

# CHEMICAL

# Information

# BULLETIN



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# Chemical Information Bulletin

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Chemical Information Bulletin

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## Message from the Chair



I attended my first ACS National Meeting in 2001, a starry-eyed undergraduate researcher visiting San Diego for the first time. It was almost dizzying, all the talks, all the posters, all the social events geared towards undergrads. I really had no concept of how broad and in-depth the world of research could be beyond the small drug discovery group I was a part of. I took a lot away from that meeting. Even now as a well-seasoned National Meeting attendee, I come away from each one completely exhausted with new ideas, new plans, and new connections. The National Meeting is an invaluable part of ACS membership, and can open up the world to students or early career scientists. CINF programming and networking is inarguably the strongest divisional value at national meetings, and our continued engagement with early career

services is a key focal point. It is important to remember how much of an impact these meetings can have when we look to planning the next one.

Yet less than 10% of ACS members attend an ACS National Meeting, speaking to the need to focus our service offerings on those who cannot. With costs rising in the large cities, and travel budgets shrinking, this number is not likely to grow. CINF has been making some strides to increase the value of division membership beyond the National Meeting, and I look forward to focusing on this mission during my term as divisional chair. I am hoping that soon the answer to the question “What value do I get with my CINF membership” will be “a lot!”

One of the items on our divisional-value docket this year is an Innovative Projects Grant to create a new CINF website. This is geared at reaching all of the division with improved communication, resources, and regular content. We hope that this will engage the entirety of the division in discussion and contribution, especially those that cannot attend the National Meetings. While this is slated to go live at the end of the year, we hope to have a beta ready for review well before. Keep an eye out for an invitation to explore, contribute, and provide feedback!

I have been delighted to see the programming at National Meetings grow and diversify over the past few years. We have experimented with new formatting and themes, more often than not with resounding success. You will notice in the upcoming San Francisco National Meeting that the CINF programming is packed through Wednesday, with no programming on Thursday. We hope that this can better accommodate speakers and attendees in one of the more expensive locations. You will also notice that CINF programming is all located in a nearby hotel. With the Moscone center undergoing renovations during the meeting, many divisions have been assigned to nearby hotels (including the other divisions we are closely connected to such as COMP, CHED, CHAS, CHAL, and ANYL). When planning your attendance, please be sure to pay attention to locations and account for commute time between them. I doubt I will be the only person frantically running between hotels.

I am super excited to work with the division on all our goals, and getting to know the members. As always, we would love to get members involved with the divisional operations; we could use more thoughts, input, and volunteers. If you are interested in helping shape CINF, drop me a line! Or if you are at a National Meeting, join us for one of our many open committee meetings.

Looking forward to meeting you!

Erin Davis, PhD  
Chair, ACS Division of Chemical Information (CINF)  
[cinfchair@gmail.com](mailto:cinfchair@gmail.com)

## Letter from the Editor

Thanks for reading the spring 2017 issue of the ACS *Chemical Information Bulletin* (*CIB*). And a special thank you to all of our authors, editors, and sponsors for contributing to the *CIB*.

In this issue we have two feature articles. The first is a tribute to Eugene Garfield from Bonnie Lawlor. Dr. Garfield greatly advanced the field of chemical information and bibliometrics; he surely will be missed. I very much enjoyed reading Bonnie's sincere tribute. The second feature article is a book review by Svetla Baykoucheva. Svetla reviewed *A Tale of Seven Scientists and a New Philosophy of Science* by Eric Scerri.

You may notice that the Division of Chemical Information (CINF) program and the cosponsored technical program, and abstracts are no longer published within the *CIB*. Due to *CIB* publishing timelines, the technical program within the *CIB* quickly became outdated by the time the *CIB* was released. Moreover, acquiring the technical program in an appropriate format for the *CIB* was not trivial as it required programmatic scripting that needed to be adjusted each time a new technical program was released. Incidentally, Dave Martinsen (ACS Publications, retired) deserves a lot of credit for his skills and ability to produce the technical program within the *CIB* for the past several years.

Moving forward, we believe, the best option for readers is to use the official ACS technical program. The official ACS technical program serves as the latest authoritative copy of the technical program and abstracts:

<https://ep70.eventpilot.us/web/page.php?page=Home&project=ACS17SPRING>

We still plan to archive a copy of the CINF (and cosponsored) technical program and abstracts alongside the *CIB*.

Lastly, CINF is now working on a modern website. As part of the update, a web-based platform for the *CIB* will be developed that will allow new opportunities for production, content, and engagement. More details will be coming soon.

I hope to see many of you at the upcoming 253<sup>rd</sup> ACS National Meeting in San Francisco, CA!

Vincent F. Scalfani, Editor  
The University of Alabama  
vfscalfani@ua.edu

# CINF Social Networking Events at the Spring 2017 ACS Meeting



Division of  
Chemical  
Information

Please Join Us at these  
Division of Chemical Information Events!

The ACS Division of Chemical Information is pleased to host the following social networking events at the Spring 2017 ACS National Meeting in San Francisco, CA.

**Sunday Welcoming Reception & Scholarships for Scientific Excellence Posters**

6:30-8:30 pm, Sunday, April 2nd – Franciscan I & II, Park Central Hotel, 50 3rd Street.

Reception co-sponsored by **Journal of Cheminformatics (Springer Nature)**,  
**Journal of Chemical Information & Modeling**,  
**Collaborative Drug Discovery, PerkinElmer, Schrödinger**  
and **Thieme Chemistry**.

Scholarships for Scientific Excellence sponsored exclusively by **ACS Publications**.

**Tuesday Luncheon** (Ticketed Event – Contact Division Chair, Erin Davis)

12:00-1:30 pm Tuesday, April 4th – Franciscan I, Park Central Hotel, 50 3rd Street.

Sponsored exclusively by the **Royal Society of Chemistry**.

**Speaker: Dr. Andrew R. Leach**

Head of Chemistry Services

European Molecular Biology Laboratory, European Bioinformatics Institute

**Presentation:** *“Molecules, Data and Models.”*

## Tuesday Luncheon Talk

Dr. Andrew R. Leach

*Molecules, Data and Models*

Andrew Leach joined EMBL-EBI as Head of Chemistry Services in August 2016, in which role he is responsible for a number of EBI's core resources including ChEMBL, ChEBI and metabolomics. Prior to joining the EBI Andrew spent more than 20 years at GlaxoSmithKline where his many roles included the development and application of computational and cheminformatics methodologies, fragment-based approaches, target class drug discovery in proteases, ion channels and epigenetics; and the development of platform capabilities to address cardiovascular safety, lead discovery and attrition reduction. Most recently he was the Global Head of Biomolecular Sciences, responsible for protein X-ray crystallography, biophysics and biological mass spectrometry platforms. He served for 12 years as Editor of the *Journal of Computer-Aided Molecular Design*, was until recently a Trustee of the Cambridge Crystallographic Data Centre, and is the author of widely used textbooks in molecular modeling and cheminformatics.

## CINF Business Meetings

Saturday, April 1: 12:30-2:30 PM

- o Education Committee: Franciscan II, Park Central Hotel
- o Awards Committee: City, Park Central Hotel
- o Program Committee: Franciscan I, Park Central Hotel

Saturday, April 1: 3:00-6:00 PM

- o Executive Committee: Franciscan I, Park Central Hotel

Sunday, April 2: 12:00-2:00 PM

- o Chemical Structure Association Trust Meeting: Franciscan II, Park Central Hotel

Wednesday, April 5: 1:00-5:00 PM

- o RDA Chemistry Research Data Interest Group: Franciscan I, Park Central Hotel





## Chemical Structure Association Trust

### Applications Invited for CSA Trust Grant for 2017 and 2018

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program and is now inviting the submission of grant applications for 2017. The deadline for receipt of proposals for the 2018 Grant is also being announced at this time.

### Purpose of the Grants:

The Grant Program has been created to provide funding for the career development of young researchers who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and compounds. One or more Grants will be awarded annually up to a total combined maximum of ten thousand U.S. dollars (\$10,000). Grantees have the option of payments being made in U.S. dollars or in British Pounds equivalent to the U.S. dollar amount. Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated. Grantees are also requested to recognize the support of the Trust in any paper or presentation that is given as a result of that support.

### Who is Eligible?

Applicant(s), age 35 or younger, who have demonstrated excellence in their chemical information related research and who are developing careers that have the potential to have a positive impact on the utility of chemical information relevant to chemical structures, reactions and compounds, are invited to submit applications. While the primary focus of the Grant Program is the career development of young researchers, additional bursaries may be made available at the discretion of the Trust. All requests must follow the application procedures noted below and will be weighed against the same criteria.

### Which Activities are Eligible?

Grants may be awarded to acquire the experience and education necessary to support research activities; for example, for travel to collaborate with research groups, to attend a conference relevant to one's area of research (including the presentation of an already-accepted research paper), to gain access to special computational facilities, or to acquire unique research techniques in support of one's research. Grants will not be given for activities completed prior to the grant award date.

## Application Requirements:

Applications must include the following documentation:

1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used (e.g., cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc.). The relevance of the above-stated purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application)
3. A brief biographical sketch, including a statement of academic qualifications and a recent photograph;
4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4. A copy of the completed application document must be supplied for distribution to the Grants Committee and can be submitted via regular mail or e-mail to the Committee Chair (see contact information below).

## Deadline for Applications:

Application deadline for the 2017 Grant is March 31, 2017. Successful applicants will be notified no later than May 9, 2017. Application deadline for the 2018 Grant is March 30, 2018. Successful applicants will be notified no later than May 9, 2018.

## Address for Submission of Applications:

The application documentation can be mailed via post or emailed to: Bonnie Lawlor, CSA Trust Grant Committee Chair, 276 Upper Gulph Road, Radnor, PA 19087, USA. If you wish to enter your application by e-mail, please contact Bonnie Lawlor at [chescot@aol.com](mailto:chescot@aol.com) prior to submission so that she can contact you if the e-mail does not arrive.

## Chemical Structure Association Trust: Recent Grant Awardees

### 2016 – Thomas Coudrat

Monash University, Australia, was awarded a Grant to cover travel to present his work at three meetings in the United States: the Open Eye Scientific CUP XVI, The American Chemical Society Spring Meeting, and the Molsoft ICM User Group Meeting. His work is in ligand directed modeling.

### 2016 – Clarisse Pean

Chimie Paris Tech, France, was awarded a Grant to cover travel to give an invited presentation at the 2016 Pacific Rim Meeting on Electrochemical and Solid State Science later this year.

### 2016 – Qian Peng

University of Oxford, England, was awarded a Grant to attend the 23<sup>rd</sup> IUPAC Conference on Physical Organic Chemistry. His research is in the development of new ligands for asymmetric catalysis.

### 2016 – Petteri Vainikka

University of Turku, Finland, was awarded a Grant to spend the summer developing and testing new methods for modeling organic solvents in organic solutions with Dr. David Palmer and his group at the University of Strathclyde, Glasgow, Scotland.

### 2016 – Qi Zhang

Fudan University, China, was awarded a Grant to attend a Gordon Conference on enzymes, coenzymes and metabolic pathways. His research is in enzymatic reactions.

### 2015 – Dr. Marta Encisco

Molecular Modeling Group, Department of Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Australia. She was awarded a Grant to cover travel costs to visit collaborators at universities in Spain and Germany and to present her work at the European Biophysical Societies Association Conference in Dresden, Germany in July 2015.

### 2015 – Jack Evans

School of Physical Science, University of Adelaide, Australia. He was awarded a grant to spend two weeks collaborating with the research group of Dr. Francois-Xavier Coudert (CNRS, Chimie Paris Tech).

### 2015 – Dr. Oxelandr Isayev

Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill. He was awarded a Grant to attend summer classes at the Deep Learning Summer School 2015 (University of Montreal) to expand his knowledge of machine learning to include Deep Learning (DL). His goal is to apply DL to chemical systems to improve predictive models of chemical bioactivity.

### 2015 – Aleix Gimeno Vives

Cheminformatics and Nutrition Research Group, Biochemistry and Biotechnology Dept., Universitat Rovira i Virgili. He was awarded a Grant to attend the Cresset European User Group Meeting in June 2015 in order to improve his knowledge of the software that he is using to determine what makes an inhibitor selective for PTP1B.

### 2014 – Dr. Adam Madarasz

Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences. He was awarded a Grant for travel to study at the University of Oxford with Dr. Robert S. Paton, a 2013 CSA Trust Grant winner, in order to increase his experience in the development of computational methodology which is able to accurately model realistic and flexible transition states in chemical and biochemical reactions.

### 2014 – M.José Ojeda Montes

Department of Biochemistry and Biotechnology, University Rovira i Virgili, Spain. She was awarded a Grant for travel expenses to study for four months at the Freie University of Berlin to enhance her experience and knowledge regarding virtual screening workflows for predicting therapeutic uses of natural molecules in the field of functional food design.

### 2014 – Dr. David Palmer

Department of Chemistry, University of Strathclyde, Scotland. He was awarded a Grant to present a paper at the fall 2014 meeting of the American Chemical Society on a new approach for representing molecular structures in computers based upon ideas from the Integral Equation Theory of Molecular Liquids.

### 2014 – Sona B. Warriar

Departments of Pharmaceutical Chemistry, Pharmaceutical Biotechnology, and Pharmaceutical Analysis, NMIMS University, Mumbai. She was awarded a Grant to attend the International Conference on Pure and Applied Chemistry to present a poster on her research on inverse virtual screening in drug repositioning.

### 2013 – Dr. Johannes Hachmann

Department of Chemistry and Chemical Biology at Harvard University, Cambridge, MA. He was awarded the Grant for travel to speak on “Structure-property relationships of molecular precursors to organic electronics” at a workshop sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) that took place October 22 – 25, 2013 in Lausanne, Switzerland.

### 2013 – Dr. Robert S. Paton

University of Oxford, UK. He was awarded the Grant to speak at the Sixth Asian Pacific Conference of Theoretical and Computational Chemistry in Korea on July 11, 2013. Receiving the invitation for this meeting provided Dr. Paton with an opportunity to further his career as a Principal Investigator.

### 2013 – Dr. Aaron Thornton

Material Science and Engineering at CSIRO in Victoria, Australia. He was awarded the Grant to attend the 2014 International Conference on Molecular and Materials Informatics at Iowa State University with the objective of expanding his knowledge of web semantics,

chemical mark-up language, resource description frameworks and other online sharing tools. He also visited Dr. Maciej Haranczyk, a prior CSA Trust Grant recipient, who is one of the world leaders in virtual screening.

### 2012 – Tu Le

CSIRO Division of Materials Science & Engineering, Clayton, VIC, Australia. Tu was awarded the Grant for travel to attend a cheminformatics course at Sheffield University and to visit the Membrane Biophysics group of the Department of Chemistry at Imperial College London.

### 2011 – J. B. Brown

Kyoto University, Kyoto, Japan. J.B. was awarded the Grant for travel to work with Professor Ernst Walter-Knapp at the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels.

### 2010 – Noel O'Boyle

University College Cork, Ireland. Noel was awarded the Grant to both network and present his work on open source software for pharmacophore discovery and searching at the 2010 German Conference on Cheminformatics.

### 2009 – Laura Guasch Pamies

University Rovira & Virgili, Catalonia, Spain. Laura was awarded the Grant to do three months of research at the University of Innsbruck, Austria.

### 2008 – Maciej Haranczyk

University of Gdansk, Poland. Maciej was awarded the Grant to travel to Sheffield University, Sheffield, UK, for a 6-week visit for research purposes.

### 2007 – Rajarshi Guha

Indiana University, Bloomington, IN, USA. Rajarshi was awarded the Grant to attend the Gordon Research Conference on Computer-Aided Design in August 2007.

### 2006 – Krisztina Boda

University of Erlangen, Erlangen, Germany. Krisztina was awarded the Grant to attend the 2006 spring National Meeting of the American Chemical Society in Atlanta, GA, USA.

### 2005 – Dr. Val Gillet and Professor Peter Willett

University of Sheffield, Sheffield, UK. They were awarded the Grant for student travel costs to the 2005 Chemical Structures Conference held in Noordwijkerhout, the Netherlands.

#### 2004 – Dr. Sandra Saunders

University of Western Australia, Perth, Australia. Sandra was awarded the Grant to purchase equipment needed for her research.

#### 2003 – Prashant S. Kharkar

Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai. Prashant was awarded the Grant to attend the conference, Bioactive Discovery in the New Millennium, in Lorne, Victoria, Australia (February 2003) to present a paper, “The Docking Analysis of 5-Deazapteridine Inhibitors of Mycobacterium avium complex (MAC) Dihydrofolate reductase (DHFR).”

#### 2001 – Georgios Gkoutos

Imperial College of Science, Technology and Medicine, Department of Chemistry. London, UK. Georgios was awarded the Grant to attend the conference, Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, (CMTPI-2001) in Bordeaux, France, to present part of his work on internet-based molecular resource discovery tools.

## Eugene Garfield, 1925–2017

### Dr. Eugene Garfield: A Visionary Information Pioneer Dies at Age 91



Eugene Garfield in 2007. Photo courtesy of the Chemical Heritage Foundation ([CC BY-SA 3.0](#)).

Dr. Eugene Garfield, the founder of the Institute for Scientific Information (ISI) (now Clarivate Analytics), and the intrepid entrepreneur who created ground-breaking products such as *Current Contents*, the *Science Citation Index*, *Index Chemicus*, and *Current Chemical Reactions*, died unexpectedly on February 26, 2017.

Most members of the Division of Chemical Information (CINF) know at least of Dr. Garfield, with many of us having developed personal and professional relationships with him over the years. He was very active in CINF, serving as Alternate Councilor from 1970-1972, as a Committee Chair, and as a frequent presenter at symposia. He was also the Herman Skolnik Awardee in 1977

and the Patterson-Crane Awardee in 1983. Eugene Garfield was a larger-than-life figure in the evolution of the chemical information industry from print through digital formats, but his was an unplanned career.

It began as a laboratory bench chemist under the tutelage of Professor Louis P. Hammett, the father of the Hammett equation, after graduating in 1949 from Columbia University with a B.S. in chemistry. By his own admission, Garfield was not successful in the lab and his career path took an unexpected turn when he attended a meeting of the American Chemical Society (ACS) in New York City and heard a presentation on the use of punch cards to handle large volumes of chemical information. He was intrigued, and ultimately took a position at Johns Hopkins University as research assistant on the Welch Medical Indexing Project: one of the first large-scale investigations into the potential of machine-based information systems. During the two years that Garfield spent on the project he learned a lot and the seeds of three concepts were planted - those of citation indexing, chemical indexing, and contents-page alerts. He ultimately left the project to study for a Master's degree in Library Sciences, which he obtained in 1954 from Columbia University. Armed with his two degrees and the concepts that he developed while at Johns Hopkins (a PhD in structural linguistics from the University of Pennsylvania was added in 1961), Garfield went on to found the Institute for Scientific Information in 1960. From that point on, until the company was sold to the Thomson Corporation in 1992, Garfield nurtured the seeds that were planted during the Welch Project, ultimately developing unique and innovative information products and services, not only in the sciences, but also in the arts and humanities and social sciences.

Yes, he was a successful entrepreneur and businessman. And while the Garfield legend is well known (he did create the early versions of *Current Contents* while working out of a chicken coop converted into a [log cabin!](#)) not everyone has been blessed to know Eugene Garfield as an employer, mentor, and friend. I, and many ISI employees, especially those of us from ISI's early days, have been so blessed. He was a creative force and was in many ways the nurturer of our careers. Regardless of age, gender or ethnicity, he supported you if you had good ideas and worked hard. It was not a bureaucratic company, but rather it had the look and feel of a family-run operation. He regarded his employees as his extended family and, to this day, we former early-day employees remain a family, although now without our fearless and tenacious leader.

With the passing of Eugene Garfield an era has ended. But his legacy lives on. Today, thousands of scientists around the globe use his products and services to advance their research, and hundreds of people owe their jobs to the result of his labor as Clarivate Analytics continues to build on his amazing foundation.

Goodbye, dear friend, and thank you for all that you gave to us through your example and teaching. You may no longer be with us in person, but you live in the hearts of the entire ISI family and in the hearts of others whom you impacted along the way. Rest well until we all meet again.

Bonnie Lawlor

For more information on Dr. Eugene Garfield, see the following:

Eugene Garfield web site: <http://www.garfield.library.upenn.edu/>

*Future of the History of Chemical Information* (ACS Symposium Series) American Chemical Society, Leah Rae McEwen (Editor), Robert E. Buntrock (Editor) 2014, ISBN 9780841229457. DOI: [10.1021/bk-2014-1164](https://doi.org/10.1021/bk-2014-1164)

Baykoucheva, S., "Interview with Eugene Garfield," *Chemical Information Bulletin*, Vol. 58, No. 2, pp. 7-9, 2006. <http://www.acscinf.org/content/interview-eugene-garfield>



## Book Reviews

Scerri, E. R. (2016). *A Tale of Seven Scientists and a New Philosophy of Science*. New York, NY: Oxford University Press. 228 pages. ISBN: 9780190232993, \$29.95 (Amazon)

For Eric Scerri, the author of the book, *A Tale of Seven Scientists and a New Philosophy of Science*, the number seven seems magical. This new book follows in the steps of his previous one, *A Tale of Seven Elements* (2013, Oxford: Oxford University Press).

Scerri is a philosopher and historian of science. The readers of the *Bulletin* may remember his interview, [A philosopher's view on the periodic table of the elements and its significance: Interview with Eric Scerri](#), and the review of his book [A Tale of Seven Elements](#). In his new work, Scerri examines the life and contributions of seven scientists considered by science historians as being marginal or whose views were looked upon as mistaken. These little-known scientists (John Nicholson, Anton van den Broek, Richard Abegg, Charles Bury, John D. Main Smith, Edmund Stoner, and Charles Janet) were either physicists or chemists (or both). Their contributions are related to the periodic table of the elements, and more specifically, to the atomic number and chemical bonding. Although their names are not familiar, except to some historians of science, these scientists paved the road to important discoveries.

Scerri disagrees with historians and philosophers of science such as Karl Popper and Thomas Kuhn who view scientific progress as a sequence of discretionary steps and revolutionary breaks. Scerri is proposing an alternative philosophy of science as “a collective enterprise... in which many individuals, some significant, others far less so, make contributions which are taken up by countless other scientists in the shared growth of the story of scientific knowledge.” He compares science to a giant living organism on a Darwinian-type gradual development path, which includes a systematic advance of scientific knowledge through both the major and minor figures in science, through trials and errors. According to this evolutionary philosophy, the fighting and competition between individual scientists resembles the struggle among different biological species for survival. In this fight, there are no winners or losers, no abrupt scientific revolutions. There are “worker-bee-like scientists who all contribute to the overall progress.” In science, says Scerri, marginal and intermediate figures are no less important than the “star” scientists.

**John Nicholson**, one of the main “heroes” in the book, is one of such less known but pivotal figures. He was an established mathematical physicist, first at Cambridge and then in King's College, London. Nicholson used astronomical data to develop his planetary model of the atom. His work is of major historical significance, because of the role he played in the revolution in physics during the early 20th century. Figures such as Nicholson are just as important as the major ones such as Niels Bohr, who had noticed the contributions of Nicholson before he presented his famous paper announcing his model of the atom. Nicholson's theory influenced the thinking of scientists in the development of the quantum theory of atoms and molecules.

**Anton van den Broek**, who was a lawyer and never held an academic appointment, was the first to discuss the key concept of atomic number, which characterizes each of the known chemical elements, even those that were not yet discovered. Van den Broek looked at the periodic table as a whole, taking into account the relationships between the elements. This was a different perspective from the one viewed by the physicists, who were focusing on just one or two elements or a specific property of an element.

**Richard Abegg**, a student of Nernst, started as an organic chemist, but then switched to physical chemistry. He was greatly influenced by his mentors Arrhenius, van't Hoff, and Ostwald. Abegg was one of the first to see the role that electrons play in chemical bonding. His work provided "a missing link" between the work of Mendeleev on valency and G. N. Lewis's novel ideas on chemical bonding in terms of number of electrons.

**Charles Bury**, whose contributions remained unknown to chemists, worked in a provincial university in Wales. Pursuing research at the border of chemistry and physics, he contributed to the elucidation of electronic configurations of the atoms of the elements. Bury criticized Langmuir for focusing on the chemical behavior of only some of the elements, and not looking at all of them. He succeeded in coming to a better and more complete set of electron arrangements that provided an improved model of the periodic table of the elements.

Although **John D. Main Smith**, a chemist from the University of Birmingham in the UK, published a comprehensive book, *Chemistry and Atomic Structure*, his work remained mostly unknown. The reason for that is that he published his papers in an obscure journal (*Chemistry & Industry*), a publication that did not have much of an influence on chemists and physicists. Main Smith courageously took on Niels Bohr, a powerful scientist, and proposed some improved electronic arrangements.

Another lesser-known scientist, **Edmund Stoner**, independently discovered the arrangements obtained by Main Smith, and contributed to the understanding of the physics of the atom and the atomic spectra. Stoner's work provided Wolfgang Pauli with a clue in solving a difficult problem when developing his idea of the Exclusion Principle.

**Charles Janet** was a fascinating figure, "a Renaissance Man," whose diverse interests took him to explore many different disciplines, including geology, entomology, biology, and chemistry. In addition to his scientific accomplishments, he also made significant contributions to world literature. Janet was 78 when he decided to turn to chemistry. His work led to renewed interest into the theoretical foundations of the periodic system of the elements. Janet developed an interesting model of the periodic system that is coherent with quantum mechanics. His so-called "left-step table," admired by Scerri, resembles a staircase arising from left to right, unlike the more uneven format used to present the periodic table.

Born in Paris and a graduate of the Sorbonne, Janet's first research interests were devoted to geology. He later turned to studying insects, particularly bees and ants, a topic on which he continued to publish throughout his life. Janet also studied freshwater algae and assembled a fossil collection with over 50,000 items that he personally classified into 400

species. Janet also had many other interests, which included making electrical inventions, icebox structures, and studying the housing conditions of early 20th-century French laborers. One of his major inventions was an artificial nest, used by biologists to observe the social behavior of ants.

At some point in his life, Janet served as director of La Brosserie Dupont, a large commercial enterprise in the l'Oise district of France, which employed 1,000 workers. His 54-room mansion included a science library that was also home to an enormous fossil collection. Scerri suggested that the fact that Janet had spread his efforts in so many different directions contributed to his lack of recognition.

The scientists discussed in this book share a common fate: they contributed to the overall development of different branches of physical science, but were forgotten or remained unknown. Their work served as a foundation for the work of others. Their contributions are the missing links in the evolution of modern atomic theory. Scerri looks at scientific progress as a development of a giant organism that is “constantly evolving, ‘trying out’ new variations and letting nature favor one or the other path of biological evolution.”

In this book, Scerri discusses the reasons why the contributions of these scientists were either neglected or downplayed. In some cases, it was the perspective that scientists at that time had on the periodic table of the elements, depending on whether they were looking at it from the point of view of physics or chemistry. The small intermediate steps in science are often ignored, and “the development of science appears to have been as a series of spectacular leaps and the architects of success in theories take on the mantle of superheroes with almost magical powers...” As Scerri says, “The more correct picture is one of incremental steps occurring almost imperceptibly and frequently carried out by unknown individuals. The history of science proceeds via evolution in which dozens of small players contribute, and not via revolutions fashioned by the few and famous.”

Scerri admits his book is radical. It presents “scientific development as an impersonal phenomenon, in which personalities, egos, or who was ‘right’ or ‘wrong’ look irrelevant. What is important is the progress made by scientists as a community.” This book brings our attention to an aspect of science that is often obscured by human desire to pay attention only to the “stars,” and it is very much worth reading.

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## Notes From Our Sponsors



Division of Chemical Information Sponsors Spring 2017



The American Chemical Society Division of Chemical Information is very fortunate to receive generous financial support from our sponsors to maintain the high quality of the Division's programming and to promote communication between members at social functions at the ACS Spring 2017 National Meeting in San Francisco, CA, and to support other divisional activities during the year, including scholarships to graduate students in Chemical Information.

The Division gratefully acknowledges contributions from the following sponsors:

<b>Gold</b>	<b>ACS Publications</b>
<b>Silver</b>	<b><i>Journal of Chemical Information &amp; Modeling</i></b> <b>Royal Society of Chemistry</b>
<b>Bronze</b>	<b><i>Journal of Cheminformatics (Springer Nature)</i></b> <b>Collaborative Drug Discovery</b> <b>PerkinElmer</b> <b>Thieme Chemistry</b>
<b>Contributors</b>	<b>Bio-Rad Laboratories</b> <b>Schrödinger</b>

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Please feel free to contact me if you would like more information about supporting the ACS Division of Chemical Information.

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In addition, we will accompany the Altmetric Attention Score with a display of total article views. This number is the [COUNTER-compliant](#) sum of full text article downloads (including PDF, ACS ActiveView PDF, and full text HTML article views). Authors and researchers can easily see the broad impact of an article by viewing both the number of full-text downloads and the Altmetric Attention Score.

"We are pleased to now be incorporating Altmetric data on our journal articles," says Jeff Lang, Assistant Director of Platform Development at ACS Publications. "This is a great opportunity for authors to gain a wider understanding of the impact of their work, while providing researchers and others with an idea of how the article has been received by a broader audience."

**Discover these new metrics by taking a closer look at the data on the following article from *ACS Energy Letters*: [100k Cycles and Beyond: Extraordinary Cycle Stability for MnO<sub>2</sub> Nanowires Imparted by a Gel Electrolyte](#)**



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## Journal of Chemical Information and Modeling

The *Journal of Chemical Information and Modeling* launched two new manuscript types last year: Application Note and Review. Application Note articles are informative peer-

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reviewed reports on novel software packages, databases, and web servers.

Review articles are peer-reviewed topical overviews of general interest to the *JCIM* community.

Both new manuscript types have been well received and we encourage interested parties to refer to [the journal's author guidelines](#) for more details. Those with review ideas and pre-submission inquiries can contact Editor-in-Chief Kenneth M. Merz Jr. at [eic@j cim.acs.org](mailto:eic@j cim.acs.org).

## RSC Advances goes gold open access

**From Issue 1, 2017 *RSC Advances*, currently the world's largest chemistry journal, will be gold open access. This change allows researchers free access to a broader scope of high-quality research articles, and offers new, affordable open access publishing options for authors around the world.**



*RSC Advances* publishes high-quality scientific research on 133 subjects, covering the entirety of the chemical sciences, including multidisciplinary and emerging areas. Since its launch in 2011, we have published over 26,000 articles, with submissions from authors in 91 countries. Transitioning the journal to gold open access enables the Royal Society of Chemistry to shape the future of open access publishing by maximizing the visibility of research in the chemical sciences, and related areas, and helping authors meet their funding and institutional requirements.

Dr. Emma Wilson, Director of Publishing at the Royal Society of Chemistry, emphasized how the journal is setting a new standard of academic publishing, "The journal has been at the forefront of innovation since its launch in 2011. The strength of support for *RSC Advances* from the community has been unprecedented in chemistry publishing, and last year we built on and increased this engagement by introducing an innovative peer-review model. The new open access model is the next step forward in the continued evolution of the journal."

We support authors' ability to choose where to publish their work, and we believe that open access publishing should be an option available to all, regardless of economic background.

We are therefore setting the article processing charge (APC) at a competitive level of £750 to ensure it is affordable to all authors. To show our commitment to affordable open access, we are offering all authors a discounted APC of £500 for the first two years.

In addition, more than 40 countries that fall under [Research4Life](#) groups A and B will receive a full waiver to the APC, with a partial discount of £250 being made available to seven further countries including India, Egypt and Pakistan.

When announcing the change, Dr. Helen Pain, Deputy Chief Executive of the Royal Society of Chemistry, explained why this approach is so important, "We want to make sure that high-impact research from emerging centers of chemistry gets the international visibility it deserves. With this in mind, we have set our APCs at one of the lowest in the industry to make it affordable for authors."

For more information on *RSC Advances* please visit [rsc.li/rsc-advances](http://rsc.li/rsc-advances).



### **Royal Society of Chemistry**

We are the oldest chemical society in the world and in 2016 we celebrated 175 years of progress and people in the chemical sciences. Throughout the year, we shared stories of how our members past and present have helped to change the world with chemistry.

With over 50,000 members and a knowledge business that spans the globe, we are the United Kingdom's professional body for chemical scientists; a not-for-profit organization with 175 years of history and an international vision of the future.

We promote, support and celebrate chemistry. We work to shape the future of the chemical sciences, for the benefit of science and humanity.

Registered charity number 207890

## Springer Nature launched SharedIt



Springer Nature wants researchers to share content easily and legally. Our Springer Nature SharedIt content-sharing initiative means that links to view-only, full-text subscription research articles can be posted anywhere, including on

social media platforms, author websites and in institutional repositories, so researchers can share research with colleagues, and general audiences.

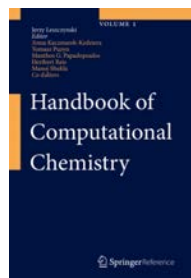
To find out how this works, and for detailed information about this service for authors, librarians, and subscribers, please go to <http://www.springernature.com/gp/researchers/sharedit>

## Research Data Policies implemented for Springer Nature journals

At Springer Nature we want to enable all of our authors and journals to publish the best research, which includes achieving community best practices in the sharing and archiving of research data. We also aim to facilitate compliance with research funder and institution requirements to share data. To help accomplish this we have introduced a set of standardized research data policies to almost 800 journals and continue to roll this out to further journals. These policies can be easily adopted, and we are developing supporting tools and services.

For more information, go to <http://www.springernature.com/gp/group/data-policy/> and read the blog post by Iain Hrynaszkiewicz, Head of Data Publishing at Springer Nature:

<http://blogs.springeropen.com/springeropen/2016/07/05/promoting-research-data-sharing-springer-nature/>



## Now published: Second edition of the “Handbook of Computational Chemistry”

Under the editorship of Jerzy Leszczynski, Jackson State University (JSU), Jackson, MS (USA), this new edition has been expanded and revised, now including sections on chemoinformatics, relativity, and solvents. For more information, go to:

[www.springer.com/978-3-319-27281-8](http://www.springer.com/978-3-319-27281-8)

## New Editors for *Journal of Cheminformatics*



At the end of 2016, Christoph Steinbeck and David Wild stepped down as Editors-in-Chief of *Journal of Cheminformatics*, handing the reins to Rajarshi Guha and Egon Willigahgen, who started their tenures as the new Editors-in-Chief earlier that year (<http://blogs.springeropen.com/springeropen/2016/09/08/new-editors-chief-journal-cheminformatics/>).

In addition to Rajarshi and Egon, the journal welcomed Geoff Hutchison (Associate Professor of Chemistry at the University of Pittsburgh and lead on the Open Babel project) and Evan Bolton (Lead Scientist at NCBI and co-winner of the 2016 Herman Skolnik Award for his work on the PubChem database) to the Editorial Board.

## Collaborative Drug Discovery (CDD)

CDD provides a modern approach to drug discovery research informatics trusted globally by thousands of leading researchers. [CDD Vault](#) is a complete platform for drug discovery informatics, hosted through an intuitive web interface. It helps your project team manage, analyze, and present chemical structures and biological assay data.

CDD cordially invites you to share your experiences with your peers in the drug discovery space. We are hosting a “Sharing Experiences in Life Science Research” [seminar](#) right after the ACS meeting on Friday April 7th, 2017, between 8:30 and 1:00 (Pacific) at The American Bookbinders Museum in San Francisco. Take full advantage of this unique opportunity to:

- ✓ Network with other drug discovery scientists
- ✓ Gain insights from seasoned lab informatics professionals
- ✓ Decompress after ACS before flying home
- ✓ Discover the upcoming innovations planned within the CDD Vault pipeline!

For more information, please visit our [website](#) or email us at [info@collaboratedrug.com](mailto:info@collaboratedrug.com).

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## PerkinElmer, Inc.

PerkinElmer is pleased to announce the release of the PerkinElmer Signals Notebook for ChemDraw, a cloud-based electronic lab notebook. This ELN solution is part of the ChemOffice Professional 16 release of the ChemDraw software, the industry's No. 1 chemical structure drawing tool which ensures the efficient design and visualization of molecules, reactions, biological entities and pathways in a publication-ready format.



The PerkinElmer Signals Notebook for ChemDraw will enable you to organize your scientific research within an electronic notebook with chemistry capabilities built-in, allowing you to eliminate your paper notebook. You will be able to organize your work in notebooks and experiments to easily build an electronic record with experimental evidence by drawing reactions, writing notes, and attaching relevant document and reference materials.

In addition to the PerkinElmer Signals Notebook for ChemDraw, the ChemOffice Professional platform also includes the ChemDraw Cloud web-based application facilitating quick, convenient, and flexible access to research anytime, anywhere, and fosters increased collaboration across organizations with the functionality to revise documents in the cloud.

Product Link: <http://www.perkinelmer.com/category/chemistry-software>

## Science of Synthesis: Prof. Fürstner Named First Editor-in-Chief, and New Version to be Released in March

### Prof. Alois Fürstner Named First Editor-in-Chief of Science of Synthesis



# Thieme

Professor Alois Fürstner, Managing Director at the Max-Planck-Institut für Kohlenforschung (Max-Planck-Institute for Coal Research), Mülheim an der Ruhr, Germany, has taken over the position of Editor-in-Chief on the Science of Synthesis (SOS) Editorial Board.

An expert in organometallic chemistry, Professor Fürstner has been a member of the Editorial Board since 2008.

“My task as Editor-in-Chief will be to work with the Editorial Board to ensure that the methods presented in Science of Synthesis continue to reflect the latest insights in synthetic chemistry,” Professor Alois Fürstner comments. Science of Synthesis content is regularly reviewed and adapted. “This large database offers both a quick overview and in-depth information on all relevant problems in chemical synthesis,” Professor Fürstner says. “That’s what makes SOS both unique and essential.” Over 1,800 renowned authors around the world contribute to the reference work. They evaluate synthetic methods in their respective fields, and select the most significant for discussion in their reviews.

### Science of Synthesis 4.7 in March 2017

A new version of Science of Synthesis will be released at the end of March 2017.

In addition to including new citation search functionality, it will include two new content volumes on *N-Heterocyclic Carbenes in Catalytic Organic Synthesis* edited by Professor Steven P. Nolan and Dr. Catherine S. J. Cazin (Ghent University, Belgium) with contributions from 79 authors. These volumes provide a user’s guide to NHC chemistry and catalysis, thus facilitating the introduction of NHCs to novices, and also helping to expand the repertoire of synthetic tools available to the more-advanced researcher, enabling the design of new catalysts and reactions.



A short video introduction shows in an entertaining way how researchers can benefit from using Science of Synthesis: [https://www.youtube.com/watch?v=rzDru\\_VLuaQ](https://www.youtube.com/watch?v=rzDru_VLuaQ).

To get access to Science of Synthesis 4.7 or a free trial please visit <https://sos.thieme.com>.

For more information about Science of Synthesis please visit the Web site at <https://www.thieme-chemistry.com/sos/>.

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## Schedule of Future ACS National Meetings

254 <sup>th</sup>	Aug. 20–24	2017	Washington, DC	Chemistry's Impact on the Global Economy
255 <sup>th</sup>	Mar. 18–22	2018	New Orleans, LA	The Food, Energy, Water Nexus
256 <sup>th</sup>	Aug. 19–23	2018	Boston, MA	Nanotechnology
257 <sup>th</sup>	Mar. 31–Apr. 4	2019	Orlando, FL	Chemistry for New Frontiers
258 <sup>th</sup>	Aug. 25–29	2019	San Diego, CA	Chemistry of Water
259 <sup>th</sup>	Mar. 22–26	2020	Philadelphia, PA	Macromolecular Chemistry: The Second Century
260 <sup>th</sup>	Aug. 23–27	2020	San Francisco, CA	Chemistry from Bench to Market
261 <sup>st</sup>	Mar. 21–25	2021	San Antonio, TX	TBA
262 <sup>nd</sup>	Aug. 22–26	2021	Atlanta, GA	TBA