



CSA Trust Newsletter

Issue 21

Spring 2013

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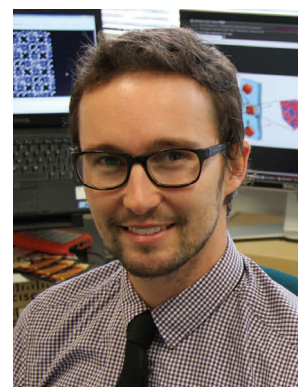
CSA Trust Grant for 2013 Awarded



Dr. Johannes Hachmann



Dr. Robert S. Paton



Dr. Aaron Thornton

The CSA Trust received eight grant proposals this year - a record number! The Board of Trustees voted to award three Grants, based upon the unanimous recommendation of the selection committee.

The first Grant was awarded to **Dr. Johannes Hachmann**, a Research Associate in the department of Chemistry and Chemical Biology at Harvard University. He leads the Harvard Clean Energy Project, a virtual high-throughput screening and design effort for the next generation of organic photovoltaic materials. It features the most extensive first-principles quantum chemical study of all times, and a massive reference database on organic electronics. This work is one of the flagship projects of the White House materials Genome Initiative and part of the Global Climate and Energy Project. Dr. Hachmann has been invited 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 will take place October 22 - 25, 2013 in Lausanne, Switzerland. He is the only invited speaker who does not hold a faculty position. The CSA Trust will allow him to travel to the meeting at which he plans to create an awareness of the value of big data and cheminformatics/materials informatics in the modeling and simulation community, a community that does not traditionally make use of these techniques.

The second Grant was awarded to **Dr. Robert S. Paton**, a University Lecturer in organic chemistry at the University of Oxford, UK. There he has established a research group focused on understanding organic structure and reactivity and on developing models to predict the outcomes of reactions to aid and inform synthesis. In particular, his group is interested in extending the use of QSAR/QSPR-type models towards understanding and predicting selectivity in reactions for which the mechanism is not unclear or too large to model atomistically, and on non-linear free energy relationships in organic chemistry. In 2012 he was appointed associate editor of the overlay —>Page 3

CSA Trustees at the ACS 2013 Spring Meeting in New Orleans



Top Left: Bill Jorgensen and Wendy Warr

Top Right: David Martinsen and René Deplanque.

Middle Left: Keith Taylor, Julien Thibault, Amir Seddik, Guenter Grethe

Middle Right: Peter Loew, Roger Schenck, Guido Herrmann

Bottom Left: Farrel Borden, Valentina Eigner-Pitto, Phil McHale, Julia Stoetzner

Bottom Right: Peter Rusch and Edlyn Simmons

Pictures taken by Wendy Warr. Used with permission from the ACS Chemical Information Division (<http://www.flickr.com/photos/cinf/>).

CSA Trust Grant for 2013 Awarded continued

journal *Computational Chemistry Highlights*. He has been invited to give numerous talks on his research including one at the Sixth Asian Pacific Conference of Theoretical and Computational Chemistry in Korea on July 11, 2013. Receiving the invitation for this meeting has provided Dr. Paton with an opportunity to further his career as a Principal Investigator and the Grant funds will allow him to travel to the conference.

The third Grant was awarded to **Dr. Aaron Thornton**, a Research Scientist in Computational and Simulation Sciences, Material Science and Engineering at CSIRO in Victoria, Australia. Dr. Thornton leads a team of three PhD students, a postdoctoral fellow and three permanent staff in the field of mathematical, computational and simulation sciences. After completion of his PhD in 2010 he started a postdoctoral fellowship on the topic of "Computational Tools for Materials Design," where he developed and collected algorithms to aid experimentalists in material design from the molecular scale. This work resulted in numerous structure-property predictive tools such as void fraction, surface area, cavity-size distribution, binding energy, gas storage and gas diffusivity. One of his tools demonstrated the concept of "Virtual Screening" where Dr. Thornton used predictive tools to guide experimentalists to the most promising candidate structures for clean energy applications, and he began establishing a workflow for screening materials based upon the computed properties. The tools he has developed are based upon existing capabilities and he wants to expand to next-generation technologies. His Grant funds will be used to attend the 2014 International Conference on Molecular and Materials Informatics at Iowa State University. The objective is to support his next career development step to expand his knowledge of web semantics, chemical mark-up language, resource description frameworks and other on-line sharing tools. He will also visit Dr. Maciej Haranczyk, a prior CSA Trust Grant recipient, who is one of the world leaders in virtual screening.

As you can see, all three of the CSA Trust Grant recipients have accomplished much at a young age and the Grant funds will help them continue their career development. All three will submit reports on their Grant-funded activities that will be published in a future edition of this newsletter.

The CSA Trust Grant Program was created to provide funding for the career development of young researchers (ages 35 or less) 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. The Grant Committee has already begun a call for the submission of proposals for the 2014 Grant Proposals must be submitted by March 13, 2014 and the total maximum value of the Grant funds awarded will be \$10,000 (U.S. dollars). For more information, go to: http://www.csa-trust.org/?page_id=9.

Previous CSA Trust Grant Award Winners

- 2012 **Tu C. Le:** CSIRO Division of Materials Science & Engineering, Clayton, VIC, Australia. Tu C. 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-Knappe 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.

Previous CSA Trust Grant Award Winners continued

- 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 **Val Gillet** and **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 **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, Dept. 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.

Picture Album from the ACS 2013 Spring Meeting in New Orleans



Pictures taken by Wendy Warr. Used with permission from the ACS Chemical Information Division (<http://www.flickr.com/photos/cinf/>).

Sheffield Chemoinformatics Group wins Jason Farradane Award



Photo: Martin White presenting the certificate to Peter Willett (image courtesy of Information Today & photovibe).

The 2012 UKeiG Jason Farradane Award has been awarded to the **Chemoinformatics Research Group** in the Information School, University of Sheffield. The Chemoinformatics Research Group has been one of the leading centres worldwide for chemoinformatics research for over forty years, and has been noted as providing "the most widely recognized and well-established research and teaching base in the field." The Group has demonstrated over many years the contributions that can be made by those with a specifically information perspective that complements more obviously chemical and biological studies. The Group's work was initiated by Michael Lynch, who came to Sheffield in 1965 from the post of Head of Basic Research at Chemical Abstracts Service.

The Award is made in recognition of the Chemoinformatics Research Group's work in raising the profile of the information profession within a field of endeavour in a way which has become an exemplar to others; demonstrating excellence in education and training; and for their major contribution to the theory and practice of information science. An important part of the Group's educational activities has been the training of students who have subsequently gone on to join the chemoinformatics workforce, with some of them now in senior positions. The nomination notes that the Group's first publication dates from 1967 and it has made very significant contributions to the theory and practice of chemoinformatics over a period of more than four decades, by means of both its published research and its extensive collaborations with industry. Their work spans search algorithms and data structures; 3D and patent (or Markush) searching; ligand docking

and pharmacophore mapping; and the detailed comparison of different tools for some chemoinformatics application to enable the identification of the most effective and/or efficient approach. The Group's industrial collaborations over the years include joint research projects with many of the world's leading pharmaceutical, agrochemical and software companies.

The Group also organizes the **Joint Sheffield Conference in Chemoinformatics**, which has been held every three years since 1998 and is one of the two largest regular conferences that focus on chemoinformatics.

The judges had no hesitation in awarding the three current members of the research group - Val Gillet, John Holliday and Peter Willett - the 2012 UKeiG Jason Farradane Award.

The presentation was made at Internet Librarian International 2012 at the Olympia Conference Centre on Wednesday 31st October.

About Jason Farradane

Jason Farradane graduated in chemistry in 1929 at what is now Imperial College and started work in industry as a chemist and documentalist. After working in research at the Ministry of Supply and the Admiralty during World War II, he first made an impact with a paper on the scientific approach to documentation at a Royal Society Scientific Information Conference in 1948.

He was instrumental in establishing the Institute of Information Scientists in 1958 and the first academic courses in information science in 1963 at the precursor of City University, where he became Director of the Centre for Information Science in 1966. Of Central European origin, his commitment to science was reflected in the name he created for himself - a combination of Faraday and Haldane, two scientists he particularly admired. On the research side his main contributions lay in relational analysis, which can now perhaps be seen as providing a precursor to work in the area of A.I., and the concept of information. He saw information science as a step towards understanding and better organizing ourselves.

Source: <http://www.ukieg.org.uk/awards/jason-farradane>

People and Places



Dimitris K. Agrafiotis Retires as Trustee of CSA Trust

With deep appreciation for all his efforts, Dimitris Agrafiotis retired from the CSA Trust on 31 December 2012.

Dimitris K. Agrafiotis is Vice President of Informatics at Johnson & Johnson Pharmaceutical Research & Development. He also serves as Adjunct Professor of Informatics at Indiana University School of Informatics and the University of Athens School of Pharmacy.

His research spans many areas of computational chemistry and biology, including computer-assisted drug design, chemo- and bioinformatics, data mining, visualization, artificial intelligence and software engineering. He is the author of 80 scientific publications and book chapters, and co-inventor of 18 patents. He serves on the Editorial Boards of the *Journal of Chemical Information and Modeling*, *Molecular Informatics*, *Chemical Biology & Drug Design*, *Journal of Molecular Graphics and Modeling*, and *Molecular Diversity*, plus boards for several organizations. He frequently delivers invited lectures, serves as symposium organizer at national and international conferences, and participates in grant review boards. Source: <http://dimitris-agrafiotis.com/> (accessed 25 May 2013).

In Memoriam



Left: Josef Brandt and Anita Meurling. (Noordwijkerhout Meeting in 1990) Right: Wendy Warr and Josef Brandt.

Emeritus Prof. **Dr. Josef Brandt** died on 20th October 2012 in his hometown near Aachen, Germany, aged 77. He studied chemistry at the *Technische Hochschule Aachen* and received his PhD there in 1963. Afterwards he worked at the Max Planck Institute in Mülheim, spending one year in Canada.

From 1974 until his retirement in 2000 he was at the Technical University of Munich, working in Prof. Ivar Ugi's Computational Chemistry group. In 1981 he attained his habilitation for work on a hierarchical classification of chemical reactions. In his approach, which can only be applied to complete reactions, including all byproducts, the first level contains all reactions that follow the same electron redistribution pattern, with refinements using free valence electrons and atomic symbols of the reaction core and neighbouring atoms.

Later research looked at the stereochemistry of reactions and the automatic identification of the reaction core by using the minimal chemical distance approach. A program for the generation of unprecedented reactions was also based on his hierarchical classification.

Josef Brandt organized major conferences including the 1985 International Conference on Computers in Chemical Research and Education (ICCCRE) in Garmisch-Partenkirchen. He also initiated an exchange of academics with the Chinese Academy of Sciences in Shanghai. He did not like flying, and always went by train and ship to Shanghai. He once travelled to an American Chemical Society meeting on a Polish freight ship, returning to Europe on the QE2 luxury liner. He was very good at interpreting bureaucratic rules, and thoroughly enjoyed (and won) the subsequent dispute with the University administration over his travel expenses.

Written by Annette von Scholley-Pfab, Munich (one of Dr. Brandt's PhD students)
Submitted by John Barnard

CSA Trust Grant Call for Applications for 2014

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 currently inviting the submission of grant applications for 2014.

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. Grants will be awarded annually up to a maximum of a total combined value of ten thousand U.S. dollars (\$10,000). 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; e.g. for travel to collaborate with research groups, to attend a conference relevant to one's area of research, to gain access to special computational facilities, or to acquire unique research techniques in support of one's research.

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; 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. Three copies of the complete application document must be supplied for distribution to the Grants Committee.

Deadline for Applications: Applications must be received no later than March 13, 2014. Successful applicants will be notified no later than May 2, 2014.

Address for Submission of Applications: Three copies of the application documentation should be forwarded 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 blawlor@nfais.org prior to submission so that she can contact you if the e-mail does not arrive.

News and Announcements

Wiley acquires assets of FIZ Chemie Berlin

"On 16 January 2013, publisher John Wiley & Sons, Inc. has announced that it has acquired the assets of the FIZ Chemie Berlin, a provider of online database products for organic and industrial chemists. The acquisition aligns with the company's long-term strategy to support research, learning, and professional practice through high quality content and services. Wiley is expanding its presence in Berlin with the new venture providing roles for more than 30 skilled information professionals.

According to Steve Miron, Senior Vice President, Scientific, Technical, Medical and Scholarly, Wiley, the FIZ suite of databases and services are a great addition to Wiley's deep reservoir of chemical databases, journals, books and references. The FIZ products and services will enable Wiley to build a new generation of information products to help boost the productivity of chemists.

The products include the ChemInform weekly abstracting service and reaction database (CIRX), as well as the abstracting journal *Chemisches Zentralblatt*, the InfoTherm database of thermo-physical properties, and eLearning tools and services."

Source: Knowledgespeak <http://www.knowledgespeak.com/newsArchiveviewdtl.asp?pickUpID=17018&pickUpBatch=2117#17018>

New Developments in Chemical Information: 'Best Practice'

RSC CICAG (Royal Society of Chemistry Chemical Information and Computer Applications Group)

A one day course for information scientists, librarians, researchers and anyone with an interest in Chemistry consisting of a series of presentations providing an impartial and critical overview of Chemical Information products/services, given by specialists.

Date: 03 July 2013 10:00 – 16:30

Venue: Royal Society of Chemistry, Council Room, Burlington House, Piccadilly, London W1J 0BA

Ticket/Registration Information: RSC CICAG members £30; Non-members £40

Booking Form:

<http://www.rsc.org/ConferencesAndEvents/conference/downloadfile.cfm?fname=3rd%20july%202013%20booking%20form%20Edoc>

Contact: Dr Keith White, Chair, RSC CICAG;
Email: whitek@matthey.com

Includes:

- "SciFinder, the Chemical Search Tool for Scientists", Yvonne Pope, Regional Sales Manager, CAS
- "Thomson Reuters Markush Data Feed: A New Way to Search and Analyse Chemical Information from Patents", Brian Lerner, Product Specialist, Thomson Reuters
- "Bringing Data Together – the National Chemical Database Service and Other e-Science Developments at the RSC", Richard Kidd, Business Development Manager, RSC
- "Extracting Knowledge from Reactions: Developments from InfoChem", Stephanie North, Allyl Consulting Ltd; representing InfoChem in the UK
- "Innovative Patent Chemistry Workflows Using SureChemDirect", Elisabeth Piveteau, Sales Manager EMEA, SureChem/Digital Science
- "The RSC Virtual Library: What Do Our Members Want?", Sheena Elliott, Manager, Member Services, RSC
- "How Accelrys Plans to Address the Remaining Challenges in Structure Representation and Searching: Chemically Modified Biologics, Non-Specific Structures, and Organometallic Compounds", Keith Taylor, Advisory Product Manager, Accelrys

Report from the American Chemical Society Council Meeting Held on April 10, 2013

The Council of the American Chemical Society met in New Orleans, LA on Wednesday, April 10, 2013 from 8:00am until approximately 12:00pm in the Grand Ballroom A-C of the Hiltons New Orleans Riverside Hotel. The meeting opened with recognition of deceased Councilors and a moment of silence in their honor. The minutes of the prior Council meeting held in Philadelphia, PA were approved as was an interim action of the Council Policy Committee who had elected Carolyn Ribes as Vice-Chair. Below are highlights of and the results of actions that were taken at the meeting.

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) identified four nominees for the office of 2014 ACS President-Elect. They were as follows: G. Bryan Balazs, Charles E. Kolb, Jr., Carolyn Ribes, and Diane Grob Schmidt. The four nominees answered questions at the Town Hall meeting that was held on Sunday, April 7th, and each gave a three minute presentation at the Council meeting. By electronic ballot, the Council selected G. Bryan Balazs and Charles E. Kolb, Jr. as candidates for 2014 President-Elect. These two candidates, along with any candidates selected via petitions, will stand for election in the Fall National Election.

Other Elections

The Committee on Nominations and Elections announced the results of the election to select *candidates* from the list of *nominees* to serve as Directors from District II and District IV on the Board of Directors for the term 2014-2016. Nominees for District II included George M. Bodner, Jed F. Fisher, Alan A. Hazari, and Robert A. Pribush. Nominees for District IV included John P. Fackler, Jr., Rigoberto Hernandez, Larry K. Krannich, and John A. Whittle. By mail ballot, the Councilors from these districts selected George M. Bodner and Alan A. Hazari as District II candidates; and Rigoberto Hernandez and Larry K. Krannich as District IV candidates. Ballots will be mailed on or before October 10 to all ACS members in District II and District IV for election of a Director from each District.

The Committee on Nominations and Elections also announced the selection of the following candidates for Director-at-Large for a 2014 - 2016 term: Susan B. Butts, Thom H. Dunning, Jr., Dor-

othy J. Phillips, and Kathleen M. Schulz. The election of two Directors-at-Large will be conducted in the fall. Ballots will be mailed to the Council on or before October 10, 2013.

Two vacancies on the Committee on Committees were created by the election of Ingrid Montes to the ACS Board of Directors and the appointment of H.N. Cheng as chair of the Committee on International Activities. Prior to the New Orleans meeting, the Committee on Nominations and Elections presented to the Council the following slate of candidates for membership on the Committee on Committees beginning 2013: Christopher J. Bannochie, Arindam Bose, David Lohse and Jason Ritchie. Christopher J. Bannochie and Jason Ritchie were selected to fill three-year and one-year terms, respectively.

ACS Dues for 2014

Council voted to accept the recommendation from the Committee on Budget and Finance with regard to the 2014 membership dues (an increase of \$3.00 - from \$151 to \$154). The increases to ACS dues are based upon an escalator defined in the ACS Bylaws (Bylaw XIII, Section 3,a). The dues are calculated by multiplying the base (current) rate "by a factor which is the ratio of the revised Consumer Price Index for Urban Wage Earners and Clerical Workers (Service Category) for the second year previous to the dues year to the value of the index for the third year previous to the dues year, as published by the United States Department of Labor, with the fractional dollar amounts rounded to the nearest whole dollar".

Base rate 2013:	\$151.00
Change in the Consumer Price Index, Urban Wage Earners, Services Category:	
December 2012 CPI-W Services:	268.661
December 2010 CPI-W Services:	262.954
Change in CPI-W Index:	2.17%
2014 Dues, fully escalated: $\$151.00 \times 1.0217 = \154.28	
2014 Dues, Rounded:	\$154.00

Report from the ACS Council Meeting Held on April 10, 2013 continued

Change in Committees

The Committee on Committees (ConC) put forth a recommendation for the continuation of the committees that have been reviewed as required by the Committee Sunset Laws. The committees reviewed were the Committees on Chemical Abstracts Service, Environmental Improvement, and Younger Chemists. Council VOTED unanimously to continue these committees until their next evaluation. Continuation of these three committees requires Board concurrence.

Petitions for Vote

Petition to Amend National Election Procedures

After some discussion, a vote to approve the Petition to Amend National Election Procedures FAILED (85% against, 15% in favor). The petition sought to shorten the campaign period for candidates for President-Elect and to charge the Committee on Nominations and Elections (N&E) with proposing two candidates for President-Elect. Currently, N&E proposes four *nominees* from which Council selects two *candidates*. Other nominees, as now, would be put forth by members by petition, and procedures for preferential balloting would remain unchanged. All candidates would then be invited to a public forum, such as a Town Hall meeting, at the fall national meeting, and would appear on the ballot. This process would shorten the campaign period, allow all candidates to be seen by Council and other members, and ease the burden on N&E. However, under this petition, Council would no longer vote on a list of nominees. In collaboration with the Committee on Nominations and Elections, the Council Policy Committee authorized a joint task force on election timelines and procedures. This task force will examine the entire election system.

It should be noted that this change was not put forth by and was opposed by the Committee on Nominations and Elections.

Revision to Charter Bylaws for the International Chemical Sciences Chapters

The Committee on Constitution and Bylaws (C&B), in cooperation with the Committee on International Activities, asked Council to approve changes in the Charter Bylaws for the International Chemical Sciences Chapters. These changes are primarily in

the Amendments section, for C&B to review bylaw changes before proposed changes are approved by the membership of the chapter. Other changes are editorial. The Council VOTED to approve changes to the Charter Bylaws for New International Chemical Sciences Chapters.

Petition to Charter One new International Chemical Sciences Chapter

One legal application had been received for the formation of the Romanian International Chemical Sciences Chapter. It consists of the Territory of Romania which is not part of any other Local Section or Chapter of the Society. The application was signed by members in good standing of the Society who reside in the Territory. It met all of the requirements and included a proposed budget for the Chapter's operations (which includes no funding from the Society). The ACS Board has authorized this action and was seeking Council approval, after which (if given) the Chapter could begin operation. The Council VOTED, in concurrence with the Board of Directors, to approve the petition to charter the Romanian International Chemical Sciences Chapter, consisting of the Territory of Romania.

Approval of Academic Professional Guidelines

The Committee on Economic and Professional Affairs (CEPA) submitted for Council approval a revision of the Academic and Professional Guidelines. It contained updates to the current version which was last revised in 2008. This was a minor revision. A more extensive revision is underway and will be presented for Council consideration in 2014. This draft was presented for Council consideration in Philadelphia and has been approved by ACS legal Counsel. The Council VOTED to approve the Academic Professional Guidelines as submitted by the Committee on Economic and Professional Affairs. These guidelines apply to those members of the academic community whose job function impacts directly or indirectly on scientists practicing the profession of chemistry.

Report from the ACS Council Meeting Held on April 10, 2013 continued

Proposed Formula to Distribute the Local Section Allocation

The Committee on Local Section Activities (LSAC) proposed a new formula for the distribution of the Local Section Allocation beginning in 2014. The proposed formula replaces an existing formula that is not tied to the Local Section Allocation, but is instead expressed in dollar amounts that is adjusted upwards each year. The present formula is being replaced because distributions may soon exceed the Local Section Allocation. The new formula will use percentages. The total base allotment of 49% of the total local Section Allocation will be shared equally among all Local Sections. The per member allotment of 43% of the total Local Section Allotment will be divided by the total number of Local Section members and distributed based upon the number of members in a Local Section. The LSAC program funds of 8% of the total Local Section Allocation will be used to support Society initiatives, strategic planning, and Board directives. The Council VOTED to approve a new formula for the distribution of allocations to individual Local Sections beginning in 2014.

Re-alignment of Electoral Districts

At the 2012 fall meeting, Councilors called for a broader and long-lasting solution to requirements that Board electoral districts have parity in member populations. At this meeting, the Committee on Nominations and Elections reported on their discussions of a revised redistricting proposal which brings all six election districts within 400-1,000 members of the mid-point of the permissible range. This proposed action is designed to eliminate the need for frequent small changes for some time to come. The proposal will be up for vote at the fall Council meeting in Indianapolis.

Society Finances

The Committee on Budget and Finance reported on the current status of ACS' finances. Despite the sluggish economy, ACS generated favorable operating results in 2012. Total revenue was \$490.7 million, which was \$6.1 million or 1.3% greater than the approved budget, and 3.9% higher (\$18.6M) than 2011. The Net from Operations was \$20.2 million, or \$4.3 million favorable to budget. This was largely attributable to better-than-expected performance by ACS Publications and CAS, and represents

the Society's 9th consecutive year of positive operating results. While operating performance was favorable, Unrestricted Net Assets declined \$1.4 million to \$100.6 million:

Net from Operations:	\$20.2M
Investment Gains:	\$28.2M
Leadscope Expense:	(\$22.6M)
<u>Pension costs:</u>	<u>(\$27.2M)</u>
	(\$1.4M)

Finally, ACS ended the year in compliance with four of the five Board-established financial guidelines.

Member Statistics

Society membership at the end of 2012 was 163,322 - 893 lower than the total for year-end 2011 despite recruiting 24,943 new members. The net loss occurred primarily in the Regular, full member category. There was continued growth in both the Student Member undergraduate and international categories, which helped mitigate the overall decline in membership. The Membership Affairs Committee approved five pilot market data tests to increase membership.

Divisional Activities Name Change Request

The Divisional Activities Committee (DAC) received a request from the Division of Colloid and Surface Chemistry to change its name to the Division of Colloids, Surfaces and Nanomaterials. Six divisions have registered opposition to the proposed name, largely due to the use of the term 'nanomaterials.' DAC will ask Council to vote on the new name in Indianapolis, with a recommendation to approve.

Attendance Report

As of the morning of Council, the spring national meeting had a total of 15,596 attendees as follows:

Regular:	8,105
Guests:	347
Students:	5,793
Exhibitors:	946
Exhibit-only:	395

Report from the ACS Council Meeting Held on April 10, 2013 continued AND Themes for Future ACS National Meetings

Spring meeting attendance since 2004 is as follows:

2004: Anaheim, CA:	14,141
2005: San Diego, CA:	15,385
2006: Atlanta, GA:	12,546
2007: Chicago, IL:	14,520
2008: New Orleans, LA:	13,454
2009: Salt Lake City, UT:	10,668
2010: San Francisco, CA:	18,076
2011: Anaheim, CA:	14,047
2012: San Diego, CA:	16,864

(as of Tuesday, March 27th)

2013: New Orleans, LA: 15,596

(as of Wednesday morning, April 10th)

A total of 11,232 papers were presented.

Special Discussion Item

A special discussion item was put on the Council agenda for this meeting. ACS President Marinda Li Wu presented and moderated a discussion on "What else should ACS do to help members to thrive in the global chemistry enterprise?" ACS has established a strategic goal to "Empower an inclusive community of members with networks, opportunities, resources, and skills to thrive in the global economy." In support of this goal, President Wu commissioned a task force entitled, "Vision 2025: Helping ACS Members Thrive in the Global Chemistry Enterprise," to identify globalization opportunities and engage members in advocacy for improving the business and job climate. Following the presentation, 29 Councilors engaged in a robust discussion on what the Society currently offers or could offer to help members thrive in the global chemistry community.

Respectfully submitted May 10, 2013

CINF Councilor, Bonnie Lawlor

Themes for Future ACS National Meetings

The future of thematic programming at ACS meetings looks bright. More and more technical divisions organize symposia related to the theme of a meeting, often cosponsored by other divisions indicating the interdisciplinary nature of chemistry. We definitely have seen a strong upwards trend in the last few meetings. Below are the themes for future ACS national meetings (F=Fall, S=Spring):



F2013 *Chemistry in Motion* (Indianapolis)

S2014 *Chemistry and Materials for Energy* (Dallas)

F2014 *Chemistry and Global* (San Francisco)

S2015 *Chemical Resources: Extraction, Refining and Conservation* (Denver)

F2015 *A History of Innovations: From Discovery to Application* (Boston)

S2016 *Computers in Chemistry* (tentative) (San Diego)

F2016 *Chemistry and Education* (tentative) (Philadelphia)

S2017 *Water and Chemistry* (proposed) (San Francisco)

F2017 *Chemistry and Globalization* (proposed) (Washington)

By Guenter Grethe, CINF Representative to Multidisciplinary Program Planning Group

Excerpt reprinted with permission from the Chemical Information Bulletin 65 (2): Summer 2013.
<http://bulletin.acscinf.org/node/468>

News and Announcements



The Sixth Joint Sheffield Conference on Chemoinformatics, 22-24 July 2013.

The conference will be held at The University of Sheffield, UK. The meeting is sponsored by the Chemical Structure Association Trust and the Molecular Graphics and Modelling Society. The conference will be held at the Edge, and ensuite accommodation will be based in Endcliffe Village adjacent to the conference venue.

Session topics include: QSAR, Virtual Screening, Algorithmic Techniques, Drug Discovery, Representation and Visualisation, and Database Analysis. For more details and to register for the conference, please see <http://cisrg.shef.ac.uk/shef2013/>

Joint CINF-CSA Trust Symposium: Semantic Technologies in Translational Medicine & Drug Discovery

246th ACS National Meeting, Indianapolis, Indiana, September 8-12, 2013: CINF Division

The last few years have seen an explosion of public and proprietary healthcare and drug discovery data, and in parallel the emergence of powerful semantic, network and visualization technologies for integrating and mining these data. These novel datasets and technologies open up many possibilities for drug discovery and translational medicine, including drug repurposing, target identification, gene-disease association and patient population mapping. In parallel, major efforts are underway, such as the US NCATS at NIH, that support translational medicine and streamlined discovery of new medical therapies in the public sphere.

This session will showcase some of the challenges in this area and the ongoing research into semantics, drug discovery and translational medicine. We encourage papers to be submitted in this scope, in particular the following areas:

- Large scale integration of heterogeneous drug discovery data using semantic technologies
- Algorithms and methodologies that use semantic drug discovery and medical data
- Semantic technologies in scientific publication, including Nanopublication
- Efforts to use semantic technologies in the pharmaceutical industry

Presentations will be 25-30 minutes, including time for questions.

Organizers:

David Wild, Assistant Professor, Indiana University School of Informatics & Computing
(djwild@indiana.edu)

Jan Kuras, Publisher, Chemistry Central (jan.kuras@chemistrycentral.com)



CSA Trust website:
<http://www.csa-trust.org>

CSA Trust Brochure:
<http://www.csa-trust.org/files/CSATBrochure.pdf>

Newsletter Calendar for 2013

Spring Issue:

Submission Deadline: May 10
Review Copy: May 27
Publication Date: June 3

Fall Issue:

Call for Content: Aug. 2
Reminder: Sept. 4
Submission Deadline: Sept. 27
Review Copy: Oct. 4
Publication Date: Oct. 7

About the CSA Trust

The Chemical Structure Association Trust (CSA Trust) is an internationally recognized, registered charity which promotes education, research and development in the field of storage, processing and retrieval of information about chemical structures, reactions and compounds. Since 2003, it has incorporated the activities of the former Chemical Structure Association.

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