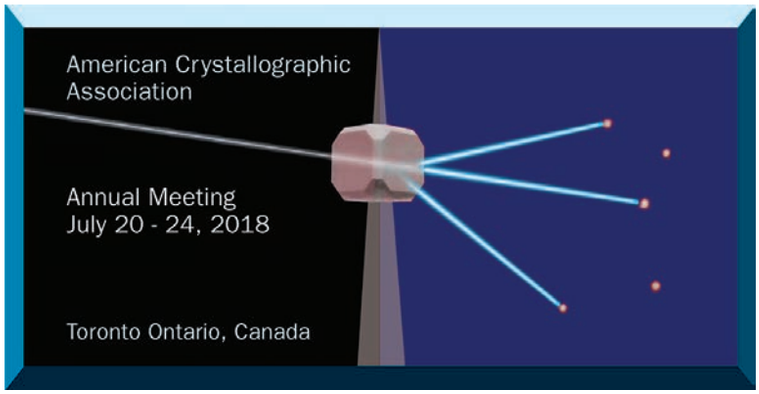
Virginia Pett:

Judy was a small-molecule crystallographer at the Laboratory for the Structure of Matter (Naval Research Laboratory) for 35 years. A steadfast supporter of the ACA, she was president in 1991, a member of the meeting site selection committee for many years, co-editor of the ACA RefleXions magazine, and one of the prime movers behind the formation of the new ACA journal Structural Dynamics. She was past president of the US National Committee for Crystallography and a former editor of the IUCr Newsletter. A long-time representative to the American Institute of Physics (AIP) Executive Committee and the Governing Board, she was elected in 2013 to the office of AIP Corporate Secretary. Judy was a passionate advocate of causes she supported and she had the ability to cut to the heart of the issue under discussion. She welcomed many of us to ACA annual meetings at the registration desk. We will miss her friendship and warmth and devotion to our society.

Jenny Glusker:

It is with great sadness that I heard of the death of Judy Flippen-Anderson. She contributed so much to structural studies by X-ray diffraction, and to the smooth running, with Connie Rajnak, of the regularly issued and informative newsletter (ACA RefleXions). Judy was a well-known and respected member of our community and will be greatly missed.

We are pleased to present the 68th meeting of the ACA in beautiful downtown Toronto, Canada!



ACA TORONTO

Friday, July 20 – Tuesday, July 24, 2018

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(Room prices are in Canadian Dollars)

Hotel Reservation Deadline: June 15, 2018

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Special Opening Keynote Speaker

John Polanyi
1986 Nobel Laureate in Chemistry

2018 ACA Awards

Simon Billinge
Warren Award

Frank Hawthorne
Buerger Award

Jason McLellan
Etter Early Career Award

WORKSHOPS

Cryo-EM – A Guide to High-Resolution Structure Determination
Molecular Art and Animation in 3D
Applications of Small Angle Scattering to Structural Biology: An Introduction
Rietveld Refinement and pdf Analyses of in situ X-ray Scattering Data within GSAS-II

SESSIONS

Transactions Symposium – Shining a Light on Structure-Based Drug Design
Structural Dynamics – in Honor of Philip Coppens
Special Sessions in Honor of Dick Marsh
Crystallography on the International Space Station
Advances in Biological Cryo Electron Microscopy
Structural Biology of Pathogens
NMR Crystallography
Neutron and X-ray Scattering of Correlated and Quantum Materials
Dynamic Crystals as Molecular Materials
Mineralogical Crystallography

For meeting sponsor information, abstracts, on-line registration, and details including room sharing feature see:
http://www.amercrystalassn.org/2018-meeting-homepage

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Nominations for 2019

ACA Awards: Nominations for the 2019 **I. Fankuchen, K. Trueblood,** and **Margaret C. Etter Early Career** awards were due by April 1, 2018. **Nominations** for **ACA Fellows** were also due by April 1.

ACA Offices and Committees: In Fall 2018 we will elect an ACA Vice- President, Treasurer, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards & Computing). To suggest a candidate for one of the above positions, please contact **Kristin Stevens: kstevens@hwi.buffalo.edu**. Full details describing the criteria for all ACA awards and offices can be found on the ACA website.

2018 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds.

NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org

Send all award nominations to: kstevens@hwi.buffalo.edu

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RefleXions Announces New Co-Editor, Ed Stevens

A native of Oregon, Ed grew up near Portland and attended Oregon State University where he received a B.S. degree in Chemistry in 1969. He then moved to the University of California, Davis and received a Ph.D. degree in Chemistry in 1973 under the direction of Prof. Håkon Hope, during which time he developed an interest in accurate x-ray intensity measurements and experimental charge density measurements. He then moved to Buffalo, NY as a postdoctoral research associate working with Prof. Philip Coppens to continue his work on charge density distributions. In 1981, after briefly working as a Research Chemist at Allied Chemical Corp. in Morristown, NJ, he joined the faculty of the Department of Chemistry at the University of New Orleans as an assistant professor. He remained at the University of New Orleans for the next 33 years teaching chemistry, conducting structural studies of energetic materials and homogeneous catalysts, and measuring charge densities using low temperature x-ray diffraction measurements. Ed retired from UNO in 2014, having attained the rank of University Distinguished Professor and having served as department chair for eight years. He moved to join his wife, Cheryl, who is currently Dean of the College of Science and Engineering at Western Kentucky University. Ed keeps busy by teaching chemistry and wine science courses at WKU, directing research projects with students, and serving as director of two research centers in the university's research park, the Thermal Analysis Lab and the Advanced Materials Institute.

ACA Member Named as 2017 AAAS Fellow

In October, 2017, **Winnie Wong-Ng**, Research Chemist and Project Leader at the National Institute of Science and Technology (NIST), was named a 2017 AAAS Fellow, an honor bestowed on scientists "whose efforts on behalf of the advancement of science or its applications in service to society have distinguished them." She has also been honored as an ACA Fellow (2014) for her sustained and meritorious service to the American Crystallographic Association and, more recently, with the Distinguished Fellow Award from the International Centre for Diffraction Data (ICDD). Her memoir may be read on the History portal of the ACA website.

2018 Ludo Frevel Scholarships Announced

Through its Crystallography Scholarship Fund, known as the Ludo Frevel Crystallography Scholarship Fund, the International Centre for Diffraction Data (ICDD) awards scholarships to aspiring crystallographers. Because crystallography is such an interdisciplinary discipline the recipients of these scholarships come from many branches of science. This year **Yu-Tsun Shao**, PhD in Material Science and Engineering at the University of Illinois at Urbana-Champaign, is one of ten recipients out of 62 applicants. He was cited for the Determination of Local Symmetry and Polarization in Ferroelectric Perovskites. He is looking at nanoscale order and symmetry fluctuations in ferroelectric crystals.

Kay Onan

2017 U. S. Crystal Growing Competition

"It is events like this that help get our students excited about sciences, especially in an underprivileged district like ours… It also allowed an organic chemist like me to go back to my days of growing crystals for X-ray." – Excerpt from thank you note from educator Bradley Harmon of J.C. Harmon High School in Kansas City, Kansas.

Kids and teachers love growing crystals! Nearly 160 teams from schools and households in 36 states (up from 80 teams in 26 states in 2016) signed up for the fourth running of U.S. Crystal Growing Competition (USCGC, http://www.uscrystalgrowingcompetition.org/). Our survey indicated that nearly 4000 kids in grades K-12 competed to grow the highest quality crystal of potassium aluminum sulfate in the 2017 USCGC! We sent out nearly 200 kg of Alum! Sponsored in part by ACA, the USCGC continues to bring the science of crystals into America's classrooms. Given the increased size and quality of the winning crystals relative to previous years, it is clear that the crystal growing abilities of the participants continues to improve.

Chemistry professor Jason Benedict (left) and chemistry PhD candidate Eric Sylvester prepare to ship crystal-growing supplies to participants in the U.S. Crystal Growing Competition. Photo: Douglas Levere/University at Buffalo.

The 2017 USCGC, which one again began during National Chemistry Week in mid-October and concluded in early December, was judged by a number of veteran judges that included University at Buffalo (UB) Professors from Chemistry: Timothy Cook, Ekin Atilla-Gokcumen, and Luis Velarde and Geologist Travis Nelson. The contest was aided by some new judges: Geologist Sue Bratcher, Georgetown University (GU) graduate student Lee Ayscue, and Chemistry Professors David Lacy (UB) and Michael Nippe (Texas A&M University). Michael is also the newest member of our team of regional coordinators that includes Fernando Uribe-Romo (University of Central Florida) and Karah Knope (GU).

(Left to right) Juniors Ely Driscoll, Hannah Ives, and Rachel Durand placed 1st for grades 9-12. Ely's crystal won best overall crystal and Hannah and Rachel's won best quality crystal! Photo: Sharon Geyer.

The Bronx High School of Science in Bronx, New York continues to dominate! For the third year in a row, Jessica Weedon took home the "Best Teacher Crystal" and a check for $100. Her students won 2nd place Overall grades 9-12. Taking home 1st prize Overall ($200) and 1st prize Quality in grades 9-12 were Sharon Geyer's students from Woodstock Academy in Woodstock, CT. Falling one spot to 3rd place Overall for grades 9-12 were Dawn Kelley's students from Lyme-Old Lyme High School (Old Lyme, CT).

Winners of the 1st place Overall Sasha and Mason Doll (Center) and 1st place Quality Danil Slater (right), all from Manhattan School Plus. Photo: Valentina Bardakova.

For grades K-8, Valentina Bardakova's students from Manhattan School Plus in New York, NY won both 1st place Overall and 1st place quality! Ms. Pelliteir's class from Raymond Elementary in Raymond, ME won 2nd place Overall. And for the second year in a row, a homeschool entry from Heather Costner (Springville,

All entries are on display on the 7th floor of the Department of Chemistry Natural Sciences Complex at the University at Buffalo. Photo: Jason Benedict.

NY) took 3rd place Overall.

New for 2017 was the addition of the 'Coolest Crystal' category where participants were tasked with growing the most neat and interesting crystal possible with two simple rules: Be safe and crystals will not be returned. While we received a number of very cool crystals, the winning entry was sent in by Jeff Yap, a teacher in Williamsville, NY. By adding the juice from a highlighter to the crystal growing solution, Jeff created a glow-in-the-dark crystal that

Image of the glow-in-the-dark 'Coolest Crystal' grown by Jeff Yap. Photo: Gage Bateman and Jason Benedict

really wowed the judges.

Growth of the contest is driven by our active use of social media to advertise and provide contest updates! The winners were announced via the contest Twitter account, @USCrystalComp. Many participants sent in pictures of their progress, which were also shared with the world via social media. Want to see the action? Check out #2017USCGC on Twitter! The USCGC has also received from exciting nation-wide exposure. The USCGC was mentioned in a recent Ted talk by Fernando. The ACA received a special shout out during my recent interview on the PRI radio show Science Friday (How to grow your own crystals)! These efforts raise public awareness of the importance of crystal-based research and organizations including the ACA that promote and support these activities.

The USCGC gratefully acknowledges the Benedict Research Group graduate students, and the support of our sponsors: ACA, National Science Foundation, Ward's Scientific/VWR, Bruker AXS, Krackeler Scientific, Cambridge Structural Data Centre, the Western New York section of the American Chemical Society, and the UB Department of Chemistry. Please consider helping with or donating to the 2018 contest. For more information, please visit the USCGC website or e-mail Jason Benedict at jbb6@buffalo.edu.

Jason Benedict

ACA History Project Update

Gautam R. Desiraju, former President of the IUCr, recounts some aspects of his multifaceted scientific career in this issue. Desiraju's innovative concept of the supramolecular synthon has been particularly useful and significant in crystal engineering. In addition, his investigation of weak C–H•••O and C–H•••F–C hydrogen bonds has generated some controversy but also led to new understanding. A major contributor to the structural science community, Desiraju organized the 24th Congress and General Assembly of the IUCr in Hyderabad last August. In addition to his outstanding scientific contributions, from my point of view, I appreciate his Twitter posts of interesting scientific articles.

Sir Fraser Stoddart gave the plenary address at the 2017 ACA meeting in New Orleans, "How Crystallography Helped to Create a New Bond in Chemistry." He calls this new bond the mechanical bond. Stoddart shared the 2016 Nobel Prize in Chemistry with Jean-Pierre Sauvage and Bernard Feringa "for the design and synthesis of molecular machines". In his inspiring lecture he detailed his journey of over 50 years in science and showed animated examples of molecular machines at work. In conclusion, he said that he would like to be remembered for mentorship of over 400 students from over 40 different nationalities, not for any prize. Thanks to Dean Johnston (Otterbein University) the video of his plenary address is now online at ACA History pages, at http://bit.ly/2G2FrML.

In case you missed it, the Living History of **I. David Brown** is now online at the ACA History pages. Brown was a professor at McMaster University until his retirement in 1996. He specialized in inorganic crystallography, and with R. D. Shannon he developed the bond valence method in coordination chemistry. He was instrumental in establishing the Inorganic Crystal Structure Database.

Please note that there are many other biographies and autobiographies of Canadian crystallographers online at ACA History pages in the section Crystallography in the Americas, http://bit.ly/2CbX2zn.

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Hydrogen bonds in Hyderabad

Gautam R. Desiraju

I have generally been reticent about conveying details of my family, upbringing or childhood activities to a professional audience, because these things are properly kept outside the discourse. So I will merely say that I was brought up in Madras and Bombay (I still use the old names because I don't think one can change history by changing place names) in the 1950s and 1960s in an upper middle class family that was no different from thousands of other such families in India, and I was, as is common, influenced by my parents and teachers. Research scientists need a lot of "consideration" and "sympathy" from their families if they are to function effectively. In this regard, I have been extraordinarily lucky in my wife Krishna for all her understanding and support over the years, which has included shielding me off from the "normal" world.

Coming to professional things now, I got into a Boeing 747 airplane in 1972 at the advanced age of 20 and travelled halfway across the world to study for a PhD in chemistry at the University of Illinois in Urbana-Champaign. This was my first journey outside India. It was a culture shock. Bombay was, even then, a huge city with 6 million people. I had lived in an upmarket neighborhood and all I had seen were multi-storied buildings, suburban trains and a lot of traffic. Urbana seemed to be a hick town, actually a village, with just 100,000 people, some cars here and there and hardly any high rise buildings, maybe just a handful. It was a small campus town with a third of it being connected directly with the university as students and teachers. The second shock, but in reverse, was the academic atmosphere there. With an undergraduate degree from a renowned but still unpretentious (in research terms) college of Bombay University, I had been suddenly thrust into one of the most prestigious and advanced chemistry departments in the U.S. In one of the first seminars I attended there, the speaker said that he was happy to be invited to the best chemistry department between Harvard and Berkeley! The year I joined, there were 110 PhD admissions, and I was the only one from India—sounds strange in today's globalized world, doesn't it? In such a place, one had to swim or sink. I guess I swam. Unusually, I had two joint advisors for my PhD, David Curtin whose name still lives as the Curtin-Hammett Principle and Iain Paul, a younger crystallographer, who had studied under the legendary J. M. Roberston in Glasgow and then gone on to be a part of R. B. Woodward's group in the B12 project. The Curtin-Paul group was one of the very few in the world who at that time were working in an area they called organic solid state chemistry. I guess I got used to the idea from them, of working in areas that no one really knew about, understood or really cared about even. I do feel that big progress in science comes from working in areas that are not easily definable in terms of standard labels. Today's bridging areas become tomorrow's mainstream. Anyway, for those of you who remember crystallography in the 1970s, my very first crystal structure was determined on a big Picker single-crystal diffractometer: you needed to climb a wooden step to mount and align a crystal and where you manually set the four angles of the initial 25 unit cell defining reflexions before the computer drove the crystal to each of them one by one. This crystal had a long axis of 44 Å! Each reflection practically merged into the next one along the long axis. I haven't seen a cell axis this big after more than a thousand crystal structures that have come out of my research group in the last 38 years. Just goes to show.

Anyway, moving along, around halfway through my short PhD tenure of three and a half years, a new object arrived in the lab. This was an automated computer controlled Syntex P21 diffractometer. Suddenly, the same structure that used to take several weeks/months to complete with paper tapes, card punch machines and so on, if all went well, could get solved in a few days' time. This was a revelation but I thought no more of it for another few years. Like many other Indian students in the U.S. in those days, I wanted to make a career of it in the U.S. and indeed I was one of the lucky few in Illinois to get an industry placement, actually two, one at 3M in Minneapolis and the other at Eastman Kodak in Rochester. It seems funny, to think about this now, but I declined the position in 3M because I thought it would be too cold out there in Minnesota and that Rochester would have a nice climate. Just tells you how little I knew about the weather patterns in the U.S. then!

Rochester was bleak and grey most of the time but this is not what impelled me to quit the job after two years and return to India cold turkey with no job in hand, and with no prospects of getting one either. While the work environment in Kodak was fine and my colleagues friendly, I wasn't happy about being in industry all my life and the prospects for an academic job for me in the U.S. were close to nil. So I returned in 1978, spent a year as a research fellow in the Indian Institute of Science, Bangalore (to which organization I returned in 2009) before taking up a position as lecturer in the fledgling University of Hyderabad, which probably gave me the job since no one else wanted it.

The University of Hyderabad was a wild place in 1979. The culture shock of the corn fields of Illinois seemed tame by comparison. This university campus was a jungle, 15 km from the nearest habitation, and with no basic amenities, like permanent buildings, telephones, schools, and hospitals for many years. Yet, there were sincere teachers and devoted students who formed my peer group and despite our travails, we succeeded in nurturing one of the best chemistry departments in India in a relatively short period of time. I have written elsewhere that I did not have access to a single-crystal diffractometer at my university for 20 years: my research was shaped by this simple fact. With no instrument in my department, and yet knowing that crystal structure determination had become relatively easy for small molecules (from seeing the Syntex diffractometer in Urbana) I did all my crystallographic work in collaboration with foreign groups. The bright side of this was that I made lasting friendships with many talented and serious crystallographers from all over the world! The other aspect of this reality was that I started thinking about the Cambridge Structural Database (CSD), which was then emerging as a research tool in structural chemistry. The seminal 1983 article by Olga Kennard, Frank Allen and Robin Taylor in *Acc. Chem. Res.* was a real eye-opener. One could actually think about crystallographic problems without having a diffractometer!

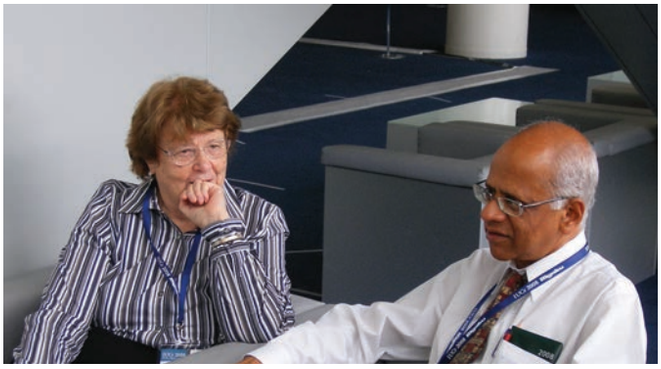
I have written elsewhere about a memorable crystallography school in Erice, organized by Aldo Domenicano, Istvan Hargittai and Peter Murray-Rust in 1985. I was one of the lucky few who were able to attend this meeting. Some meetings linger on long after they are formally over. The 1985 Erice School was one of them. I think many of us small-molecule crystallographers, at least in my age group, were facing similar professional issues each from our individual situations—we had all been trained to do something, namely determine small-molecule crystal structures, but this was fast transforming from a research area to a technique. I had started thinking about "Crystal Engineering" not in terms of designing solid state reactions, as had been envisaged originally by Gerhard Schmidt, John Meurig Thomas and Mendel Cohen, but rather as an expanded discipline where one could try and correlate the structures of molecules with the crystal structures that they form. This became known as the molecule → crystal problem, and to tackle it, one needed to appreciate the properties of intermolecular interactions as they are manifested in crystal structures. We were made aware of the magnificence of the subject of hydrogen bonding by George Jeffrey, and the utility of the Cambridge Structural Database in understanding patterns of interactions in related crystal structures by Jenny Glusker. I still remember the kindness of Ken Trueblood at that meeting. I was pretty nervous talking to him and I think he sensed this—he quietly said that it was a real pleasure to talk with me and that anyway I would very soon be attending many more such meetings than he would. I felt at that time that he was just trying to put me at ease, but he might have known better. Olga Kennard was not there but Frank Allen, from her group, was and a lifelong friendship with him began at that meeting in 1985. I was greatly saddened by his passing in 2011.

Hydrogen bonding is "the" principal interaction in crystal packing and its understanding is the cornerstone of crystal engineering. In the late 1980s and early 1990s, all of us in the field knew this interaction was very important. If a molecule contained good hydrogen bond donors and acceptors, hydrogen bonds would undoubtedly appear in the crystal structure. Anyone would have been able to rationalize the crystal structure in terms of strong and dependable hydrogen bonds. But the reverse was practically impossible—given a molecule, it would be extremely difficult to predict how its crystal structure was going to look like. A series of beautiful papers by Olga Kennard and co-workers told us that hydrogen bond geometries especially N–H…O were quite predictable, but the next step, namely molecule → crystal was impossible to handle and this is the key question in crystal engineering. The graph set approach, suggested by Margaret Etter in 1990, never did appeal to me and I have shied away from it because it has seemed to me as being merely taxonomical with no predictive value. Prediction of crystal structures must arise from chemical considerations: if close packing is everything, as suggested by Kitaigorodskii, then a computer would predict every small molecule crystal structure with ease.

During 1988-89, I spent a year in DuPont CR&D in Wilmington as a visiting scientist. By that time, I had notched up a couple of papers in good journals, most notably one on Cl…Cl and C–H…O interactions in *Acc. Chem. Res.* with my first student J. A. R. P. Sarma but the question of obtaining an extended scope for crystal engineering was concerning me. There was, I felt, still too much emphasis on 2+2 cycloaddition reactions in the solid state. The time in DuPont allowed me to complete a book called *Crystal Engineering: The Design of Organic Solids* where I wrote that directional interactions, like hydrogen bonding, move a crystal structure away from Kitaigorodskii's close packed model, and that because of this, directional interactions provide the basis for systematic crystal structure design. This book became very well known.

It's actually impossible for me to recount all my numerous professional experiences after 1989. Within the limitations of this article I cannot possibly hope to recollect all the crystallographers and chemists I have met, the places I have been to, the band of dedicated students and post-docs I have had the privilege to work with, my fans, my detractors, my experiences with being involved in the starting of new journals, landmark papers from my group and from those of others, scientific disputes, science administration including my work in IUCr, my daily professional life in Hyderabad till 2009 and in Bangalore after that, my colleagues at work, science politics, and the general business of doing all of this out of India, which in itself would make a long story. I have rarely spent long spells outside India after 1991, a week to 10 days at the most, very often less. There is no exact English translation for the Sanskrit word karmabhoomi; an imperfect translation would be "land of one's work" but this is what Hyderabad became for me and almost all the work, for which I acquired a certain degree of recognition, arose from my years in Hyderabad. Here I am shown in 2014 with J. A. R. P. Sarma and T. S. Thakur, my first and last PhD students from the University of Hyderabad.

Since I am unable to do any comprehensive justice to my research experiences after 1989, I have decided to focus on one particular paper I wrote in 1991, as a case study, and also to illustrate how a work may be conceived and how it may be received—and how these two features may be largely unconnected. The paper in question was called "Hydration in Organic Crystals. Prediction from Molecular Structure" and it was published in *Chemical Communications* in 1991; the journal, incidentally, remains one of my favorites. At one point in the 1990s, Jenny Glusker graciously told me that she was retaining her personal subscription to that journal so that she could get to read my papers there quickly.



Jenny is a remarkable scientist and human being—there is much I have learned from her in terms of prioritizing goals and in setting goals that are realistic. A week's visit that she and her husband Don made to Hyderabad in the mid-1990s and the time my wife and I spent with them will always remain in my memory. I was really pleased to have been able to invite her, as IUCr President, to deliver the keynote lecture on 100 years of crystallography in the inauguration ceremony of the International Year of Crystallography (IYCr) in UNESCO, Paris in 2014.

Another ceremony in Poznan, Poland where I unveiled a plaque commemorating Max von Laue, in his primary school building there, stays on as a memory of IYCr and my time as President, IUCr. Of course, in Laue's time, Poznan, Poland was Posen, Germany but this is history mocking at you again. Fittingly, however, the function there in 2014 was organized jointly by the crystallographic societies of Poland and Germany. Science, it would seem, had the last laugh.

The origins of my 1991 *Chem. Comm.* paper (incidentally, one my very few original research papers—not reviews—which are single author) actually began in my year in DuPont where their scientists wanted to determine the crystal structure of 2,5-dinitrosalicylic acid in a project connected with second order non-linear optical effects. I did this structure with two highly competent DuPont crystallographers, Joe Calabrese and Dick Harlow, two people from whom I have learned a lot.

The first unusual thing about this structure is that it is non-centrosymmetric in space group C2, and the acid molecules are not held together as dimers—which would be common for aromatic carboxylic acids—but rather as catemers which are strung together with water molecules. When I tried to add a drop of water to several crystals, they would dissolve readily in this small quantity of solvent almost instantaneously. On the other hand, 5-nitrosalicylic acid remained stubbornly insoluble in water. Many strange things happening together: this is always a sign to me that there is some underlying factor that will explain all of it.

It's easiest to quote from my 1989 book, where I postulated a possible reason for the solubility and hydration of 2,5-dinitrosalicylic acid. On page 141, I wrote *"The interesting question is, of course, why this unusual crystal structure is adopted at all. A possible rationale is obtained by considering that the number of hydrogen bond donors (2) and acceptors (7) is quite unbalanced. In order that the maximum number of acceptors may be incorporated in the hydrogen bonding scheme, three-center interactions would appear inevitable. However, an alternative possibility is to redress the donor-acceptor imbalance by including a water molecule. The presence of water in the hydrogen bond pattern opens up possibilities other than the centrosymmetric motif and the crystal structure actually adopted is probably determined by the stabilization conferred by all hydrogen bonds, weak and strong"*. As to any possible relationship between the high solubility of the acid and its propensity for hydration, I was silent.

Back in Hyderabad in 1989 and restarting my research group after the year-long absence in the U.S., I had time to work by myself on the CSD, and I began to wonder if the behavior of 2,5-dinitrosalicylic acid was more general. To go from the specific to the general is almost addictive to a scientist. Would compounds with a hydrogen bond donor/acceptor imbalance render a compound more susceptible to hydration? The CSD showed that of the 3696 non-metal atom containing solvates in the 1988 version of the database, as many as 2566 were hydrates. This was surprising because water is not the first choice solvent for crystallizing a molecular organic solid—many of these compounds tend not to be water soluble. Enumerating the donors and acceptors in these molecules had to be performed manually—2566 hydrates was too large a number to manage and I further narrowed the test group to 411 structures, chosen arbitrarily, on the basis of journal of publication. The histogram of these hydrated structures according to donor/acceptor ratios was revealing. There were far more hydrated structures formed by acceptor rich molecules, and it seemed to me that my extrapolation from a single

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compound, 2,5-dinitrosalicylic acid, was reasonable. I wrote up the result, and to my recollection, there were no adverse referee comments; the paper was published speedily. In truth, I did not think more about this paper for many years; over the first 18 years, the paper picked up just 40 citations. In the following eight years, however, it secured as many as 63 citations. Last year, it had as many as seven citations. Something is going on.

What is going on is in fact not revealed in these citation statistics, although they begin to hint at something interesting. During the intervening years, the properties of solid forms of drugs became of major interest to the pharmaceutical companies and many legal issues became connected with crystal engineering and properties of solid forms, things like polymorphism, and solvation notably hydration. The matter becomes quite simple: given a particular drug molecule, if it is possible to predict whether or not it is going to form a hydrate, then the crystallization of any particular hydrate will not constitute grounds for non-obviousness in a patent application for the hydrate. Unknown to me, pharmaceutical companies had become quite interested in my 1991 paper that had been written in an earlier era with totally different objectives in mind: crystal structure prediction and hydrogen bond patterns and propensities. If this paper was broadly correct, then it could have legal implications on patentability of new hydrates of drugs. If not, then supposedly one could keep patenting new hydrates merrily.

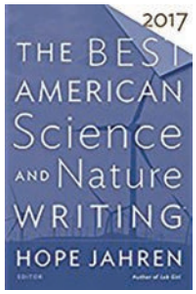
I suspect this is why several groups began looking at my 1991 paper more seriously, perhaps even with the idea of proving me wrong. Notably, I will recall a 2006 paper in *CrystEngComm* by Sam Motherwell and others from the Cambridge Crystallographic Data Centre (CCDC) where they tried to show that hydration had not much to do with donor/acceptor imbalances. However, the drawback of their paper is that it gets lost in detail, and in several subsequent conversations I have had with pharmaceutical company scientists and their attorneys, the merits or otherwise of such studies were never seriously considered. Legal arguments continue to be made on the basis of my 1991 paper. This example is possibly common in science: work gets done with certain motivations but others glean new things from the work motivated by a totally different perspective that might not even have existed when the original work was done. And citations don't tell the whole story! Many of my papers have received many more citations than this simple 1991 single-author Chem. Comm. article, but this is the paper that seems to have attracted the attention of industry more than any other.

What I will say is that in many of these matters concerning crystal engineering and crystal structure prediction and design, one needs to go back to Kitaigorodskii who famously said that "It is more advantageous to have a rough theory applicable to most molecular crystals than a fine theory useful only for crystals of benzene and urotropin". It's a hard fact of life that complex systems are bedeviled by the need to simultaneously optimize both generality and accuracy. This dilemma has confronted me practically every working day of my life, and I have never hesitated to pick generality over accuracy. Even while using the CSD, I have followed this precept. An exception to the rule has never made me nervous because I feel that with a sufficient accumulation of new data, the exceptions will constitute a new rule. Not all practitioners of crystal engineering agree with me, and this is to be expected because crystal engineering itself is now a very wide subject and people come to this discipline from very varied backgrounds that have differing degrees of respect for the quantitative and the qualitative.

I feel remarkably grateful in my research career of 45 years, of which 39 have been spent in pursuing independent research. Many a time I have chosen the road not often travelled and yet I have always felt exhilarated by my non-conformism. I declined admission to the prestigious Indian Institutes of Technology at the age of 17, gave up a U.S. green card at the age of 26, and refused to accept a so-called career shaping award in India when I was 43, simply because I didn't feel these things were correct for me. I have never regretted these decisions and on the contrary, these experiences have enabled me to see life in its entirety and as I have said in one of my better known papers, in a "holistic" manner. It's practically a cliché for an Indian to quote Mahatma Gandhi but my favorite quotation from his works is "Be the change you want to see". During my years in Hyderabad and now in Bangalore, I have always enjoyed my interactions with my students, post-docs, associates and collaborators, many of whom participated vigorously in the very memorable 24th Congress and General Assembly of the IUCr that I

organized in Hyderabad in August, 2017, with their substantial assistance and advice. Without their very real work, support and loyalty, I would scarcely have begun to be able to do anything at all. To all of them, I offer my sincere and heartfelt thanks.

Gautam R. Desiraju



The Best American Science and Nature Writing 2017, Edited by Hope Jahren, Houghton Harcourt Mifflin Publishing Co., New York, 2017, 352 pages ISBN: 978-1328715517.

Despite the name, The Best American Science and Nature Writing contains an expertly curated set of exemplary pieces from 2016, culled by biologist/science writer Hope Jahren. Jahren is well known for her memoir Lab Girl, which offered brutally honest insight into the pursuit of science as a woman in the past few decades.

The Best contains 24 pieces of science and nature writing from American publications. Jahren sorted the pieces into three categories: Emergent Fields, Changing Land and Resources, and The "Real Life" of Scientists. That essentially boils down to "new stuff," "climate change", and "profiles" (not every story fits into those narrower categories, but the pieces that stood out the most certainly did).

Writing a good, compelling long-form science story is hard. Especially when you are describing an emergent field—something that is at the forefront of human understanding. As a writer, you are faced with explaining a concept to your audience that even the scientists who specialize in the subject don't yet fully understand. That said, the four pieces in "Emergent Fields," by Sarah Everts, Maria Konnikova, Kim Tingley, and Nicola Twilley, do a fairly good job of just that. But like any piece on emergent science—though certainly important—they leave the reader wanting more, which is decidedly unsatisfactory. But given the nature of the work, it seems inevitable. Konnikova's "Altered Tastes," originally published in The New Republic, was particularly intriguing. She explicates a brief history of food science in the context of the study of neurogastronomy—essentially the relationship between your stomach and your brain (and the rest of your body).

Part II, Changing Land and Resources, had ten pieces. Given the current political climate (and the current climate climate), many of these pieces resonated more than those in the previous section. We live in a world where its "most powerful man" is a vehement climate change denier, and that is quite frankly, deeply upsetting. Two of the works from this section resonated in particular—Adrian Glick Kudler's "Something Uneasy in the Los Angeles Air" and Nathaniel Rich's "The Invisible Catastrophe," originally published in Curbed and The New York Times Magazine respectively. Kudler's piece, on the Santa Ana winds—their history, their devastation, and the fascination they inspire—seemed particularly relevant given the devastating fires that wracked the greater Los Angeles area this past winter. The Santa Ana winds have always blown—but the role of climate change in increasing the extent of their devastation is a harder causality to pinpoint. Rich's piece (also on the greater Los Angeles area) tells a story about an old, drained J. Paul Getty oil field in Aliso Canyon that was bought by Pacific Lighting in the 1970s. Pacific Lighting used the land to store excess supplies of natural gas—methane. Fast forward to 2016—residents of a housing development on the land above this methane storage ground were reporting strange phenomena—painful headaches, dying pet parrots, even cancer. This story seems like déjà vu—and should, at least for anyone who saw the Academy-Award winning, based on a true story Erin Brokovich, almost 20 years ago—or more recently, the documentary Gasland or its sequel Gasland II. It is definitely discouraging to say the least.

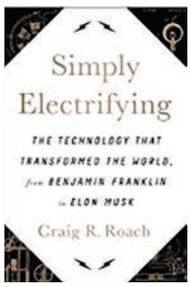
Part III, The "Real Lives" of Scientists, had more memorable pieces than the other two, but that might just be the nature of the writing. Profiles have an inherently human element, and that element makes

it easier to form a compelling narrative. Included in this section are Azeen Ghorayshi's "He Fell in Love with His Grad Student—Then Fired Her For It," from Buzzfeed and Kathryn Joyce's "Out Here, No One Can Hear You Scream" from Huffington Post Highline/ The Nation Institute Investigative Fund—both are horrifying tales of sexual harassment towards female researchers perpetrated by their male coworkers. Given the recent outbreak of scandals pouring out of every industry, particularly entertainment, these pieces resonate—these stories need to be told, and they deserve attention.

But the standout piece from the whole book actually ended up being the longest: David Epstein's "The DIY Scientist, the Olympian, and the Mutated Gene," from ProPublica. Epstein, the author of The Sports Gene, a book that details the possible relationship between genetic predisposition and athleticism, tells a story about the aftermath of his book. Long story short, a woman who suffered from a rare form of muscular dystrophy reached out to Epstein, wanting to be put in contact with an Olympic athlete who she suspected suffered from a similar condition. You'll have to read Epstein's piece if you want to find out what ensued.

Jahren includes a list of dozens of other noteworthy pieces from 2016—which are worth hunting down and reading, if you haven't already.

Review by Jeanette S. Ferrara, MA



Simply Electrifying: The Technology that Transformed the World, from Benjamin Franklin to Elon Musk, by Craig R. Roach, BenBella Books, Inc., Dallas, 2017, 400 pages, ISBN: 978-1944648268

Joe Ferrara: Full disclosure, Dr. Roach is my brother-in-law and I was reluctant to print this review because I did not want give the impression of favoritism. However, this title appeared in JPMorgan's Next List for 2018 so I think it is reasonable to print Jeanette's review here.

A world without electricity would be a dark one indeed (both literally and figuratively). That's where Craig R. Roach starts Simply Electrifying: by asking the reader to imagine their world without the innumerable technologies that make our daily lives so much easier--technologies that predominantly run on electricity.

So who do we have to thank for this incredible energy that powers our lives? You've probably heard the story about how electricity was "discovered"--it involves founding father Benjamin Franklin, a kite, a key, and a lightning storm. Roach elaborates on the historical accuracy of this story and the impact of Franklin's experiment in his first chapter.

But what is electricity, really? When did it become something to be taken for granted? Where does it actually come from? How do we harness it? And who regulates how we use it?

These are all important questions Roach answers in his book--so even someone with little to no understanding of the "science" behind what electricity is (moving electrons), or the history of electricity (it's a rich one!), can read Simply Electrifying and walk away with a newfound knowledge of such a key aspect of their life.

Simply Electrifying is divided into five parts, or "ages" of electricity: The Age of Franklin, The Age of Edison, The Age of Big, The Age of Harm, and The Age of Uncompromising Belief.

Roach follows Franklin's discovery with James Watt's steam engine--an over two hundred year-old invention that cemented our modern dependence on coal-burning for electric power. Then, he takes a slight detour into the realm of the theoretical history of electricity: Faraday's Law of Induction and Maxwell's Equations.

After laying the groundwork, Roach details various inventors and their creations that employed the newfound electricity to power them, like Samuel Morse's telegraph and Thomas Edison's light bulb. He touches on the Tesla-Edison AC/DC debate, and the mass deliverance of electricity to American homes.

Then Roach moves on to FDR's New Deal policies, which included bringing electricity to rural areas of the United States in an effort to combat unemployment. Hoover Dam and hydroelectricity, coal power, and Einstein's e = mc^2 all make appearances.

The dangers of electricity--namely the potential hazards of nuclear power and pollution from coal-powered plants--along with California's electricity crisis in the 1990s and the fall of Enron come next.

Finally, Roach ends with Obama's Clean Power Plan (how will it really impact the American public?), George Mitchell's shale gas revolution (fracking!) and the man many see as a real-life Tony Stark and the future of

electricity: Elon Musk.

Simply Electrifying is not a light read--clocking in at 375 pages, not counting footnotes and indices--but it reads like one. Roach's prose hits the delicate balance between informative and compelling, covering all the bases in an objective and still interesting way.

Review by Jeanette S. Ferrara, MA

Soonish: Ten Emerging Technologies That'll Improve and/or Ruin Everything by Kelly and Zach Weinersmith, Penguin Press, New York, 2017, 368 pages, ISBN: 978-0399563829

Soonish is a marriage of science fact and science humor--which makes sense, given that the authors, a scientist and a comic strip creator, are married.

The authors divided the book into three sections: the universe, stuff, and you. Translation: space exploration, gadgets and robots, and human biology.

In The Universe, Soonish, the authors detail everything from the impracticalities of a space elevator, to the pitfalls and potential struggles of asteroid mining, to Elon Musk and his SpaceX program. Aside from the practicality of execution, the main roadblock on the highway to space exploration is cost. Although, as the authors casually observe--if you stop worrying about getting explorers back to Earth alive, you could cut a lot of the costs.

Next, in Stuff, Soonish, fusion power, augmented reality, and robots take the lead, along with programmable matter (it's exactly what it sounds like--both perplexing and riveting) and synthetic biology (CRISPR!*). Fusion power seems a long way off for practicality reasons but, if it could be achieved--what a way to power your microwave (and fridge and toaster and pretty much everything else). Augmented reality--anyone who has been run over by an overeager Millenial or Gen Z teenager playing Pokémon Go knows the pitfalls--has numerous applications, and not all of them involve playing app-based phone games. Robots, the authors somewhat jokingly posit, are going to take over in 2027--the sooner you accept that inevitability, the sooner you can be open to the incredible advances in robotics and how they can help you in the next decade.

Finally, in You, Soonish, the human body takes the stage--namely precision medicine and bioprinting. Every person's body processes prescription medication and treatments in a different way. Two people with Stage 3 cancer can be given the exact same drug regimen-- one might survive while the other does not. The idea behind precision medicine is that by studying a patient's DNA--and even potentially modifying it--you can cure someone of a chronic condition before they even present symptoms. And, as for bioprinting,it presents a possible solution for a real problem. Roughly one person dies every hour in the United States waiting for an organ--liver, heart, lung, kidney,take your pick. That's over 8,000 people per year--and that's just in the U.S. The U.S. only accounts for 4.4% of the world population--you can do the math. 3D-printing of cells, and, eventually, whole organs, means dying people around the world won't have to wait for someone to donate an organ (whether by generosity or death) to survive.

The intermittent comics add a colorful and playfully sardonic tone to a book that covers emergent technologies with a combined sense of wonder, skepticism, and even a healthy dose of fear. Soonish is a fun look at the future of technology--which like the present and the past, isn't always fun.

*The authors deserve some serious bonus points for giving Jennifer Doudna and Emmanuelle Charpentier their due credit for developing CRISPR--there is an ongoing patent battle between these phenomenal women in science and their mostly male collaborators at the Broad Institute of MIT and Harvard.

Jeanette S. Ferrara

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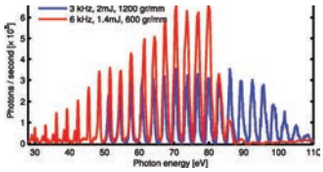
Celebrating 5 Years in Publication

This year, Structural Dynamics publishes its 5th volume. The submissions have grown 200%, downloads have grown 540%, while our average number of days to acceptance has decreased to 58 days, providing fast turnaround to our continuously growing author base. Structural Dynamics is ranked in the top 10 journals in the Clarivate category "Atomic, Molecular, & Chemical Physics".

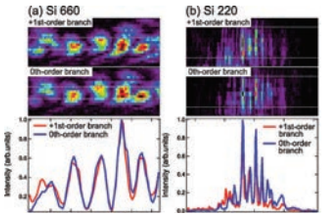
Our Editor-in-Chief, Majed Chergui, shared his thoughts on the 5th year anniversary. “I am very proud of the great start of the journal and I am excited to see how it may serve the growing community of scientists working on ultrafast structural science. This journal is their venue!"

In celebration of this milestone, we have compiled a list of ten highly cited articles. As an open access journal, articles in Structural Dynamics are always freely available to read, download, and share without a subscription.



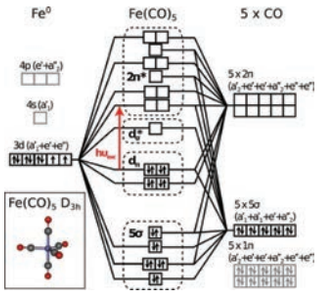
Harmonium: A pulse preserving source of monochromatic extreme ultraviolet (30–110 eV) radiation for ultrafast photoelectron spectroscopy of liquids

J. Ojeda, C. A. Arrell, J. Grilj, F. Frassetto, et al.



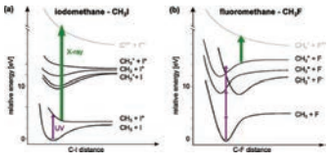
A beam branching method for timing and spectral characterization of hard X-ray free-electron lasers

Tetsuo Katayama, Shigeki Owada, Tadashi Togashi, Kanade Ogawa, et al.



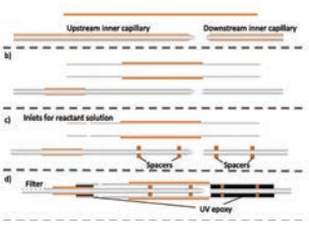
Identification of the dominant photochemical pathways and mechanistic insights to the ultrafast ligand exchange of Fe(CO)5 to Fe(CO)4EtOH

K. Kunnus, I. Josefsson, I. Rajkovic, S. Schreck, et al.



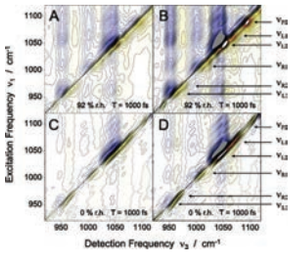
Charge transfer in dissociating iodomethane and fluoromethane molecules ionized by intense femtosecond X-ray pulses

Rebecca Boll, Benjamin Erk, Ryan Coffee, Sebastian Trippel, et al.



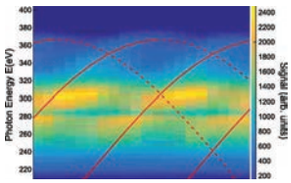
Mixing injector enables time-resolved crystallography with high hit rate at X-ray free electron lasers

George D. Calvey, Andrea M. Katz, Chris B. Schaffer, Lois Pollack



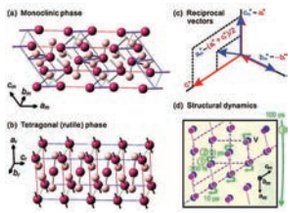
Ultrafast vibrational dynamics of the DNA backbone at different hydration levels mapped by two-dimensional infrared spectroscopy

Biswajit Guchhait, Yingliang Liu, Torsten Siebert, Thomas Elsaesser



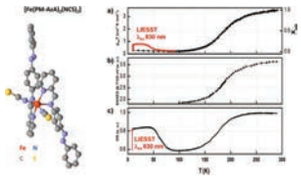
Measurement of sulfur L2,3 and carbon K edge XANES in a polythiophene film using a high harmonic supercontinuum

A. S. Johnson, L. Miseikis, D. A. Wood, D. R. Austin, et al.



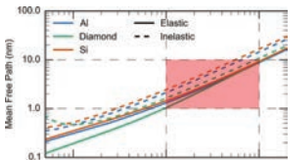
Ultrafast electron crystallography of the cooperative reaction path in vanadium dioxide

Ding-Shyue Yang, Peter Baum, Ahmed H. Zewail



Activation of coherent lattice phonon following ultrafast molecular spin-state photo-switching: A molecule-to-lattice energy transfer

A. Marino, M. Cammarata, S. F. Matar, J.-F. Létard, et al.



Ultrafast electron diffraction optimized for studying structural dynamics in thin films and monolayers

D. S. Badali, R. Y. N. Gengler, R. J. D. Miller

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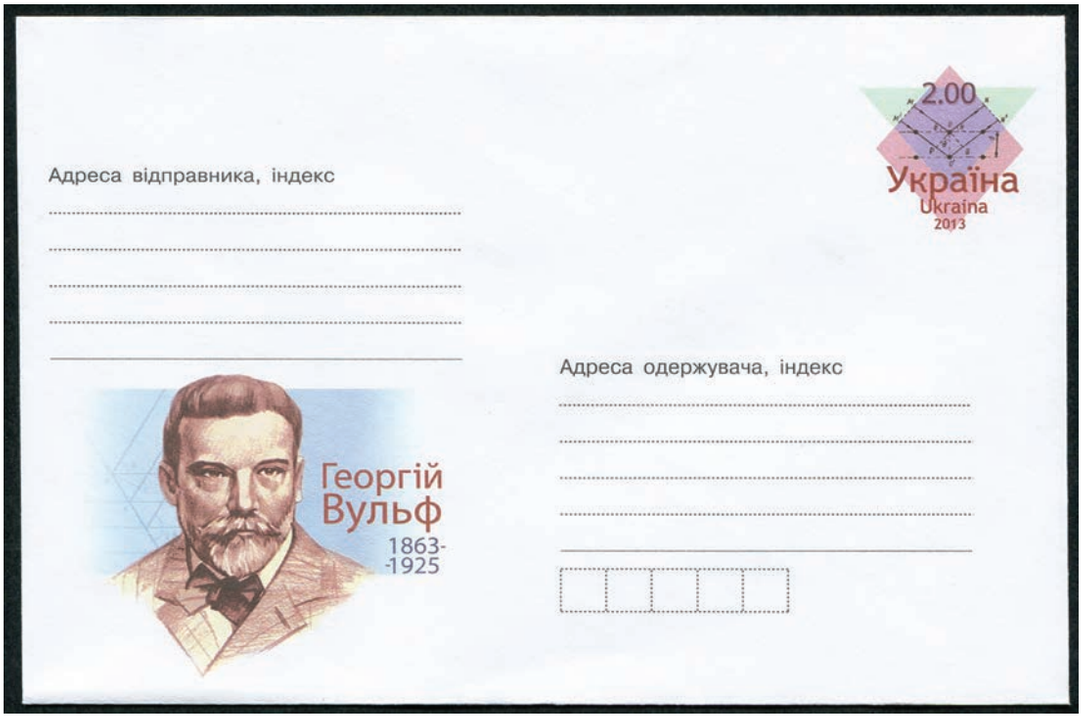
George Wulff: Bragg's Law before the Braggs?

Daniel Rabinovich

Priority disputes are nothing new in science and many well-known cases can be found, for example, in the discovery of new chemical elements. Such is the story beautifully told by Carl Djerassi and Roald Hoffmann in their play Oxygen, which relates the trials and tribulations of a fictitious retro-Nobel Prize Committee to ascertain the essential element's paternity among Lavoisier, Priestley, and Scheele. As for the issue of settling priority disputes, the fame (but not necessarily the fortune!) often goes to the first individual who publishes a new finding, even if other researchers made the same discovery or arrived at the same conclusion independently and almost simultaneously.

That is what happened with Bragg's law ($n\lambda = 2d \sin\Theta$), with which most readers of RefleXions are likely to be familiar. On 11 November 1912, William Lawrence Bragg described for the first time at a meeting of the Cambridge Philosophical Society the relationship between the wavelength of the incident radiation (e.g., X-rays), the angle of reflection, and the interplanar distance in a crystal. His lecture appeared in print in the corresponding Proceedings on 10 January 1913. Meanwhile, the Ukrainian crystallographer George Wulff (1863-1925), who established the first X-ray laboratory in Russia and was also familiar with the work of Max von Laue on X ray diffraction by crystals, independently derived the same reflection law before Bragg's Proceedings paper reached Moscow. He submitted his results to the prestigious German journal Physikalische Zeitschrift on 3 February 1913, and his paper was published shortly thereafter, in the 15 March issue. Thus, in the relatively short span of four months two brilliant crystallographers developed the same equation even though W.L. Bragg usually gets credit for it since his paper came out a couple of months earlier than Wulff's. The stamped envelope illustrated below was issued in Ukraine in 2013 to celebrate the 150th anniversary of George Wulff's birthday.



Puzzle Corner

For this issue, we have a crossword puzzle with crystallographic theme words by **Guest Puzzler** Joe Ferrara, a new DISORDERED puzzle, the solution to Crystal Connections puzzle #13 and mention of those who provided solutions to previous puzzles.

Solution to Crystal Connections #13 - All relate to Toronto, site of the next ACA meeting

1) "And farther below Lake Ontario takes in what Lake Erie can send her." (From The Wreck of the Edmund Fitzgerald, Gordon Lightfoot, 1976).

2) (Fibonacci number following 610) + 6! +192 - 43 + 5 987 + 720 + 361 – 64 + 5 = 2009 (The year of the last ACA meeting held in Toronto).

3) Irish spelling of loch – Lough (Alan Lough is manager of the X-ray crystallography facility in the Department of Chemistry, University of Toronto).

4) 553.3 meters tall, completed in 1976 – The CN Tower is a landmark of downtown Toronto.

5) Members of species Cyanocitta cristata, in a yarn by Mark Twain from A Tramp Abroad – The Blue Jays are the Toronto major-league baseball team.

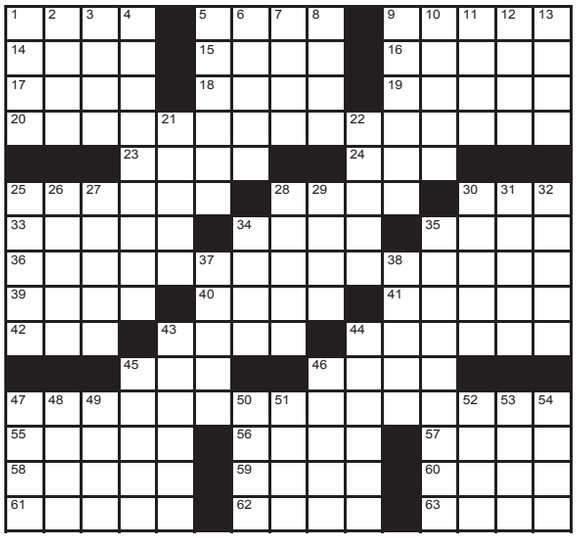
6) Published the structure of rubber in 1954 – Stanley Nyburg did superlative crystallography at the University of Toronto, 1964-1987.

7) Earnest Hemingway wrote for this newspaper around 1920. – The Toronto Star.

Tim Royappa (Univ. of West Florida) provided the solution to Crystal Connections #13.

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Guest Puzzlers are especially welcome!

Frank Fronczek – ffroncz@lsu.edu

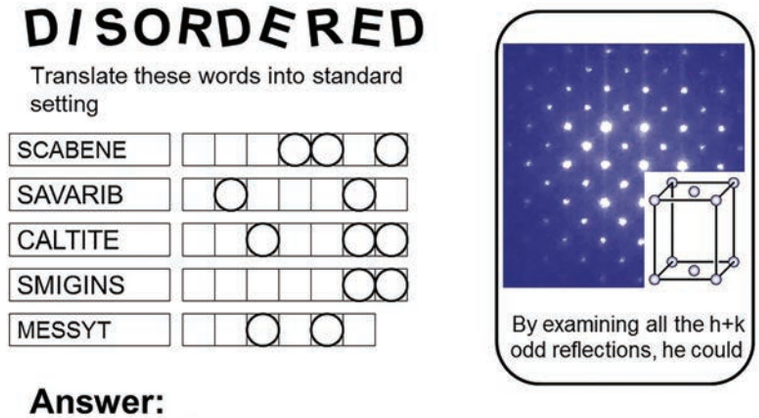


Across

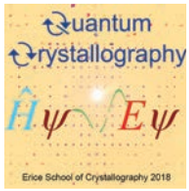
1. Basis of a Maryland treat
5. Wise one
9. Weds
14. Yorkshire river
15. Team's burden
16. Target
17. "Excuse me ..."
18. Function
19. ~
20. Theme phrase
23. Loo user
24. ___ Day
25. Son of Jesus
28. Shoelace problem
30. Infection clue
33. Looks at lustfully
34. Continue
35. Use an atomizer
36. Theme word
39. Olde English denizen
40. Bill
41. Bay window
42. Pig pen
43. Tom Jones's "___ a Lady"
44. Pigment
45. Simon and Garfunkel, eg.
46. Doozy
47. Theme phrase 3
55. Take forcibly
56. Knitting step
57. Screen symbol
58. Boot camp boss
59. Yen
60. "Giovanna d'___" (Verdi opera)
61. Potato, e.g.
62. Opening
63. Faithful

Down

1. Old Ethernet cable
2. German industrial region
3. Offshore
4. Please do
5. Dash
6. Up in the air
7. VW model
8. Pitcher
9. Garfield
10. Kwanzaa principle
11. Songs for one
12. Edible part of the taro plant
13. Spotted
21. Thomas Jefferson, by faith
22. In the company of
25. Not geeks
26. Wading bird
27. Like the fox
28. They're nuts
29. Secluded spot
30. Small songbird
31. One who puts you in your place
32. Newspaper section
34. Kind of club
35. Wallaby, for example
37. Dislike intensely
38. Stirs
43. _ mirrors
44. That which is fired
45. Sad song
46. Florida's Key ___
47. Iron (III) oxide
48. Biblical twin
49. Restrain
50. Major work
51. Arm motion
52. Field measure
53. Chewed stimulant
54. Keto tautomer



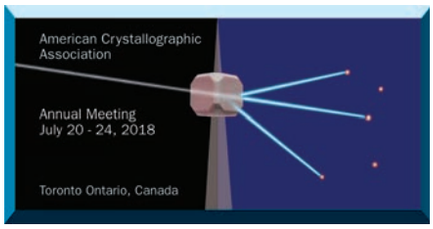
JUNE 2018



1-10 **51st Erice Course: Electron Crystallography** &
52nd Erice Course: Quantum Crystallography. Erice, Italy
http://crystalerice.org

JULY 2018

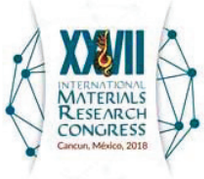
8-13 **Sagamore XIX**. Halifax, NS, Canada
http://www.sagamore2018.ca



20-24 **ACA 2018 Annual Meeting**. Toronto, ON, Canada
http://www.AmerCrystalAssn.org

24-28 **ACNS-2018**. College Park, MD
https://www.mrs.org/acns-2018

AUGUST 2018



19-24 **XXVII International Materials Research Congress.** Cancun, Mexico
http://www.mrs.org/imrc-2018

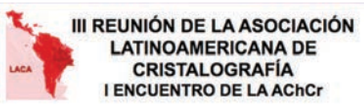
22-27 **31st European Crystallographic Meeting.** Oviedo, Spain
http://ecm31.ecanews.org

SEPTEMBER 2018

23-27 **Hot Topics in Contemporary Crystallography 3.** Bol, Croatia
http://htcc2018.org/

OCTOBER 2018

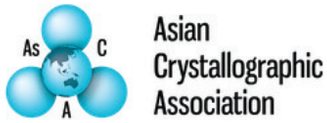
3-5 **III Meeting of the Latin American Crystallographic Association**. Valparaíso, Chile
https://cristalografia.cl/3rdlacameeting



15-30 **X-ray Methods in Structural Biology**. Cold Spring Harbor, NY
https://meetings.cshl.edu

DECEMBER 2018

25-30 **AsCA 2018**. Auckland, NZ
http://asca.iucr.org



JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
http://www.AmerCrystalAssn.org

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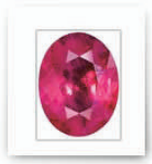

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Anton Paar

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