



### History of Chemistry Technical Division Administration Form 2011

Technical Division Administration Form - Governance	
1. Does the Division have a Vision and/or Mission Statement?*	<input checked="" type="radio"/> Yes <input type="radio"/> No
2. What was the date of the last Division long range/strategic planning session?*	4/7/2008
3. What are the primary challenges confronting your Division?*	We do not have enough volunteers to increase our programming options. We continue to work on options for programming at regional meetings as well as national meetings.
4. Were Division elections conducted according to its Bylaws?*	<input checked="" type="radio"/> Yes <input type="radio"/> No
5. Please indicate the elected positions filled	
i. Chair-Elect*	<input checked="" type="radio"/> Yes <input type="radio"/> No
ii. Secretary*	<input type="radio"/> Yes <input checked="" type="radio"/> No
iii. Treasurer*	<input type="radio"/> Yes <input checked="" type="radio"/> No
iv. Secretary /Treasurer*	<input checked="" type="radio"/> Yes <input type="radio"/> No
v. Councilor*	<input checked="" type="radio"/> Yes <input type="radio"/> No
vi. Alternate councilor*	<input checked="" type="radio"/> Yes <input type="radio"/> No
vii. Member-at-Large*	<input type="radio"/> Yes <input checked="" type="radio"/> No
Other Position Filled	
a. Were any positions of the Executive Committee left vacant last year?	<input type="radio"/> Yes <input checked="" type="radio"/> No
b. If 5a is YES, list the vacant positions	
6. What additional support do you need from DAC or ACS staff?	We believe that DAC or ACS staff should provide an option for e-voting.
7. What can DAC do to improve the Annual Review Process?	We have no specific recommendations.
8. Did you hold an Executive Committee meeting at one or both National ACS Meeting(s)?	<input checked="" type="radio"/> Yes <input type="radio"/> No

Technical Division Administration Form - Member Relations	
1. Did your total membership increase or decrease in 2011?*	Increase
2. Please indicate the approximate number of active volunteers in your Division.*	25
a. How did you get volunteers?*(Check all that apply.)	<input checked="" type="checkbox"/> E-mail <input checked="" type="checkbox"/> Website <input type="checkbox"/> Phone <input checked="" type="checkbox"/> Other- Bulletin for the History of Chemistry
3. Is your Division encountering difficulty in securing an adequate number of volunteers to run the Division?	<input type="radio"/> Yes <input checked="" type="radio"/> No
a. If the answer to 3 (above question) is YES, please explain the degree of the problem, and steps taken to address it.	
4. How does your Division recognize its volunteers?*(Check all that apply.)	<input checked="" type="checkbox"/> Certificates <input type="checkbox"/> Gift <input type="checkbox"/> Awards <input type="checkbox"/> Letter to employer <input checked="" type="checkbox"/> Recognition at an event <input type="checkbox"/> Other
5. How does your Division use its website to serve its members?*	The website allows us to notify members of current news and events. It is also the gateway to the Division journal, The Bulletin for the History of Chemistry. It serves as an active archive of Division business, including minutes, the current Exec. Committee and officers, upcoming symposia, and awards given.
6. When was your Division's website last updated?*	1/9/2012
7. How does your Division provide meeting content to its members?*(Check all that apply.)	<input checked="" type="checkbox"/> ACS Symposium Series publication <input type="checkbox"/> Webinars <input type="checkbox"/> Databases <input checked="" type="checkbox"/> Recorded meeting content <input checked="" type="checkbox"/> Other- meeting abstracts in newsletter
8. What are the most important benefits your Division provides to its members?*(Check all that apply.)	<input type="checkbox"/> Electronic balloting <input checked="" type="checkbox"/> Web access to programming <input type="checkbox"/> Career counseling <input type="checkbox"/> Wiki <input type="checkbox"/> Blogs <input checked="" type="checkbox"/> Other- Bulletin for the History of Chemistry
9. How does the Division provide information to its members on Divisional activities?	<input checked="" type="checkbox"/> Newsletter <input checked="" type="checkbox"/> Website <input checked="" type="checkbox"/> E-mail <input type="checkbox"/> Other Electronic Methods(Facebook, Twitter, etc.) <input checked="" type="checkbox"/> Meetings

Technical Division Administration Form - Programming	
1. In general, how would you assess the programming your Division delivered during 2011 ACS national meetings?*	Our division programmed several excellent symposia at both national meetings, including a symposium highlighting the centennial of the Gibbs Medal that was a fairly large draw for ACS members across several divisions. In addition, a new HIST Tutorial Series was added to the programming in 2011. The presentations in this ongoing series are slightly longer talks acting as a review tutorial on a historical subject to educate HIST members and the general ACS community on a historical topic of general interest. The topics of these tutorials are also aimed to align with thematic programming. The Division was asked by Immediate Past President Joe Francisco to add a historical segment to the <a href="http://acs.org/governance">acs.org/governance</a> section. This included listing all of the past ACS presidents plus starting the development of links for each on their life, career, and contributions. This website was introduced at a HIST symposium at the Fall Denver meeting. In addition, HIST and the Past President's funds supported a symposia at the Southwest Regional meeting in Austin TX. HIST also made both financial and programing contributions to a symposia at the Western Regional meeting in Pasadena CA on the Chemical History of California.
2. How far in advance does your Division plan its national meeting programming?*	<input type="radio"/> Less than 1 year <input type="radio"/> 1 Year <input checked="" type="radio"/> 2 Years <input type="radio"/> 3 Years <input type="radio"/> 4+ Years <input type="radio"/> Others
3. Do you have a Regional Meeting Coordinator for your Division?*	<input checked="" type="radio"/> Yes <input type="radio"/> No
a. If the answer to 3 (above question) is YES, provide contact information for your Division's Regional Meeting Coordinator.	
i. First Name	E. Thomas
ii. Last Name	Strom
iii. Phone	817-272-5441
iv. E-Mail	tomstrom@juno.com
b. Did someone attend a planning session last year?	<input checked="" type="radio"/> Yes <input type="radio"/> No
4. Do you have a Program Chair for your Division?*	<input checked="" type="radio"/> Yes <input type="radio"/> No
a. If the answer to 4 (above question) is YES, provide contact information for your Division's Program Chair.	
i. First Name	Seth
ii. Last Name	Rasmussen
iii. Phone	701-231-8786
iv. E-Mail	seth.rasmussen@ndsu.edu
b. Did someone attend a planning session last year?	<input checked="" type="radio"/> Yes <input type="radio"/> No
5. Do you have Multidisciplinary Program Planning Group (MPPG) Representative for your Division?*	<input checked="" type="radio"/> Yes <input type="radio"/> No
a. If the answer to 5 (above question) is YES, provide contact information for your Division's Multidisciplinary Program Planning Group (MPPG) Representative.	
i. First Name	Joe
ii. Last Name	Jeffers
iii. Phone	870-245-5216
iv. E-Mail	jeffers@obu.edu
b. Did someone attend a planning session last year?	<input type="radio"/> Yes <input checked="" type="radio"/> No

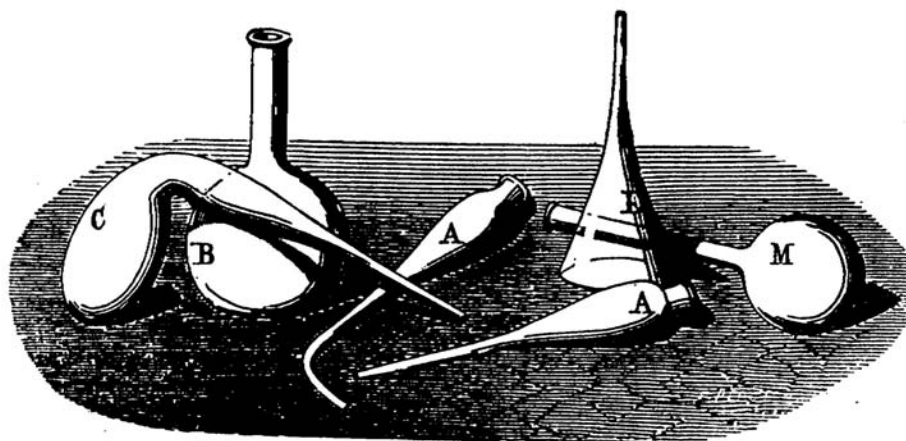
## Technical Division Administration Form - Supporting Materials

File Name	File Size	Brief Description
2011.pdf	0.02 MB	Quicken Summary 2011
HIST Spring 2011 Abstracts Program Only.pdf	0.34 MB	HIST Program and Abstracts Spring 2011
HIST Fall 2011 Abstracts Program Only.pdf	0.25 MB	HIST Program and Abstracts Fall 2011
HIST 2011 Annual Report - Financial.xls	0.25 MB	HIST Financial Report - Excel Version

---- END OF REPORT ----



American Chemical Society  
**DIVISION OF THE HISTORY OF  
CHEMISTRY**



**PROGRAM AND ABSTRACTS**

241<sup>st</sup> ACS National Meeting  
Anaheim, CA  
March 27-31, 2011

*S. C. Rasmussen, Program Chair*

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# HIST

## DIVISION OF THE HISTORY OF CHEMISTRY

Final Program, 241st ACS National Meeting, Anaheim, CA, March 27-31, 2011

S. C. Rasmussen, *Program Chair*

**BUSINESS MEETING:**  
**HIST Executive Committee Meeting, 5:00 pm:Sun**

### SUNDAY AFTERNOON

Disney's Paradise Pier – Redondo

#### General Papers

S. C. Rasmussen, *Organizer, Presiding*

**1:30**—Introductory Remarks

**1:35**—**1.** HIST Tutorial: Early history of metallurgy. **S. C. Rasmussen**

**2:15**—**2.** Materiapolymérica: Natural rubber. **G. D. Patterson**

**2:45**—Intermission

**3:00**—**3.** Chemistry in 1803: A living history outreach. **P. L. Rambo**

**3:30**—**4.** Edward Teller: Chemist, physicist, “Father of the hydrogen bomb”. **I. Hargittai**

**4:00**—**5.** Associates of Fred Sanger: Elizabeth Blackburn, Nobel Laureate 2009. **J. S. Jeffers**

### MONDAY MORNING

Disney's Paradise Pier – Redondo

#### Pioneers of Quantum Chemistry

E. Strom, *Organizer, Presiding*

A. Wilson, *Organizer*

*Cosponsored by COMP and PHYS*

**8:55**—Introductory Remarks

**9:00**—**6.** Free-electron model: From Otto Schmidt to John Platt. **W. B. Jensen**

**9:30**—**7.** George Wheland: Forgotten pioneer of resonance theory. **E. T. Strom**

**10:00**—**8.** Pioneering quantum chemistry in concert with experiment. **I. Hargittai**

**10:30**—Intermission

**10:45**—**9.** Michael J. S. Dewar: Quantum theory for organic chemists. **M. K. Holloway**

**11:15**—**10.** Molecular Orbital Theory for organic chemists. **A. Streitwieser**

**11:45**—**11.** H. C. Longuet-Higgins: Contributions to theoretical chemistry. **W. T. Borden**

## MONDAY AFTERNOON

Disney's Paradise Pier – Redondo

### Pioneers of Quantum Chemistry

E. Strom, *Organizer, Presiding*

A. Wilson, *Organizer*

*Cosponsored by COMP and PHYS*

**1:45— 12.**Atoms, molecules and bonds.**K. Ruedenberg**

**2:15— 13.** John Pople, the man and his science. **J. E. Del Bene**

**2:45— 14.**History of the Quantum Chemistry Program Exchange (QCPE).**V. V. Mainz**

**3:15—** Intermission

**3:30— 15.**Development of the ideas of orbital symmetry control. **R. Hoffmann**

**4:00— 16.** Golden years at Chicago (LMSS) and San Jose (IBM): Lessons that are relevant today. **P. S. Bagus**

**4:30 — 17.** Quantum chemistry: 1950 - 1960. **H. F. Schaefer**

## MONDAY EVENING

Anaheim Convention Center, Hall B

### Sci-Mix

S. C. Rasmussen, *Organizer*

**8:00 - 10:00**

**1.** See previous listings.

**18.** See subsequent listings.

## TUESDAY MORNING

Disney's Paradise Pier – Redondo

### What's In a Name? Histories of Units and Constants

C. Giunta, *Organizer, Presiding*

*Cosponsored by CHED and NTS*

**8:30—** Introductory Remarks

**8:35— 18.**Avogadro, his hypothesis, and his number.**C. J. Giunta**

**9:05— 19.**Redefinition of the kilogram and the mole.**P. F. Rusch**

**9:35— 20.**Faraday and his constant.**G. D. Patterson**

**10:05—** Intermission

**10:20— 21.** Radioactivity: Why becquerels? **P. J. Karol**

**10:50— 22.**Curie and Rutherford - Interplay of personalities and philosophies.**J. L. Marshall**, V. R. Marshall

**11:20— 23.** SI units on stamps: We've come a long way from fathoms and furlongs, baby! **D. Rabinovich**



## TUESDAY AFTERNOON

Disney's Paradise Pier – Redondo

### General Papers

S. C. Rasmussen, *Organizer, Presiding*

**2:00**— Introductory Remarks

**2:05**— **24.** Immunoassays: A historical perspective. **A. W. Coates**

**2:35**— **25.** Use of lead and its deadly consequences: A historical perspective. **T. L. Viaene**

**3:05**— Intermission

**3:20**— **26.** Chemical and petroleum industries of the Newtown Creek of the late 19<sup>th</sup> and early 20<sup>th</sup> centuries. **P. Spellane**, R. Michals

**3:50**— **27.** Materiapolymérica: Polystyrene. **G. D. Patterson**

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## Abstracts

### HIST 1: HIST Tutorial: Early history of metallurgy

*Seth C Rasmussen*<sup>(1)</sup>, *seth.rasmussen@ndsu.edu*, NDSU Dept. 2735, P.O. Box 6050, Fargo ND 58108-6050, United States. (1) Department of Chemistry and Biochemistry, North Dakota State University, Fargo ND, United States

It is difficult to think of modern technology without basic metal materials. However, prior to the development of smelting, the only known metallic species were primarily copper, silver, and gold, and even these were somewhat rare. In fact, the very word *Metal* originates from the Greek *metallan*, "to seek after". The extraction of metals from their ores did not begin until ~5,000 BC with the smelting of copper, a landmark moment in history. In contrast, the smelting of iron was a relatively late discovery due to the much higher temperatures required in comparison to that of copper. As a result, the history and technology of early metallurgy is also closely tied to the early history of the furnace and related pyrotechnology. An overview of the early history and chemistry of smelting, metals, and alloys will be presented.

### HIST 2: Materiapolymérica: Natural rubber

*Gary D Patterson*<sup>(1)</sup>, *gp9a@andrew.cmu.edu*, 4400 Fifth Avenue, Pittsburgh PA 15213, United States. (1) Department of Chemistry, Carnegie Mellon University, Pittsburgh PA 15213, United States

One of the most important substances that provided the vision to see forms of matter that could only be understood in terms of macromolecules is natural rubber. Its remarkable properties have been known for millennia. Serious scientific study of the purified tree sap was carried out in the 19<sup>th</sup> century by Faraday and others. Even in the absence of vulcanization (crosslinking by sulfur), stretched rubber becomes birefringent and shrinks upon rapid heating under tension. The empirical formula was established very soon after such procedures were widely known. Destructive distillation yielded isoprene. The scientific path that led from a view of natural rubber as a colloid formed from isoprene to a macromolecule of polyisoprene will be presented.

### **HIST 3: Chemistry in 1803: A living history outreach**

**Patricia L. Rambo**<sup>(1)</sup>, *patricia.rambo@mnsu.edu, Ford Hall, Mankato Minnesota 56001, United States. (1) Chemistry, Minnesota State University, Mankato, Mankato Minnesota 56001, United States*

I will describe my outreach efforts at area living history events. These events (called Rendezvous) occur year round in various locations throughout the country, and typically focus on the fur trade era (up to 1840) in the United States. During these events I portray a chemist named Wilhemina Buch, and present chemistry demonstrations to elementary students in a manner that is consistent with the chemistry that was known in the year 1803. I will describe my demonstrations as well as the research efforts into the activities. The challenge of doing chemistry from an 1803 perspective is to talk only about what was known at that time, and not talk about atomic theory, electrons, and elements that were not yet isolated. Additional challenges were acquiring period equipment and doing safe demonstrations while in period dress.

### **HIST 4: Edward Teller: Chemist, physicist, “Father of the hydrogen bomb”**

**Istvan Hargittai**<sup>(1)</sup>, *istvan.hargittai@gmail.com, P.O. Box 91, Budapest Budapest 1521, Hungary. (1) Hungarian Academy of Sciences and Budapest University of Technology and Economics, Hungary*

Edward Teller was a most influential, controversial, and brilliant scientist.\* Some of his contributions to chemistry have proved to be of long-lasting significant, including the determination of the rotation barrier in ethane, the BET equation, and the Jahn–Teller effect. Much of Teller's oeuvre was devoted to the defense of the United States. His contribution to the hydrogen bomb helped secure peace between the superpowers for decades. Other deeds, such as opposition to the nuclear test ban, belittling the consequences of fallout, his role in SDI, and his Machiavellian handling of human interactions greatly damaged his image. Whether by merit or default, he contributed to the victory of democracy and the demise of the Soviet Union.

\*I. Hargittai, *Judging Edward Teller: A Closer Look at One of the Most Influential Scientists of the Twentieth Century* (Amherst, NY: Prometheus, 2010)

### **HIST 5: Associates of Fred Sanger: Elizabeth Blackburn, Nobel Laureate 2009**

**Joe S. Jeffers**<sup>(1)</sup>, *jeffers@obu.edu, 410 Ouachita Street, Box 3786, Arkadelphia AR 71998, United States. (1) Chemistry, Ouachita Baptist University, Arkadelphia AR 71923, United States*

Elizabeth Blackburn shared the 2009 Nobel Prize in Physiology or Medicine "for the discovery of how chromosomes are protected by telomeres and the enzyme telomerase." Elizabeth is the third graduate student of Fred Sanger to be awarded a Nobel Prize. Fred Sanger himself is a two-time Nobel Laureate. The life and work of Elizabeth Blackburn will be presented.

### **HIST 6: Free-electron model: From Otto Schmidt to John Platt**

**William B. Jensen**<sup>(1)</sup>, *jensenwb@ucmail.uc.edu, ML 0172, Cincinnati OH 45221, United States. (1) Department of Chemistry, University of Cincinnati, Cincinnati OH 45221, United States*

The talk will trace the history of the application of the free-electron model to problems of chemical bonding and spectroscopy from the work of the German chemist, Otto Schmidt, in the late 1930s through that of John Platt and his associates at the University of Chicago in the 1960s. It will also address the issue of the nature and use of radically approximate models in both research and teaching.

## **HIST 7: George Wheland: Forgotten pioneer of resonance theory**

*E. Thomas Strom*<sup>(1)</sup>, *tomstrom@juno.com*, Box 19065, 700 Planetarium Place, Arlington TX 76019-0065, United States. (1) Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington TX 76019-0065, United States

George W. Wheland, although little remembered today, is forever linked to resonance theory through three seminal papers in the '30's coauthored with Linus Pauling and through his magisterial 1955 monograph "Resonance in Organic Chemistry." At Chicago Wheland carried out research on acids and bases while continuing to publish papers on resonance. Sadly, his scientific career ended long before his death because of his contracting neurological disease. This paper gives an overview of his career with emphasis on his influence on resonance theory.

## **HIST 8: Pioneering quantum chemistry in concert with experiment**

*Istvan Hargittai*<sup>(1)</sup>, *istvan.hargittai@gmail.com*, POBox 91, Budapest Budapest, Hungary. (1) Hungarian Acad. of Sci. and Budapest Univ. of Tech. and Economics, Budapest, Hungary

Computation and experiment perform best when they act in concert, and the quantum chemistry pioneers kept this in mind from the beginning. Linus Pauling discussed theory and experimental information in a concerted way. He deduced from theory that the peptide bond should be planar. The theory of resonance went through bumpy periods in the Soviet Union in the early 1950s and its proponents were made to suffer for their ostensibly succumbing to foreign decadent ideologies. For a while there was a great battle between the more eloquent VB and the more useful MO approaches. Charles Coulson showed the way to shift toward MO theory and applications. Thanks to John Pople, quantum chemistry has become an integral part of chemical research. He pointed the way to estimating the "experimental error" of calculations thus developing quantum chemistry computations to be an equal partner in the realm of all "physical" techniques.

## **HIST 9: Michael J. S. Dewar: Quantum theory for organic chemists**

*M. Katharine Holloway*<sup>(1)</sup>, *kate\_holloway@merck.com*, Bldg. 53F-301, West Point PA 19486, United States. (1) Department of Chemistry, Modeling, and Informatics, Merck Research Laboratories, West Point PA 19486, United States

Michael J. S. Dewar was one of the first organic chemists to apply quantum theory to organic chemistry problems. His studies in quantum chemistry under Charles Coulson and subsequent work with Robert Robinson, a famous organic chemist, rendered him uniquely qualified for this role.

While still a post-doctoral fellow at Oxford in 1945, he deduced the correct structure for stipitatic acid, which included the first 7-membered aromatic ring system for which he coined the term tropolone. In 1949, as a young professor at Queen Mary College, he published a revolutionary book, *The Electronic Theory of Organic Chemistry*, that attempted to introduce physical organic chemists to molecular orbital ideas. And in 1952, more than 10 years before the Woodward-Hoffman rules, he published a seminal series of six back-to-back papers in the Journal of the American Chemical Society which made the case for the use of molecular orbital, rather than resonance theory, arguments in the understanding of standard organic chemistry reactions. He is well-remembered for his vigorous debate on the mechanistic details of cycloaddition reactions and the structures of carbenium ions. However, Dewar is perhaps best known for his development in the '70s and '80s of the semi-empirical MO methods MINDO/3, MNDO, and AM1, which enabled quantitative molecular orbital computations on large organic molecules, including novel ions, organic reaction mechanisms, and even enzyme catalysis.

In addition to his professional achievements, Dewar was a splendid conversationalist who often espoused rather unorthodox views in order to stimulate discussion. He was also a wonderful storyteller and a

legendary host, along with his wife Mary (an English Tudor historian). He had many diverse interests outside of chemistry, from astronomy and geology to oriental cooking and science fiction novels.

### **HIST 10: Molecular Orbital Theory for organic chemists**

**Andrew Streitwieser**<sup>(1)</sup>, *astreit@berkeley.edu, Dept of Chemistry, Berkeley CA 94720-1460, United States. (1) Department of Chemistry, University of California, Berkeley CA 94720-1460, United States*

In 1931 Erich Hückel published his treatment of benzene with a method now generally referred to as the Hückel MO (HMO) method. He showed how cyclic arrays of 2, 6 and 10  $\pi$ -electrons form closed shells that provide enhanced stability. By the middle thirties he had applied his approach to other aspects of organic chemistry but thereafter did no further original work. Extensive theoretical and experimental work on his concepts was done by others. "Molecular Orbital Theory for Organic Chemists" was written a quarter century later and documented brilliant syntheses of new "4n+2" molecules as well as numerous applications of HMO theory to redox processes, aromatic substitution, carbocation and carbanion reactions, rearrangements, as well as "Frontier Orbital" perturbation approaches. The era reviewed was predominantly the chemistry of  $\pi$ -electrons but was followed shortly by various treatments of  $\sigma$ -electrons in what can now be recognized as the next era of quantum chemistry.

### **HIST 11: H. C. Longuet-Higgins: Contributions to theoretical chemistry**

**Weston T Borden**<sup>(1)</sup>, *borden@unt.edu, 1155 Union Circle #305070, Denton Texas 76203-5017, United States. (1) University of North Texas, United States*

During the quarter of a century between the publication in 1943 of H. C. Longuet-Higgins' paper, "The structure of the boron hydrides" (written when he was still an Oxford undergraduate), until he left chemistry in 1967 (to cofound the Department of Machine Intelligence and Perception at the University of Edinburgh), H. C. Longuet-Higgins was one of the world's most creative and insightful theoretical chemists. This lecture will describe some of the many contributions made by H. C. Longuet-Higgins to theoretical chemistry.

### **HIST 12: Atoms, molecules and bonds**

**Klaus Ruedenberg**<sup>(1)</sup>, *ruedenberg@iastate.edu, Osborn Drive, Ames Iowa 50011, United States. (1) Department of Chemistry and Ames Laboratory USDOE, Iowa State University, Ames Iowa 50011, United States*

Over the last two centuries, the concept of the atom has undergone significant modifications: from the hard corpuscle whose motions yield the gas pressure, to a thought model for explaining chemical reactions and properties, to the planetary orbits and then the standing waves of electrons around isolated nuclei and, finally, to the as yet poorly-understood wave mechanical electronic substructures that form around nuclei within molecules. Correspondingly challenging has been the elucidation of chemical bonding beyond numerical calculations. Understanding its physical *origin* is difficult due to the kinetic energy operating differently in wave mechanics than in classical mechanics. Unraveling the great *variety* of bonding interactions and their mixtures is difficult because it requires complex molecular energy analyses to identify *intrinsic* features that are transferable as well as interpretable. The quest for the wave mechanical understanding of atoms and bonds in molecules that was begun by R.S. Mulliken is still ongoing.

### **HIST 13: John Pople, the man and his science**

*Janet E. Del Bene<sup>(1)</sup>, jedelbene@ysu.edu, 116 Pinehurst Drive, SE, Warren Ohio 44484, United States. (1) Department of Chemistry, Youngstown State University, Youngstown Ohio 44555, United States*

Sir John A. Pople was the dominant theorist of the second half of the twentieth century. He and his work were given the ultimate recognition in 1998 when John was awarded the Nobel Prize in Chemistry. This talk will briefly outline his biography, but will focus primarily on his science as viewed through the eyes of his students and research collaborators.

### **HIST 14: History of the Quantum Chemistry Program Exchange (QCPE)**

*Vera V Mainz<sup>(1)</sup>, mainz@illinois.edu, 142B RAL, Box 34 Noyes, 600 S. Mathews Ave., Urbana IL 61801, United States. (1) School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana IL 61802, United States*

The Quantum Chemistry Program Exchange was formed in 1962 at Indiana University to distribute quantum chemistry codes. It is no longer active. This was a unique source for access to hundreds of computational chemistry/physics programs. The author will attempt to present a short history of this valuable resource.

### **HIST 15: Development of the ideas of orbital symmetry control**

*Roald Hoffmann<sup>(1)</sup>, rh34@cornell.edu, Cornell University, Baker Lab, Ithaca NY, United States. (1) Cornell University, United States*

A personal account will be given of my work with RB Woodward from 1964-1969 on the role of molecular orbitals in controlling the course of chemical reactions, the complex of ideas now known as the Woodward-Hoffmann rules.

### **HIST 16: Golden years at Chicago (LMSS) and San Jose (IBM): Lessons that are relevant today**

*Paul S. Bagus<sup>(1)</sup>, bagus@unt.edu, 1155 Union Circle #305070, Denton Texas 76203-5017, United States. (1) Department of Chemistry, University of North Texas, Denton Texas 76203-5017, United States*

Presentations at the 1959 Boulder conference on Molecular Quantum Mechanics showed the potential of rigorous non-empirical, *ab initio*, quantum chemical calculations to address and solve chemical problems. About 25% of the papers in the conference proceedings, published in Reviews of Modern Physics, were contributions from the Laboratory of Molecular Structure and Spectra, LMSS, directed by Roothaan and Mulliken, at the University of Chicago. During the 1960's several people from LMSS moved to Clementi's department at the IBM Research Laboratory in San Jose, California to continue the development and application of programs for the calculation of Hartree-Fock and correlated wavefunctions. Because of limitations of available computers calculations often had to be individually designed to contain the correct chemistry and still be computationally feasible. A selection of work from LMSS and IBM San Jose, whose ideas and concepts are relevant to the way we use and understand calculations today, will be reviewed.

### **HIST 17: Quantum chemistry: 1950 - 1960**

*Henry F. Schaefer<sup>(1)</sup>, fri@uga.edu, 1004 Cedar Street, Athens GA 30602, United States. (1) Center for Computational Chemistry, University of Georgia, Athens GA 30602, United States*

Although *ab initio* computational quantum chemistry produced virtually no predictions of chemical interest during the 1950's, an important foundation for future work was laid during this decade. Much of this fundamental computational research was carried out in the laboratories of Frank Boys in Cambridge

(England) and Clemens Roothaan and Robert Mulliken in Chicago. Other senior contributors to *ab initio* chemical theory during this period include Klaus Ruedenberg, Robert Parr, John Pople, Robert Nesbet, Harrison Shull, Per-Olov Löwdin, Isaiah Shavitt, Albert Matsen, Douglas McLean, and Bernard Ransil.

### **HIST 18: Avogadro, his hypothesis, and his number**

**Carmen J Giunta**<sup>(1)</sup>, *giunta@lemoyne.edu*, 1419 Salt Springs Rd., Syracuse NY 13214-1399, United States.  
(1) Department of Chemistry and Physics, Le Moyne College, Syracuse NY 13214-1399, United States

In 1811, Amedeo Avogadro published a proposal that reconciled John Dalton's atomic theory with Joseph-Louis Gay-Lussac's observations about the combining volumes of gases. Although Avogadro was not alone in this insight, his proposal did not win widespread acceptance for several decades. Today we call this hypothesis Avogadro's law, that equal volumes of gases under the same temperature and pressure contain equal numbers of molecules. Avogadro never had any idea of what that number is, but the number of fundamental entities in the SI base unit mole is now named after him. This presentation will touch on Avogadro's life, his hypothesis, and the constant named after him.

### **HIST 19: Redefinition of the kilogram and the mole**

**Peter F. Rusch**<sup>(1)</sup>, *PFRusch@aol.com*, 162 Holland Court, Mountain View CA 94040, United States. (1) Department of Chemical Information, Rusch Consulting Group, United States

The Avogadro constant permits chemists to connect the microscopic atomic world to the macroscopic world of the laboratory through the current definition of the mole relating mass to a number of entities. Proposed redefinitions of the kilogram and the mole and what they mean to the practice of chemistry will be reviewed.

### **HIST 20: Faraday and his constant**

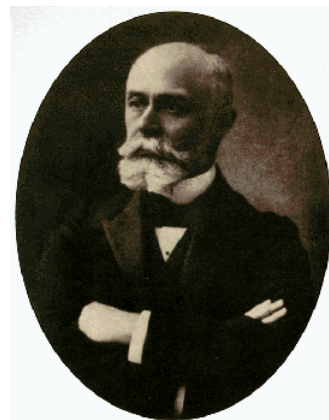
**Gary D Patterson**<sup>(1)</sup>, *gp9a@andrew.cmu.edu*, 4400 Fifth Avenue, Pittsburgh PA 15213, United States. (1) Department of Chemistry, Carnegie Mellon University, Pittsburgh PA 15213, United States

Studies at the Royal Institution established that Chemistry was inherently electrical in nature. Substances could be modified by subjecting them to electric current. What Davy initiated, Faraday completed. Faraday's Law of electrolysis established that there was a linear relationship between the mass of substance liberated by electrolysis and the amount of current that flowed. The constant of proportionality depends on the electric charge per mole of electrons, called the Faraday constant:  $F=96485.3399 \text{ C mol}^{-1}$ . The present paper will follow the details of Faraday's original research and trace how this fundamental finding was translated into a universally recognized constant of Chemistry. Full circle was achieved by Jean Perrin who showed that the Faraday constant is equal to the charge on a single electron (measured by himself and J.J.Thomson) times the Avogadro number (one of Perrin's lifelong passions).

### **HIST 21: Radioactivity: Why becquerels?**

**Paul J Karol**<sup>(1)</sup>, *pk03@andrew.cmu.edu*, Chemistry Department, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh PA 15213, United States.  
(1) Department of Chemistry, Carnegie Mellon University, Pittsburgh PA 15213, United States

The phenomenon of radioactive decay was discovered in the second half of the nineteenth century. With a migration to the SI system in the second half of the twentieth century, the unit for radioactive decay rate was cast as *becquerels* for “reasons of human safety”. I will retrace the trail of events leading up to the discovery of radioactivity and the intriguing role of Henri



Becquerel's scientific family in this fascinating and influential spectacle of nature.

## **HIST 22: Curie and Rutherford - Interplay of personalities and philosophies**

**James L Marshall**<sup>(1)</sup>, [jimm@unt.edu](mailto:jimm@unt.edu), 1155 Union Circle, Denton TX 76203-5017, United States; Virginia R Marshall<sup>(1)</sup>. (1) Department of Chemistry, University of North Texas, Denton TX 76203, United States

The rutherford and the curie are two units measuring radioactive decay, named for Ernest Rutherford (1871-1937) and Marie Curie (1867-1934), whose investigative work, perhaps above all others, elucidated the nature of this phenomenon. In this presentation a historical account will be made of the interplay and evolution of the differing scientific thinking of scientists in Great Britain and on the Continent, as exemplified by the research of these two scientists and their colleagues, as an understanding of radioactivity matured in the first quarter of the twentieth century.

## **HIST 23: SI units on stamps: We've come a long way from fathoms and furlongs, baby!**

**Daniel Rabinovich**<sup>(1)</sup>, [drabinov@uncc.edu](mailto:drabinov@uncc.edu), 9201 University City Boulevard, Charlotte North Carolina 28223, United States. (1) Department of Chemistry, The University of North Carolina at Charlotte, Charlotte North Carolina 28223, United States

The International System of Units (SI) is the most widely used array of units of measurement and is internationally recognized as the standard metric system. Playing a key role in commerce and science, it relies on the use of seven base units (meter, kilogram, second, ampere, kelvin, mole, candela) that are often associated with prefixes to indicate multiples or submultiples of a given quantity. This presentation will feature some highlights of the history of the development of the International System of Units, as illustrated on postage stamps and other postal matter. Philatelic vignettes of a number of derived SI units (newton, hertz, coulomb, volt, tesla, etc.) and their scientific namesakes will also be included in this presentation.



## **HIST 24: Immunoassays: A historical perspective**

**Andrew W Coates**<sup>(1)</sup>, [awcoates@ucdavis.edu](mailto:awcoates@ucdavis.edu), One Shields Ave, Davis California 95616, United States. (1) Environmental Toxicology, University of California, Davis, Davis CA 95616, United States

Many fondly remember the 1950s for poodle skirts, chocolate malts, and Adlai Stevenson's numerous runs for the Presidency. However, another fashionable trend at this time was the immunoassay, the highly useful and adaptive technique for bioanalysis. It was at this time that Rosalyn Yalow and Solomon Berson started their groundbreaking work in immunoassay. For this work they were awarded the Nobel Prize in the 1970s, garnering the headline referring to Yalow, "She Cooks! She Cleans! She Wins the Nobel Prize!" This is just one example of the relevance of immunoassay throughout history. From the turn of century to the culmination of biotechnology and the rise of nanotechnology, immunoassay has played a significant role in scientific understanding and is still growing strong today. As such, this presentation will analyze immunoassay through a historical perspective. Over the years, immunoassay has earned much international esteem and this nostalgic look at the history of immunoassay is sure to be a great way to celebrate the International Year of Chemistry.

## **HIST 25: Use of lead and its deadly consequences: A historical perspective**

*Tajae L. Viaene<sup>(1)</sup>, tajae.l.viaene@ndsu.edu, NDSU Dept 2735, P.O. Box 6050, Fargo ND, United States. (1) North Dakota State University, United States*

Lead is one of the earliest metals known to man and its uses throughout history are vast. Lead has been an additive in household products such as cosmetics, paints, and pottery. Interestingly, the latin word for lead, *plumbum*, has coined the word “plumbing” because of the use of lead in the vast network of pipelines that kept the cities of the Roman Empire supplied with water. From its uses in alchemy, to additives in food and wine by the Romans, and the content of lead in gasoline, lead has had significant impact on society. Today, knowledge of the toxic effects of lead ingestion have led to a number of changes such as its removal in household paints and products, along with the implementation of unleaded fuel in automobiles. A historical survey of the uses and toxicity of lead will be discussed.

## **HIST 26: Chemical and petroleum industries of the Newtown Creek of the late 19<sup>th</sup> and early 20<sup>th</sup> centuries**

*Peter Spellane<sup>(1)</sup>, pspellane@citytech.cuny.edu, 300 Jay Street, Brooklyn New York 11201, United States; Robin Michals<sup>(2)</sup>. (1) Department of Chemistry, New York City College of Technology (CUNY), Brooklyn New York 11201, United States (2) Department of Advertising Design and Graphic Arts, New York City College of Technology (CUNY), Brooklyn New York 11201, United States*

The Newtown Creek, a channel-like body of water located near the center of New York City, became in the 19<sup>th</sup> century one of the most important petroleum refining and chemical production sites in the US. In this talk, we employ period maps, photographs, and accounts of then-current technical and business practices to inform descriptions of the chemical technologies practiced along the Newtown Creek and the technical and environmental impact of these practices. In September 2010, The U.S. Environmental Protection Agency (EPA) added Newtown Creek to its Superfund National Priorities List of the country's most hazardous waste sites. This talk will focus on several significant technologies practiced at the Newtown Creek from 1870 through the mid-20<sup>th</sup> century and emphasize the technical and commercial interactions between industrial entities along the Creek. These technical and commercial realities provide background for understanding the recent EPA NPL designation.

## **HIST 27: Materiapolymérica: Polystyrene**

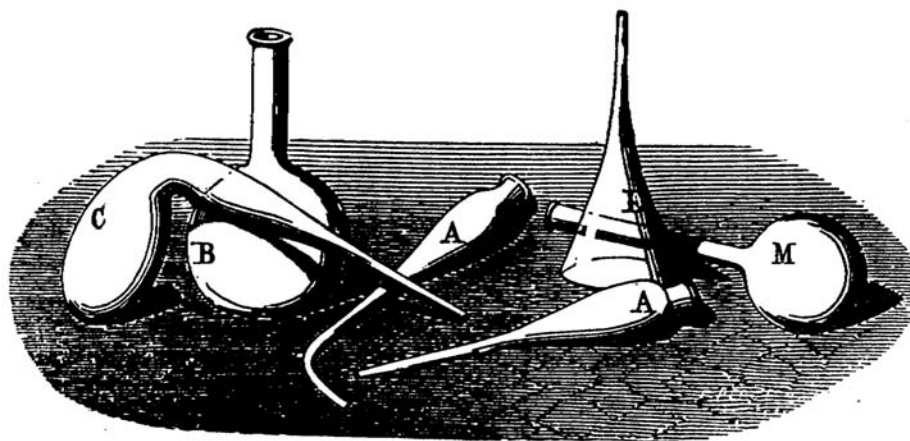
*Gary D Patterson<sup>(1)</sup>, gp9a@andrew.cmu.edu, 4400 Fifth Avenue, Pittsburgh PA 15213, United States. (1) Department of Chemistry, Carnegie Mellon University, Pittsburgh PA 15213, United States*

Tree sap has provided humankind with interesting materials from antiquity. Storax resin was widely available in the 19<sup>th</sup> century. It was noticed that it spontaneously resinified under heating. Early experiments by Berthelot examined the “polymerization” of the active ingredient in Storax resin: styrene. As the theory of chemical structure developed, there was an effort to place styrene within its proper chemical context. The present paper will trace the history of the conceptualization of the resinification of styrene. It will also present the history of the concepts necessary to understand polystyrene as a stereotactic molecule. The geometric description and understanding of polystyrene conformation will also be followed. All these concepts were extant long before polymer science was a coherent field of study.





American Chemical Society  
**DIVISION OF THE HISTORY OF  
CHEMISTRY**



**ABSTRACTS**

242<sup>nd</sup> ACS National Meeting  
Denver, CO  
August 28 - September 1, 2011

*S. C. Rasmussen, Program Chair*

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# HIST

## DIVISION OF THE HISTORY OF CHEMISTRY

Final Program, 242nd ACS National Meeting, Denver, CO, August 28 - Sept 1, 2011

S. C. Rasmussen, *Program Chair*

**BUSINESS MEETING:**  
**HIST Executive Committee Meeting, 5:00 pm: Sun**

### SUNDAY MORNING

Colorado Convention Center – Four Seasons BR 4

#### **Empowering Tomorrow's Science Super Heroes (PRES)**

*Cosponsored by ANYL, BMGT, CHED, CINF, COMSCI, FUEL, GEOC, HIST, I&EC, INOR, MEDI, PHYS, PROF, and YCC*

### SUNDAY AFTERNOON

Sheraton Denver – Terrace

#### **Gibbs Medal Centennial**

K. Fivizzani, *Organizer, Presiding*

*Cosponsored by COLL, COMSCI, I&EC, INOR, ORGN, PETR, and PHYS*  
*Financially supported by Chicago Local ACS Section*

**1:00** — Introductory Remarks.

**1:05** — **1.** History of the Gibbs Medal and selection process. **K. P. Fivizzani**

**1:30** — **2.** Josiah Willard Gibbs – Genius of science and mathematics. **K. S. Kostecka**

**1:55** — **3.** Fuel from sunlight and water. **H. Gray**

**2:25** — Intermission.

**2:40** — **4.** DNA-mediated signaling. **J. K. Barton**

**3:10** — **5.** Irreproducibility in the scientific literature: How often do scientists tell the whole truth and nothing but the truth? **R. G. Bergman**

**3:40** — **6.** Three-cornered hat. **J. M. Thomas**

**4:10** — **7.** My life with LIF. **R. N. Zare**

Colorado Convention Center – Four Seasons BR 4

#### **Science on the Hollywood Screen (PRES)**

*Cosponsored by ANYL, BMGT, CHED, CINF, COMSCI, FUEL, GEOC, HIST, I&EC, INOR, MEDI, PHYS, PROF, and YCC*

## MONDAY MORNING

Sheraton Denver – Terrace

### General Papers

S. C. Rasmussen, *Organizer, Presiding*

**7:45 — 8.** HIST tutorial: Gases of the atmosphere. **C. J. Giunta**

**8:25 — 9.** Fifty years of Vaska's compound. **R. U. Kirss**

**8:55 — 10.** 80 Years of terpyridine chemistry. **A. Winter**, G. R. Newkome, U. S. Schubert

**9:25 — 11.** Extroverted confusion – Linus Pauling, Melvin Calvin and porphyrin isomers. **M. O. Senge**

**9:55 —** Intermission.

**10:10 — 12.** John William Baker and the development of the Baker-Nathan effect. **M. D. Saltzman**

**10:40 — 13.** Arnaldo Piutti and the discovery of enantioselectivity in receptor-mediated biological activity. **J. Gal**

**11:10 — 14.** Early 20<sup>th</sup> century opinion on engineering training for chemistry undergraduates. **R. A. Egolf**, P. A. Khoury

**11:40 — 15.** Inner meanings of physical chemistry: Understanding the atom and nuclear reactions. **A. Galadari**

## MONDAY AFTERNOON

Sheraton Denver – Terrace

### Gibbs Medal Centennial

K. Fivizzani, *Organizer, Presiding*

*Cosponsored by COLL, COMSCI, I&EC, INOR, ORGN, PETR, and PHYS*

*Financially supported by Chicago Local ACS Section*

**1:30 — 16.** Developments in field of electron and related transfers - now and then. **R. A. Marcus**

**2:00 — 17.** Reactions at surfaces: Delving below and beyond. **S. T. Ceyer**

**2:30 — 18.** Gibbs Medal Award. Galloping cyclohexane conformations. **J. D. Roberts**

**3:00 —** Intermission.

**3:15 — 19.** Molecular recognition of DNA by small molecules, a historical perspective. **P. B. Dervan**

**3:45 — 20.** Ionic reactions and solvation. **J. I. Brauman**

**4:15 — 21.** Structure property relationships in molecular wires. **R. Breslow**

Sheraton Denver – Beverly

### Gibbs Medal Centennial Reception

**4:45 - 6:30**

## MONDAY EVENING

Colorado Convention Center – Hall D

### Sci-Mix

S. C. Rasmussen, *Organizer*

**8:00 - 10:00**

**8, 9, 14.** See previous listings.

**33.** See subsequent listings.

## TUESDAY MORNING

Sheraton Denver – Terrace

### IYC'11: A Philatelic Celebration

R. Hill, *Organizer*

D. Rabinovich, *Organizer, Presiding*

*Cosponsored by CHED*

**8:30** — Introductory Remarks.

**8:35** — **22.** Chemical philately: Classroom applications. **M. A. Morgan**

**9:05** — **23.** The Joseph Priestley House; A philatelic remembrance. **J. B. Sharkey**

**9:35** — **24.** Gibbs, thermodynamics, visualization - all for just 37 cents! **K. R. Jolls**

**10:05** — Intermission.

**10:20** — **25.** Chemical philately and the story of the quantum. **C. Lang**

**10:50** — **26.** Curie semipostal stamps of 1938. **R. Hill**, D. Rabinovich

**11:20** — **27.** Aluminum on stamps: A tribute on the 125th anniversary of the Hall-Héroult process.

**D. Rabinovich**

## TUESDAY AFTERNOON

Sheraton Denver – Terrace

### Profiles of Past ACS Presidents

J. Francisco, *Organizer*

J. Hayes, *Organizer, Presiding*

*Cosponsored by PRES*

**2:00** — Introductory Remarks.

**2:05** — **28.** Why does ACS need an accessible history of its presidents? **J. S. Francisco**

**2:30** — **29.** What does an ACS president do besides pontificate? **W. F. Carroll**

**2:55** — **30.** Who were the first ACS Presidents? **P. L. Perez**

**3:15** — Intermission.

**3:30** — **31.** Anna J. Harrison: After 102 years, the first ACS woman president. **L. P. Eubanks**

**3:55** — **32.** Reflections on the ACS presidents at the end of the 20th century. **B. E. Bursten**

**4:20** — **33.** Do you want to know more about the ACS presidents? Select [acs.org](http://acs.org) instead of Wikipedia? **J. M. Hayes**

**4:45** — Reception.

## **ABSTRACTS**

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### **HIST 1: History of the Gibbs Medal and selection process**

**Kenneth P Fivizzani**<sup>(1)</sup>, *kfivizzani@wowway.com*, 4251 Colton Circle, Naperville IL 60564, United States. (1) ACS Chicago Local Section, United States

In May 2011, the 100<sup>th</sup> Willard Gibbs Medal was presented to a scientist “who because of eminent work in and original contributions to pure or applied chemistry, is deemed worthy of special recognition by the jury.” The list of recipients is a who's who of chemistry. Each recipient is selected by the Jury of the Willard Gibbs Medal, which consists of twelve members elected from the ACS. Bylaw XV of the Chicago Section Bylaws contains the rules for the Gibbs Medal selection process and the presentation of the medal. The selection process begins each year on July 1; the Chair-elect of the Chicago Section is the Chair of the Jury through the presentation of the award.

### **HIST 2: Josiah Willard Gibbs – Genius of science and mathematics**

**Keith S KostECKA**<sup>(1)</sup>, *kkostECKA@colum.edu*, 600 S. Michigan Avenue, Chicago Illinois 60605, United States. (1) Department of Science and Mathematics, Columbia College - Chicago, Chicago Illinois 60605, United States

Josiah Willard Gibbs (1839-1903), best known for his work in chemical thermodynamics and physical chemistry, was also well known for his accomplishments in physics and mathematics. These achievements were throughout his life in: his early years; young adulthood and also his senior years. Gibb's formative years were centered on Hopkins Grammar School and Yale University where he graduated from in 1858 with honors in mathematics. His young adult years saw Gibbs complete his Ph.D. in engineering, tutor at Yale and then go to Europe to study chemistry and thermodynamics. From 1873 to 1878 Gibbs, back at Yale as a professor of mathematical physics, published a series of papers where he applied thermodynamics to interpret physicochemical phenomena. Gibb's senior years saw him develop vector analysis and further the development of statistical mechanics. He also won the Copley Medal in 1901; in the years following his death there would be many honors.

### **HIST 3: Fuel from sunlight and water**

**Harry Gray**<sup>(1)</sup>, *hbgray@caltech.edu*, 1200 E Calif Blvd, Pasadena California 91125, United States. (1) Department of Chemistry, California Institute of Technology, Pasadena California 91125, United States

We are working on rugged light absorbers and catalysts made from Earth abundant materials that have the potential to split water as efficiently as natural photosynthesis. We have recruited hundreds of students to join a Solar Army whose mission is the discovery of brand new metal-oxide catalysts for solar water splitters.

### **HIST 4: DNA-mediated signaling**

**Jacqueline K. Barton**<sup>(1)</sup>, *jkbarton@caltech.edu*, 1200 E. California Blvd., Pasadena CA 91125, United States. (1) Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena CA 91125, United States

DNA charge transport chemistry provides an opportunity to carry out redox chemistry at a distance. Many experiments have now shown that DNA-mediated charge transport can arise over long molecular distances but in a reaction that is exquisitely sensitive to perturbations in the DNA base stack. Studies are described to characterize biological roles for DNA charge transport. This chemistry may be used advantageously within the cell in long range signaling to DNA-bound proteins, both to regulate transcription and to activate DNA repair under conditions of oxidative stress.

## **HIST 5: Irreproducibility in the scientific literature: How often do scientists tell the whole truth and nothing but the truth?**

**Robert G Bergman**<sup>(1)</sup>, [rbergman@berkeley.edu](mailto:rbergman@berkeley.edu), Latimer Hall #1460, Berkeley CA 94720-1460, United States . (1) Department of Chemistry and Chemical Sciences Division, University of California, Berkeley and Lawrence Berkeley National Laboratory, Berkeley, Berkeley CA 94720-1460, United States

This lecture will address reports of scientific misconduct that have appeared in recent years, as well as other issues of scientific ethics, from the point of view of an active worker in synthetic organic and inorganic chemistry. After a discussion of primary scientific fraud, such as plagiarism and data fabrication, the general question of scientific data reproducibility will be considered. The talk will assess the level of reproducibility of most research in the synthetic chemical literature, and then focus on two journals, Organic Synthesis and Inorganic Synthesis, which are among the only organs that provide a source of direct information about irreproducibility. The talk will consider the question of whether trying to insure reproducibility necessarily acts as an effective means of protecting science from fraud, and will close by consideration of other ethical issues: “semi-fraud”, the conscious and unconscious manipulation of data, how experimenters manipulate data (and how it manipulates experimenters), ethical problems in peer review, and ethics in interpersonal scientific behavior.

## **HIST 6: Three-cornered hat**

**John Meurig Thomas**<sup>(1)</sup>, [jmt2@cam.ac.uk](mailto:jmt2@cam.ac.uk), CB2 3QZ, Cambridge Cambridge, United Kingdom . (1) Department of Materials Science, University of Cambridge, Cambridge CB2 3QZ, United Kingdom

A whirlwind account is to be given of: the popularization of chemical science, seen vicariously through the eyes of Davy and Faraday; the essence and applicability of single-site heterogeneous catalysts (SSHC); and revolutionary advances in chemical electron microscopy. The thoughts, actions and styles of Humphry Davy and Michael Faraday, two contrasting geniuses, speak to us down through the ages. SSHCs offer a strategy for the design of powerful new catalysts well suited to manufacture commodity-scale and fine chemicals in an environmentally responsible manner. The modern high-resolution electron microscope is arguably one of the single most powerful instruments that the chemist has at his or her disposal.

## **HIST 7: My life with LIF**

**Richard N. Zare**<sup>(1)</sup>, [zare@stanford.edu](mailto:zare@stanford.edu), Department of Chemistry, Stanford CA 94305-5080, United States . (1) Stanford University, United States

Laser-induced fluorescence (LIF) offers many advantages. It gives a bright signal against a dark background enabling detection limits to be pushed to that of a single molecule. LIF permits preparation of a well-defined excited states whose properties — radiative and collisional — can be studied in great detail. It allows probing of molecules in extremely hostile environments, such as flames, arcs, and sparks. LIF can also be used in other amazing ways, from sorting cells, one at a time, to sequencing the human genome. I will present a personal account of my own work with LIF, beginning with the birth of the laser.

## **HIST 8: HIST tutorial: Gases of the atmosphere**

**Carmen J Giunta**<sup>(1)</sup>, [giunta@lemoyne.edu](mailto:giunta@lemoyne.edu), 1419 Salt Springs Rd., Syracuse NY 13214-1399, United States. (1) Department of Chemistry and Physics, Le Moyne College, Syracuse NY 13214-1399, United States

Once upon a time, air was considered an element by those astute enough even to realize that it was matter. In the 18th century, it became apparent that air was actually a mixture of distinct "airs" (or gases to use the modern term). This presentation will focus on how the major components of the atmosphere came to be characterized and recognized as separate substances. It will include all of the most abundant components of

dry air and a few trace gases as well. Attention will be focused on, but not limited to, the pneumatic chemists of the 18th century.

## HIST 9: Fifty years of Vaska's compound

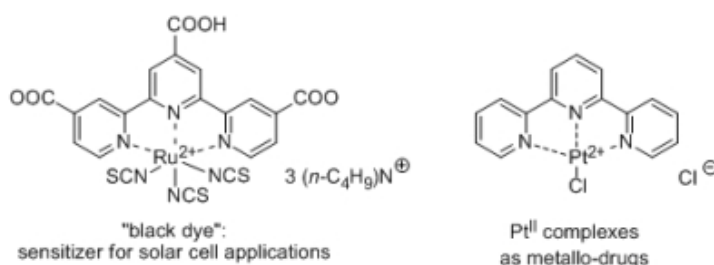
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Textbooks in organometallic chemistry list bis(triphenylphosphine)carbonyl iridium (I) chloride alongside the name “Vaska's compound”. This year (2011) represents fifty years since the synthesis and characterization of Ir(PPh<sub>3</sub>)<sub>2</sub>(CO)Cl by Prof. Lauri Vaska. Who is Lauri Vaska and what path led him to discover the compound which bears his name? In this paper we will explore the road to Ir(PPh<sub>3</sub>)<sub>2</sub>(CO)Cl, how the complex came to bear Lauri Vaska's name, and the significance of the complex in organometallic chemistry. Lauri Vaska's work on group 8 and 9 transition metal compounds led to the discovery of a number of low valent complexes during the early days of a rapidly emerging field of organometallic chemistry. Vaska reported hydrogenation of olefins in 1965, the same year as Wilkinson reported on ClRh(PPh<sub>3</sub>)<sub>3</sub>. Vaska's compound adds many small molecules and activates aldehydes in an early example of metal catalyzed decarbonylation of aldehydes used in organic synthesis today.

## HIST 10: 80 Years of terpyridine chemistry

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In 1931, Morgan and Burstall obtained 2,2':6',2"-terpyridine (tpy), along with other N-containing products, from a reaction of pyridine with anhydrous FeCl<sub>3</sub> in an autoclave (340 °C, 50 atm, 36 h). The instantaneous coordination of Fe<sup>II</sup> ions gave rise to the first indication of metal complex formation. Within the last eight decades, tpy and its derivatives evolved from a rather chemical oddity to highly versatile ligands in modern supramolecular chemistry and outstanding applications of terpyridines and their metal complexes have been derived. In this respect, the “black dye” and Pt<sup>II</sup> complexes as powerful sensitizer in photovoltaics and potent metallo-drug, respectively, have to be named. In this contribution, the historic benchmarks as well as today's applications of terpyridines in the fields of polymer science, nanotechnology, photo-physics, medicine and catalysis will be highlighted.



## HIST 11: Extroverted confusion – Linus Pauling, Melvin Calvin and porphyrin isomers

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Isomeric porphyrins such as porphycenes and N-confused porphyrins have become a mainstay of contemporary supramolecular and coordination chemistry. Notably, the N-confused (2-aza-21-carbaporphyrins) were discovered in 1994 by Furuta *et al.* and Latos-Grażyński and coworkers and opened a whole new area of heteroatom substituted tetra- and oligopyrrole research. Historically, Melvin Calvin proposed "carboporphyrins" in 1943 and, unbeknownst to contemporary science, Linus Pauling analyzed



the existence and stability of such fundamental porphyrin isomers in 1944. What he called "isoporphyrins" with "extroverted pyrrole rings" are clearly the isomeric 2-aza-21-carbaporphyrins of today.

### **HIST 12: John William Baker and the development of the Baker-Nathan effect**

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In 1935 John William Baker(1898-1967) and Wilfred Samuel Nathan(1911-1961) of Leeds University proposed a novel explanation for anomalous results that they had obtained in their studies of the rates of reaction in certain alkyl-substituted compounds. This involved the assumption that the electrons in a carbon-hydrogen bond adjacent to an unsaturated carbon were able to be delocalized. This explanation was applied to many other situations and soon the Baker-Nathan effect was applied to many other anomalous results by Baker and other investigators. This paper will initially discuss the life and chemical work of John William Baker and in the second part will review the experimental work that led to the development of the Baker-Nathan effect . Finally the reasons why the Baker-Nathan effect as originally proposed is no longer in favor.

### **HIST 13: Arnaldo Piutti and the discovery of enantioselectivity in receptor-mediated biological activity**

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The first example of biological enantioselectivity, a difference in the microbial metabolism of the tartaric acid enantiomers, was discovered by Louis Pasteur in 1857. Nearly 30 years later, in 1886, Arnaldo Piutti (1857-1928), an Italian chemist, discovered the first example of enantioselectivity in what is considered today a receptor-mediated biological activity. Natural (*L*) asparagine had first been isolated in the early 1800s but D-asparagine was unknown. Piutti separated D-asparagine from the L-enantiomer obtained from germinated vetch. From 650 kg of vetch he obtained 20 kg of L-asparagine and 100 g of the pure D enantiomer. The two enantiomers crystallized in enantiomorphous forms and had equal but opposite optical rotations. Most importantly, Piutti found that L-asparagine was without taste but the D-enantiomer was intensely sweet. This was the first reported observation of enantioselectivity in what is now known to be a receptor-mediated biological action, an important and widely occurring phenomenon.

### **HIST 14: Early 20<sup>th</sup> century opinion on engineering training for chemistry undergraduates**

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This paper will explore the variety of opinions held by early 20<sup>th</sup> century leaders in academic chemistry and chemical industry on the relative value of engineering education compared to traditional chemical education for students planning careers in chemical manufacturing and research.

### **HIST 15: Inner meanings of physical chemistry: Understanding the atom and nuclear reactions**

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The study looks into deep meanings of the atom and nuclear reactions. The atomic age is relatively modern, but arguably the philosophy of the atom existed through human history. Examples include how kings' palaces resembled the nucleus of the atom, where the eunuchs used to serve the king's household,

while the remainder of society were not allowed to cross through the walls of the palace. The king's household is likened to the protons in the nucleus and the eunuchs are likened with the neutrons inside the nucleus. Parallels are made from historic kings' palaces and the atom and how the interactions in the past resemble interactions within the atom. The paper also delves into the inner meanings of the periodic table of elements and its historic significance, as well as the inner meanings of nuclear reactions. This paper unlocks some spiritual aspects of alchemy that existed in the ancient times.

### **HIST 16: Developments in field of electron and related transfers - now and then**

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The electron transfer field has developed in numerous directions in the past half century. The subfields range from biological electron transfer (ET) to solar energy conversion, from ET in enzymes to ET in semiconductors, from transfer between molecules or ions in liquids to between liquids and between liquids and electrodes. They include ET's that are photoinduced and those that, instead, are light emitters. Studies now range from ET in ensembles to ET in the complementary field of single molecules. Some of the concepts developed originally for electron transfers, such as the dependence of reaction rate constant on standard free energy of reaction, and the cross-relation, have been extended to atom and group transfers, though with a very different model for the potential energy surface. The usual pair of parabolas for ET was replaced by a more usual description of atom transfers. The model still gave the cross-relation for the rate constants (it works well) but not the inverted effect, a difference understood from the difference in topography of the potential energy curves for the ET and for the atom or group transfer. The developments of very fast ET introduced a new element and focused attention on solvent dynamics and the long neglected Kramers theory. In this lecture we summarize and discuss some of this history and current directions, including those related to solar energy conversion and to intermittent fluorescence of nanoparticles.

### **HIST 17: Reactions at surfaces: Delving below and beyond**

*Sylvia T. Ceyer<sup>(1)</sup>, stceyer@mit.edu, 77 Mass Ave, 6-217, Cambridge MA 02139, United States. (1) Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA 02139, United States*

Catalytic surface reactions depend not only on adsorbed species but also on absorbed species. Specifically, a H atom embedded in Ni bulk emerges onto the surface and in so doing, hydrogenates adsorbed ethylene and acetylene while absorbed H does not. Their distinct reactivities arise from different energetics. These results demonstrate that absorbed H is a reactant with a chemistry of its own. In a second system, Si dangling bonds abstract a F atom from XeF<sub>2</sub> forming an adsorbed F and scattered XeF. Some XeF dissociates as a result of exothermicity partitioning to the XeF rovibrational continuum. The F and Xe are shown to arise from gas phase dissociation by demonstrating that angle-resolved velocity distributions of F, Xe, and XeF conserve momentum, energy, and mass. Knowledge and inclusion of abstraction and gas phase dissociation of a surface reaction product are critical to development of accurate models for etching and vapor deposition.

### **HIST 18: Gibbs Medal Award. Galloping cyclohexane conformations**

*John D. Roberts<sup>(1)</sup>, robertsj@caltech.edu, Crellin Laboratory 184-39, Pasadena CA 91125, United States. (1) Division of Chemistry and Chemical Engineering, California Institution of Technology, Pasadena California 91125, United States*

The Willard Gibbs Medal is a very prestigious award for chemistry, with its 100-year life span, not much less than the 110-year life span of the Nobel Prize in Chemistry, indeed it is rather simiir in scope, only

lacking a \$1,000,000 honorarium. It differs from the Nobel tradition in awarding the honor mostly to US researcher, only 6 out of 100 from other countries. Being much older than the average of male American chemists, I was fortunate to be acquainted with 72 of the past awardees and it is a great group. A bit slow in recognizing women, but there were three in the last five years and before, only Marie Curie (1921). The subject of this talk will be the use of NMR to follow conformational and preferences changes in 1,2-trans- and 1,3-cis-cyclohexanedicarboxylic acids.

### **HIST 19: Molecular recognition of DNA by small molecules, a historical perspective**

*Peter B. Dervan<sup>(1)</sup>, dervan@caltech.edu, Mail Code 164-30, Pasadena CA 91125, United States. (1) Division of Chemistry & Chemical Engineering, California Institute of Technology, United States*

Small molecules that bind specific DNA sequences would be useful tools in biology, biotechnology and potentially in human medicine. The field has its origins in the 1950's in natural products isolation and the search for antimicrobial and antitumor agents. I will attempt to trace this historical development from early concepts such as Lerman's "intercalation model" (1961) to the "Py-Im pairing rules" (1998) for minor groove recognition of the DNA double helix.

### **HIST 20: Ionic reactions and solvation**

*John I Brauman<sup>(1)</sup>, brauman@stanford.edu, Department of Chemistry, Stanford University, Stanford CA 94305-5080, United States. (1) Department of Chemistry, Stanford University, Stanford CA 94305-5080, United States*

We usually observe ions in condensed phase, where the energies of solvation are very large. These large solvation effects often overwhelm the intrinsic "chemical" differences that might otherwise determine the chemistry of these ions. By studying the isolated ions in the gas phase we learn something about their intrinsic chemistry as well as the effects of solvation. Thermodynamics (acidity and basicity), kinetics (reaction dynamics) and mechanisms ( $S_N2$ , carbonyl addition) are all dramatically affected by solvation. I will discuss some of the experiments and conclusions that can be drawn from these studies.

### **HIST 21: Structure property relationships in molecular wires**

*Ronald Breslow<sup>(1)</sup>, rb33@columbia.edu, 3000 Broadway, New York NY 10024, United States . (1) Department of Chemistry, Columbia University, New York New York 10027, United States*

The electrical conductivities of molecular wires, measured using a gold break junction, have been studied using various contacts. Extremely high conductivities were seen with gold atom contacts that directly incorporate into the gold electrodes. In other studies, conduction through stacked benzenes and through molecules with differing amounts of aromaticity and antiaromaticity are also of theoretical and practical interest.

### **HIST 22: Chemical philately: Classroom applications**

*Michael A. Morgan<sup>(1)</sup>, mmorgan@lausd.net, 1200 North Cornwell Street, Los Angeles CA 90033, United States . (1) Francisco Bravo Medical Magnet High School, United States*

The History of Chemistry, its predecessor Alchemy, and the people involved in it are often portrayed on postage stamps. Stamps showing chemical formulae, structure, and laboratory glassware are especially enjoyable topics for postage stamps. In addition scientific units and constants have been honored on philatelic issues. The metric system and mathematical equations related to chemistry can be found on many issues. Stamps of the world relating to chemistry and its history will be discussed.

### **HIST 23: The Joseph Priestley House; A philatelic remembrance**

**John B Sharkey**<sup>(1)</sup>, *jsharkey@pace.edu, 1 Pace Plaza, New York New York 10038, United States . (1) Department of Chemistry, Pace University, New York New York 10038, United States*

The temporary closing of the Priestley House in 2010 is a reminder of the fragile nature of many of our historic landmarks. Even though Joseph Priestley lived in Northumberland, PA for only ten years, the Joseph Priestley House remains today a site of major scientific importance. As part of this philatelic symposium celebrating the IYC, this paper will review some of the scientific meetings that have taken place at Priestley House over the past two centuries, and the philatelic evidence of these meetings. I will also briefly discuss some of Priestley's postal correspondence from Northumberland. Although the state staff was furloughed at the Priestley House, the site still operates through the generosity of The Friends of the Priestley House.

### **HIST 24: Gibbs, thermodynamics, visualization - all for just 37 cents!**

**Kenneth R. Jolls**<sup>(1)</sup>, *jolls@iastate.edu, 2114 Sweeney Hall, Ames Iowa 50011-2230, United States . (1) Iowa State University, United States*

J. Willard Gibbs was too early to win a Nobel Prize. He didn't become a household name like Einstein, Pauling, or Watson and Crick. He didn't develop a popular audience as did Carl Sagan. And people didn't smile at him the way they did with Richard Feynman. But Josiah Willard Gibbs prescribed the analytical methods that have placed some of nature's most formidable powers into the hands of those who would try to wield them. "Strange, abstract, deep, difficult, impenetrable" -- all words that have been applied to the tools of Gibbsian thermodynamics. But not so! The careful observer will find in them not only scientific but artistic beauty and explanations that satisfy both sides of the brain. And now also the front side of an envelope.

### **HIST 25: Chemical philately and the story of the quantum**

**C. Marvin Lang**<sup>(1)</sup>, *cmlang@uwsp.edu, Chemistry Department, Stevens Point WI 54481-3897, United States. (1) Chemistry Department, University of Wisconsin – Stevens Point, United States*

When someone asks you “*What's new?*” have you ever considered responding ... “*c over lambda!*” To the chemist and physicist, such a play on words suggests an understanding of the concepts of quantum theory. An equal response to “*What's nu?*” might be “*E over h.*” These and many other theoretical principles are expressed on postage stamps and philatelic materials issued by many nations of the world. This presentation will attempt to weave a thread between individuals and their respective contributions to Quantum Theory.

### **HIST 26: Curie semipostal stamps of 1938**

**Ronald Hill**<sup>(1)</sup>, *hillwright@mac.com, 7590 West Caley Drive, Littleton Colorado 80123, United States ; Daniel Rabinovich<sup>(2)</sup>. (1) *NA, United States* (2) *University of North Carolina at Charlotte, United States**

Marie and Pierre Curie were commemorated on a special omnibus issue of semi-postal stamps issued around the world in the fall of 1938. France and 21 of its colonies issued special stamps with an added surcharge to raise funds for the l'Union Internationale Contre le Cancer (l'UICC), which raised funds for the study, treatment and (ideally) the cure of cancer. Stamps of Monaco, Cuba and Afghanistan related to this effort will also be illustrated in this presentation, as is a detailed description of the design of these stamps.

## HIST 27: Aluminum on stamps: A tribute on the 125th anniversary of the Hall-Hérout process

**Daniel Rabinovich**<sup>(1)</sup>, [drabinov@uncc.edu](mailto:drabinov@uncc.edu), 9201 University City Boulevard, Charlotte North Carolina 28223, United States . (1) The University of North Carolina at Charlotte, United States

The industrial production of aluminum by the high-temperature electrolysis of alumina ( $\text{Al}_2\text{O}_3$ ) dissolved in molten cryolite ( $\text{Na}_3\text{AlF}_6$ ) was developed independently and almost simultaneously in 1886 by Charles Martin Hall in the United States and Paul Hérout in France. This presentation will literally describe the world of aluminum from cradle to grave, from the mining and purification of bauxite throughout the world to the recycling of discarded aluminum products, as illustrated on postage stamps and other philatelic materials (maximum cards, first day covers, special cancellations, etc.). The unique combination of physical properties that this ubiquitous metal exhibits (low density, high electrical conductivity, malleability, resistance to corrosion) and its impact on society, including the construction, transportation, and food industries, will also be highlighted in this presentation.



## HIST 28: Why does ACS need an accessible history of its presidents?

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How did the Past Presidents Project (P3) originate? What is contained in the P3? How did the idea of this project develop to include an accessible history of the ACS presidents? What information will be on each president's web page now and in the future? Why does the project look for patterns in the backgrounds, experiences, and achievements of the presidents? Is it not intriguing that the history will never be completed, that every ACS member is a potential contributor?

## HIST 29: What does an ACS president do besides pontificate?

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Why does a person run for the office of ACS president, and become a part of a three-year journey as president-elect, president and immediate past president? In addition to serving as a national and international representative of the chemical sciences to other chemists, a member of the ACS presidential succession interacts with students at all levels, the general public, government bodies, and the media. They carry out many activities in order to achieve their presidential goal(s), whatever they might be. Further, the president presides at two national meetings, visits several regional meetings and a score of other Board meetings and activities. In order to manage all these tasks, they must possess excellent communication skills, strong powers of persuasion, lots of energy and the support of staff, colleagues, bosses and family.

## HIST 30: Who were the first ACS Presidents?

**Patricia L Perez**<sup>(1)</sup>, [PatTheChemProf@yahoo.com](mailto:PatTheChemProf@yahoo.com), 776 Teakwood Lane, San Dimas CA 91773, United States . (1) Project Inclusion, San Dimas CA 91773, United States

In this presentation I will explore the beginnings of our organization, the American Chemical Society. This historical overview will focus on the experiences, careers and years of service of the first five (5) ACS presidents. The presidents were John W. Draper (1876), J. Lawrence Smith (1877), Samuel W. Johnson (1878), T. Sherry Hunt (1879), and Frederick A. Genth (1880). Each of these individual chemists brought his own background and vision that laid the foundation for the current American Chemical Society.

### **HIST 31: Anna J. Harrison - After 102 years, the first ACS woman president**

*Lucy P. Eubanks<sup>(1)</sup>, eubankslucy@bellsouth.net, 335 Woodland Way, Clemson SC 29631, United States .  
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In 1978, Anna Jane Harrison became the first woman to be elected ACS President. This major leadership role was an appropriate recognition of her career as a pioneer educator and researcher and honored the traditions of excellence set by her predecessors. Her impact upon me, her former student, was significant, expanding my networks and enriching my understanding of the relationships among science and society. Her vision and leadership in guiding the policies of the ACS and other scientific organizations was profound, improving interactions with regulatory agencies, developing programs for non-science majors as well as majors, and expanding our understanding of what it means to be a professional chemist. Anna Harrison received the ACS Award in Chemical Education in 1982, and her humility and vision of leadership were captured in this quotation from her award address: “The fundamental reason for joining any professional society is that we achieve collectively that which none of us can achieve individually.”

### **HIST 32: Reflections on the ACS presidents at the end of the 20th century**

*Bruce E. Bursten<sup>(1)</sup>, bbursten@utk.edu, 418 Buehlen Hall, Knoxville TN 37996, United States. (1)  
Department of Chemistry, University of Tennessee, Knoxville, Knoxville TN, United States*

From my point of view as the 2008 ACS president, I would like to reflect on the impact of the presidents of the American Chemical Society in the 1980s and 1990s. What were their major accomplishments and successes? How did their actions and decisions affect the direction of ACS policies and activities over this particular period of time? How did they influence the interactions of the ACS with other scientific societies, in the United States and abroad? And how did these actions become the foundation for my term of service?

### **HIST 33: Do you want to know more about the ACS presidents? Select [acs.org](http://acs.org) instead of Wikipedia?**

*Janan M Hayes<sup>(1)</sup>, janan.hayes@yahoo.com, 6829 Barbara Lee Cir, Sacramento CA 95842, United States.  
(1) Project Inclusion, Sacramento CA 95842, United States*

This P3 project started because one had to go to Wikipedia to get a complete list of the ACS presidents. One result of the project is a collection of the vast amount of information on our past presidents. We will report some interesting trends and statistics gleaned from that information. One of the major products of this project is a new page on [acs.org](http://acs.org). This page, ACS Past Presidents, will be introduced at this symposium. Not only will there be a complete list of the presidents but also a link to a page for each with a picture and basic information. Behind that page will be a growing series of pages with more detailed information and links for each president. This will be a dynamic source for the future use of ACS members, educators, students and the general public.