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Chemistry Division

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News from the Chemistry Division

Chemistry Division — William Armstrong, Chair

The Chemistry Division is concerned with chemistry and chemical technology, and the economics, educational advances, and information handling of developments in the field of chemistry and related subjects.

Let me begin this message by thanking all those who helped make this year's Chemistry Division programs at SLA Annual in Philadelphia a success. Among those instrumental in helping put together this year's event were the Planning Committee, consisting of Jim Martin and Mindy Peters; the Sponsorship Committee, with Teri Vogel, Loren Mendelsohn and Luray Minkiewicz; and the Professional Development Committee, headed by Ted Baldwin. In addition, as always, we had some wonderful volunteers who pitched in during the sessions in Philadelphia to make sure things ran smoothly and to report on activities. These included Louise Deis, Marty Rhine, Denise Callahan, Valerie Tucci, Theo Jones-Quarty, Mindy Peters, Meghan Gamsby, and Margarite Bower. There were others, as well, who graciously offered to assist in activities.

I would like to single out our teachers who always make the CE Courses such successful events and did a wonderful job in Philadelphia. This year's instructors were Judith Currano, Sue Cardinal, Denise Callihan, and Dawn French who, in various combinations, taught three separate courses, including a new one this year for advanced searchers entitled, Extreme Structure Searching. We had very good attendance at all three and are looking forward to offering another set of outstanding CE courses in Chicago.

We wish to thank our sponsors, without whom this conference would not be possible. We value our partnership with them, not just in these events, but throughout the year as we all work towards improving the production and dissemination of scholarly information through sharing of ideas, problems, and solutions. Our generous sponsors for this year's Annual were: ACS Publications; The Royal Society of Chemistry; Elsevier-Reaxys; Springer; Knovel; Chemical Abstracts Service; ASTM; IHS; John Wiley & Sons; and Global Language Translations and Consulting, Inc.

Our programs were well attended and sparked some good discussion. Summaries of some of these programs appear later in this newsletter. I would like to call your attention to the two awards that were presented at the Division's Business Meeting and Breakfast. One was the Sparks Award, presented to Courtney Hoffner; the other was the brand new Wiggins-Roth Award, bestowed upon Grace Baysinger from Stanford University. Please see the separate write-ups on these awards appearing in this edition of *SciTech News*.

Our sincere thanks go to Elsa Atson, who provided an excellent tour of the Chemical Heritage Foundation the final day of the conference. It is a fascinating place and Elsa and crew have done an excellent job in organizing and cataloging their extensive resources. If you have not toured the museum yet, by all means, do so next time you are in Philly. You won't regret it. (Additional note of interest to Division members: our archives are located there.)

Marie Fraties-Block, Chair-Elect, and Norah Xiao, Planning Committee Chair for 2012, are busy putting together another exciting program for next year's conference. If you have any ideas, suggestions, comments, please contact either Marie or Norah.

Other events/activities/items of interest:

Earlier this year a revision and update comprising the second edition of "Information Competencies for Chemistry Undergraduates: the elements of information literacy" was completed and is posted on the SLA Chemistry Division website (http://units.sla.org/division/dche/il/cheminfolit.pdf). Marion Peters spearheaded this effort, joined by Grace Baysinger and Cory Craig as co-editors. Members of the Division reviewed the document during its revision, providing helpful comments.

This second edition is a joint publication of the SLA Chemistry Division and the American Chemical Society Division of Chemical Information (CINF). We are indebted to Marion, Grace, and Chuck Huber for their efforts in securing the endorsement of ACS-CINF and look forward to more joint projects in the future.

Our web master, Linda Maddux, is currently hard at work developing a model for the Chemistry Division's new website which will use WordPress. The new site should offer better functionality and flexibility along with increased interactive capabilities, which we hope will make the site more useful and relevant to our membership in the coming years. We will keep you posted regarding progress and actual migration date.

Though final arrangements have not yet been completed, we do hope to hold another Fall web conference featuring the posters at the All Sciences Poster Session in Philadelphia. Announcements about this will be forthcoming as details are finalized.

As always, the Chemistry Division Board welcomes and encourages input and involvement from its membership. As thoughts occur to you about activities you feel the Division should be engaged in, or ways in which you would like to help, please contact me or any of the Board members (listed on web site). And be persistent! We all get bogged down in our regular job activities from time to time and so can't always respond immediately; and despite our best efforts, some things inevitably fall through the cracks. But we will do our best to help you get involved at whatever level of activity is possible for you.

I look forward to hearing from you and to bringing you updates regarding Division news as the year progresses. ❖

Bill Armstrong, Chair
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2011 Wiggins-Roth Award for Outstanding Service

Submitted by William Armstrong, Chair; and Cory Craig, Chair, Awards Committee

The SLA Chemistry Division was delighted to honor Grace Baysinger at the 2011 SLA Annual Conference as the first winner of the Wiggins-Roth Award for Outstanding Service. The Wiggins-Roth Award recognizes outstanding contributions to the field of chemical information and is named in honor of Gary Wiggins and Dana Roth. Not only was this the first time this award has been presented, but the recipient has the distinction of having been nominated by both individuals for whom the award is named, a singular honor and well deserved.

The presentation ceremony took place during the Chemistry Division's annual Business Meeting and Breakfast on June 14th. On behalf of the Chemistry Division, the Chair, Bill Armstrong, presented Grace with a check for $1,000 and a certificate of achievement. Assisting in the presentation was Dr. James Phimister, representing our generous sponsor for this award, Elsevier-Reaxys,

About the Award Winner

Grace is currently the head librarian at the Swain Library of Chemistry and Chemical Engineering at Stanford University. She began her career as a chemistry librarian in 1985, as the head of the University of Michigan, Chemistry Library.

Grace is known for her bright outlook, well-thought-out opinions, and significant contributions to academic libraries, chemical information, and chemical publishing. Throughout her career, Grace has developed significant contributions to chemical information reference, these include: web guides, tutorials, slides, and other materials. She has generously shared these materials with the larger community of chemical information professionals. The entire chemical information community has benefitted from Grace's effectiveness in making the case for changes and improvements in chemistry-related databases, software, and printed products.

Grace's contributions also include extensive service to American Chemical Society (ACS) including significant roles in the Chemical Information Division (CINF), National Chemistry Week, Chemists Celebrate Earth Day, and major ACS Committees including: ACS Joint Board-Council Committee on Chemical Abstracts Service (CCAS); Chair of the ACS Joint-Board Council Committee on Publications from 2005-2007 (member 2001-2009); and Chair of the Copyright Subcommittee from 2005-2009 (member 2001-2009). Grace was the first librarian to be appointed Chair of ACS JBCCP. She was awarded the Stanford University Marshall D. O'Neill Award in 1996, and the ACS CINF Meritorious Service Award in 2004.

Grace is one of only two U.S. librarians currently serving on the Editorial Board of XCITR (Explore Chemical Information Teaching Resources). Grace was nominated for this award by Gary Wiggins and Dana Roth. ❖

Grace Baysinger receives the Wiggins-Roth Award from Chemistry Division Chair William Armstrong.

2011 Marion E. Sparks Award for Professional Development

Submitted by Cory Craig, Chair, Awards Committee

The SLA Chemistry Division (DCHE) awarded the 2011 Marion E. Sparks Award for Professional Development to Ms. Courtney Hoffner at the 2011 SLA Annual Conference in Philadelphia.

Ms. Hoffner has been a librarian at the UCLA Science & Engineering Library since November 2010. She obtained her master's degree in Library Science from UCLA in 2008. DCHE presented Ms. Hoffner with a $1,500 check and award certificate to support her attendance at the 2011 SLA Annual Conference in Philadelphia.

The Sparks Award is named to honor Marion E. Sparks, a pioneering and influential chemistry librarian who worked at the University of Illinois from 1913 through 1929. ❖

Courtney Hoffner receives the
2011 Marion E. Sparks Award for Professional Development

2011 Marion E. Sparks Award for Professional Development 2011 Conference Report

Submitted by Courtney Hoffner, University of California, Los Angeles

With the help of the Marion E. Sparks Award for Professional Development, I enjoyed an informative and engaging SLA conference as a first-time attendee. This travel award allowed me to connect with colleagues, attend relevant conference sessions, and learn about innovative trends in science and academic librarianship.

My first SLA started off with the Sunday preconference CE course "Chemical Information Sources, Requests, and Reference" taught by Judith Currano (University of Pennsylvania) and Dawn French (Millennium Inorganic Chemicals Library). As a new chemistry librarian, this course gave me a great background in the basics of chemistry librarianship. I gained knowledge of the structure of chemical literature and channels of information used by chemists, learned techniques for chemical information retrieval, worked through examples of chemical information queries, and was introduced to substructure and sequence searching. After the preconference course, I took advantage of a few free hours to explore the city before the opening keynote speaker with lunch at the Reading Terminal Market and a trip to the Philadelphia Museum of Art, one of the largest art museums in the United States. My first day concluded with a thought-provoking keynote address by Thomas Friedman, Pulitzer Prize winner and columnist for the *New York Times*, where he spoke on the importance of creativity in a globalized society.

The next two days of the conference were filled with informative sessions that covered a range of topics that matched the diversity of my professional duties here at UCLA. I attended sessions ranging from library design and user experience to science visualization and collaboration. A few sessions that I particularly enjoyed included the spotlight sessions "Collaborations Across Disciplines" and "Design Thinking for Better Libraries." In the "Collaborations Across Disciplines" session, representatives from Mendeley, VIVO, BibApp, and Elsevier spoke about their efforts in developing collaborative tools for faculty and researchers. A few of these are open-source products that allow for researchers at an institution to connect with each other and also allow one to view scholarly communications and publications patterns within an institution. As a result of this session I have started conversations with my colleagues at UCLA about hosting a similar dynamic tool for our own faculty and researchers. In "Design Thinking for Better Libraries," Stephen Bell of Temple University gave an overview of design theories and emphasized how design thinking can be a catalyst for improving user experience in the library. A few ideas I learned from this session that I hope to explore further include how to create our libraries experiential brand statement, the totality of library user experience and how it all works together (e.g. the website, circulation, reference, the OPAC, etc.), and creating emotional user connections with the library.

A few other highlights of my SLA experience included the Chemistry Division Business Meeting and Breakfast and the All-Sciences Poster Session. At the Chemistry Division Business Meeting and Breakfast, I was exposed to my first professional association business meeting and most importantly it gave me the opportunity to connect with my chemistry librarian colleagues. I especially valued meeting my fellow UC and other California librarians. Everyone was welcoming and extended insightful advice. The All-Sciences Posters Session allowed me to catch a glimpse of cutting-edge trends in science libraries. I was especially interested in UC Irvine's pilot project on using QR codes in the stacks as the use of this technology in public service has been a topic of conversation here at UCLA. Not only did I take away ideas about how to connect users with e-books and mobile databases through the use of QR codes, but also was interested to learn about their techniques in promoting the service.

I am extremely grateful to the SLA Chemistry Division for this opportunity to attend the 2011 SLA Conference in Philadelphia. The conference proved to be an inspirational and educational experience. As my career as a science librarian grows I expect to participate more in the SLA organization and hope to see you all at future SLA conferences! ❖

Chemistry Division Conference Session Reports

Chemistry Division Academic Roundtable & Breakfast

Monday, June 13, 2011
Moderators: Sue Cardinal, University of Rochester; Linda Galloway, Syracuse University
Sponsor: ACS Publications

Reported by: Linda Galloway, Syracuse University

The DCHE Academic Roundtable was a well-attended and enjoyable event. After our stellar breakfast, we broke into discussion groups to talk about aligning library services with institutional needs. The discussion topics included: facilitating partnerships with chemistry faculty, InChi, Discovery platforms, embedded librarianship, budgetary concerns, e-books, mobile technologies and data curation.

After lively conversations and ample networking time, moderators Sue Cardinal and Linda Galloway wrapped up the Roundtable by asking a member of each group to briefly report on the topic discussed. All participants were then able to hear about the various discussion topics and learn about potential solutions. This program was a great start to the 2011 SLA Annual Conference.

Developments in Informatics

Tuesday, June 14, 2011
Moderator: William Armstrong, Louisiana State University
Division Sponsors: Chemistry; Physics-Astronomy-Mathematics; Sci-Tech Divisions
Vendor Sponsors: ACS Publications; ASTM International; IET Inspec; OSA – Optical Society of America

Reported by: Thurston Miller, University of Notre Dame

I. *Cheminformatics*

Dr. Steve Heller, Project Director of the InChI Trust spoke about InChI, the IUPAC International Chemical Identifier (InChI), which is a freely available, non-proprietary identifier for chemical substances that can be used in electronic data sources allowing easier linking of information from many different data compilations.

Dr. Heller explained that InChI was needed because there are too many existing and competing chemical identifiers from structure diagrams to connection tables (MolFiles, SMILES, etc.) to index names (IUPAC, CAS 9th CI Name, etc.) to index numbers (EINECS, Bielstein and CAS Registry Numbers, etc.). InChI offers the ability find existing information and data that is housed in diverse sources more easily and more accurately.

He estimated that 99% of the compounds indexed in computer databases can be described with InChI. However, there are some areas of chemistry that are not yet covered, such as Organometallics, Electronic States, Inorganics, and InChI for reactions (RInChI).

What are the advantages?

- Freely available and non-proprietary.
- More advanced and complete presentation of chemical information than other codes.
- Unambiguous, e.g., caffeine has one InChI and 172 SMILES.
- Indexed by major search engines such as Google (InChI Key).
- All the major structure drawing programs (ChemDraw, ISIS Draw, Jmol, etc.) now have the ability to generate an InChI. The standard InChI proved to be too long to easily search so InChI Key was created. The InChI Key is a shortened version of the standard InChI.

InChI Trust is a not-for-profit organization that oversees current and future developments. Organizations may decide to become dues paying members of the Trust thereby allowing them to influence the direction, priority, and speed of Trust activities. One can also become a non-paying supporter of the Trust. Contact Steve Heller for an application.

Presentation slides: http://www.hellers.com/steve/pub-talks/sla-6-11.pdf.

II. *Bioinformatics*

Dr. Diane Rein (University of Buffalo) spoke about Bioinformatics, beginning with a brief history of the field. In 1865, the field of Genetics was created and, in 1871, the field of DNA

was created. By 1950, the two separate fields were combined when Watson & Crick discovered the double-helix structure of DNA. GenBank was created in 1982 as a location for supporting material. The Human Genome Project was proposed at a workshop in 1985 and the projects started in 1990, ending in 2003. GenBank records are divided into many different databases.

Now there is a 1,000 Genomes Project that will sequence the genomes of a large number people to provide a resource on genetic variation. The information can be used to create personalized drugs for medical ailments. All of the data associated with these sequences is publicly available.

In addition, there has been an explosion in the amount of local data that needs to be managed. The NSF now requires a data management plan to be included in grant applications.

Who practices bioinformatics? – Biologists, Chemists, Physicists, Civil Engineers, Pathologists, Forensics, Biomedical, Psychologists, Anthropologists, etc.

Bioinformatics was done previously at the bench, but now it is being done at computers. It is a predictive information science that is discovery-driven. Someone searching databases is, in fact, doing research. As a result, it is easy for librarians to embed themselves in research groups. Bioinformatics librarians are divided into two groups – Researchers ('at the bench') and Bioinformaticians (creators of databases/ discovery tools).

Presentation slides: Unfortunately, Dr. Rein's presentation slides are not at the moment available due to externally imposed copyright restrictions.

III. *Astroinformatics*

Dr. Alberto Accomazzi (NASA Astrophysics Data System) spoke about Astroinformatics.

Astronomy is government funded. There is little to no commercial interest and the literature is published in behalf of non-profit societies.

"Astroinformatics is the formalization of data-intensive astronomy and astrophysics for research and education." (Kirk Bourne, et al. 2010)

The first conference in Astroinformatics, "Practical Semantic Astronomy," was February 2008 at Caltech.

We are at the beginning of a data deluge. The Sloan Digital Sky Survey released 49.5 terabytes of data to the public in January 2011. The Large Synoptic Survey Telescope is projected to create 15 petabytes (15,000 terabytes) of data when the survey is completed in 2015.

Fourth Paradigm: Data-Intensive Scientific Discovery by Jim Gray.

The fourth paradigm of discovery will be based on data mining and visualization. There is not enough bandwidth to transfer data to one location, so data processing will go to the data. The data archives are the "new telescope" and the software to mine the data can be called the "new instrument." Gray calls for the establishment of digital libraries and funding for the development of new authoring tools and publication models.

Some examples of digital libraries in astronomy include: ASD, Simbad, VAO in US, VizieR, Observatories.

Examples of authoring tools in astronomy are: Open Access (ScienceWISE), ArXiv curation workflow (CDS), Crowdsourcing (Galazy Zoo), VAO & Data Conservancy, VAO and ADS.

Data Curation and Libraries and Preservation Principles:

- Scientific research requires repeatability.
- The lifecycle of a research project should be documented by capturing all artifacts.
- Data, Processes, Results need to be properly described, accessible, and linked together.
- Provenance information should be attached to curated metadata throughout the process.

ADS Labs created an improved method for searching the literature using semantic interlinking concept. Some examples from the ADS beta search were shown.

Dr. Accomazzi's parting thought was that Librarians have a major role to play in the curation of metadata, both bibliographic and observational.

Presentation slides: (will be made available on

the Chemistry Division's web site

International Year of Chemistry: Perils and Promises of Modern Communication
Tuesday, June 14, 2011
Moderator: William Armstrong, Louisiana State University
Sponsors: ACS Publications; The Royal Society of Chemistry

Reported by: Louise Deis, Princeton University

The two speakers for this event were Dr. Lawrence Souder, Associate Professor of Communication; and Dr. Jean-Claude Bradley, Associate Professor of Chemistry and Learning Coordination for the College of Arts & Sciences. Both are professors at Drexel University.

Professor Souder spoke first, his talk entitled, "Rhetoric of Science: How to adapt messages to audiences." He gave several recently revealed examples of published scientific mistakes, shoddy research, or fraud and special interest (Vioxx). Grant writers have been known to withhold ideas. Double-blind studies have revealed discrimination against women authors/researchers. (He has compiled an extensive bibliography that is enlightening and will be made available on the Chemistry Division's web site.)

"Much of our knowledge rests on the trust in the ethics and morals of those practicing [science]." He gave examples of mistrust of peer review, and of retraction by a journal because the article was also published elsewhere. He mentioned the power of blogs, using the example of the panning of the "research" that erroneously made a case for the use of arsenic in place of phosphorus in a microbe.

Souder spoke of citizen (collaborative) science, and of Craig Venter, who had the wherewithal to sequence the human genome on his own – so to speak.

Trust is extremely important in science and in the communication of science for the benefit of society. How long does it take for errors to be purged? Perhaps misinformation can be corrected in less time than in the past, with such a proliferation of communication channels.

He is optimistic about the adoption of scientific networks and collaborations and the paradigms of open source, open access, and open peer review.

Talk: http://www.scivee.tv/node/31170

Slides: http://www.slideshare.net/jcbradley/souder-trust-in-science-sla-2011

Bibliography: will be made available on the Chemistry Division's web site.

Professor Bradley then spoke on "Trust in Science and Open Melting Point Collections," discussing the role of trust in science research, in scientific data, in day-to-day situations. He and his students from the Fall 2010 Chemical Information Retrieval class at Drexel performed a case study by compiling melting point data from several traditional trusted sources, including: CRC Handbook, Merck Index, chemical vendor catalogs, and peer-reviewed journals. They obtained 567 measurements for 24 compounds. Their faith in the "trusted sources", including SciFinder results, was, as a result, shaken: "No dataset was immune to errors." Peer review doesn't cover data. But technology is promising for the future. Wikipedia will become our new trusted source model.

Bradley's blog can be found at http://usefulchem.blogspot.com/2011/01/chemical-information-validation-results.html

Bradley is a pioneer in Open Notebook Science (ONS). Open Notebook Science is conducive to sharing data. ONS is defined in Wikipedia which also provides links to ONS resources. Resources from Bradley's ONS site can be found at http://usefulchem.wikispaces.com/All+Reactions.

See also: http://www.makeuseof.com/tag/started-open-notebook-science/ posted by Beth Ritter-Guth on March 8, 2010, "How To Get Started With Open Notebook Science."

Bradley quipped that there are "no facts in chemistry, only measurements embedded with assumptions." "Trust becomes proof." He urged the use of free hosted tools like Wikispaces and Google spreadsheets for calculations. Science will make faster progress with open resource collaboration on the web. "Make research transparent and discoverable," he said.

Presentation slides: http://usefulchem.blogspot.com/2011/06/my-talk-at-sla-on-trust-in-science-and.html

Chemistry Division Corporate Roundtable & Breakfast
Wednesday, June 15, 2011
Theme: "Communicating Value through Strategic Alignment."
Moderator: Mindy Peters, Carpenter Technology Corporation
Sponsors: The Royal Society of Chemistry; Global Language Translations and Consulting (GLTaC)

Reported by: Theo Jones-Quartey, W. R. Grace & Co.

This event was well attended and discussion was lively. Each of the three tables of participants was given a list of topics to discuss and report on.

Topic 1: How do you convey the relevancy of the library, its resources, and staff to your organization?

Table A: Constantly obtain feedback from customers. Recognize that people want self-service, they come in when they need help in using resources. Provide the right resources; teach/coach them how to use them and help with complicated searches. Become the go-to person. Use library branding (e.g., "brought to you by the library"). Make sure to show that the library has an input to the bottom line. It's a continuum of services and showing value.

Table B: Use professional seminars (with vendors) to promote services; also webinars, email announcements, library announcements on company websites, and work with library "champions" to spread the word. Use ROI studies (tracking usage/value over time), whitepapers, and case studies to demonstrate value.

Table C: Publish newsletters, annual reports (containing, mission, strategic plan, metrics/usage stats, and success stories), and use case studies.

Topic 2: Does the word "library" communicate the value of the services and quality of the library staff to your organization? How do you feel about name changes and the emerging trend of not using the term "library"?

Table A: It's up to us to change the perception of what the library is.

Table B: We have names other than "library" such as Research Information Services and North American Information Center. There is a decline in physical "library" space but we are still referred to as the "library." Knowledge or Resources in the name helps. Use of "Information," however, makes people think "IT." While we dislike the association, we must have rapport with IT to facilitate systems.

Table C: We have many names: RIC, Information Services, TIS, Knowledge Center, and also Library. We report into a variety of areas including Legal, IT and HR. The best is R&D.

Topic 3: How do you market services and resources to your organization? How are new databases and resources launched? How do you determine the target audience?

Table A: Use focus groups, training newsletters and bulletin board postings. Contact new employees by email; work with HR to provide them with library leaflets; present at orientations (some people are not included in their company orientations); and get in on sales/marketing meetings to make presentations. There is a need to get creative with email messages about library services; many users delete or do not pay attention to them and then seem ignorant about changes and training that has occurred.

Table B: Use of e-Readers with books on them. Concerns include limited access time and how to market this. The IT relationship is important to get prominence on the intranet.

Table C: Have email taglines, publish news features on the company website, and use survey tools.

Topic 4: Do metrics play a role in communicating your value? Do you utilize case studies? Which is more effective and what benefit does it bring?

Table A: Do a case study to show, for example, how you helped the R&D department accomplish XYZ. Use metrics to show you are contributing to the bottom line. Make sure your goals are in line with that of the company.

Table B: Capture metrics and success stories. Knovel did some case studies which can be used in your own marketing. Do anecdotal poll-

ing and usage reporting. Publishers are keen to get usage feedback to demonstrate the value of their products; share this with your customers.

Table C: Use metrics to justify value; ours and new products.

Topic 5: In public library circles there is often talk of running your library like a business. What about a corporate library? Is this also a business within a business? Do you charge for services? Do you offer any services to the public? Does this mentality help or hurt your library?

Table A: No discussion.

Table B: Yes, it is a business; market and track like a business for better metrics. Do not offer services to the public except for ILL.

Table C: Charge for services and obtain better metrics through tracking.

Topic 6: Where will corporate libraries be 10 years from now? Growing, closing, evolving? What is the future of this specialized environment?

Table A: The younger, tech-savvy generation tends to do their own research and only request assistance when they cannot find what they're looking for. They use IM even when only a few doors away.

Table B: Research now goes to China and may come back in 10 years.

Table C: Libraries are changing, shrinking in physical space but not going away. We are needed to acquire, manage collections – chemists do not want to do that. We need to become better at content management, vendor relations, enforcing policies. Vendors could profile libraries and highlight them in vendor marketing which can be used to promote users' support and enthusiasm. ❖