

the Catalyst



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March 2017
Volume 102, No. 3



Edgar Fahs Smith Lecture
Dr. Peter J. Rossky, Rice University

HIGHLIGHTS

Comments From the Chair	39
News Atoms	40
Speaker's Abstract and Biography	42
Nominations for Section Award	44
Calendar of Activities	48

ADVANCE NOTICE

APRIL MEETING

Thursday, April 20, 2017

5:00 PM

Student Scholastic Achievement Awards

Presenter: Mary Virginia Orna

Professor, The College of New Rochelle

Lost Elements

McCall Conference Center
Lynn Blvd., Upper Darby PA

See the APRIL issue of *the Catalyst* for details,
call the Section Office at (215) 382-1589 or email PhilaACS@gmail.com.

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CONTENTS

April Advance Notice	37
Comments From the Chair	39
News Atoms	40
Delaware Valley Science Fairs	40
March Meeting.....	41
Speaker's Abstract and Biography.....	42
Call for ACS Section Award Nominations	44
CCN Notice	45
Volunteers Needed for PAGES™	46
Directory of Services	47
Calendar of Activities.....	48

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Comments From the Chair



Deborah Cook

As I was doing year-end organizing, I came across the “The ACS Philadelphia Section Centennial Year Review Edition” of *the Catalyst*, Vol. 84, No. 10, December 1999. The volume was subtitled “Celebrating the Section’s 100th Anniversary April 1899-April 1999”. The volume is a treasure trove of our Section’s history. Philadelphia Section was the 12th Section to be organized and was granted a charter on April 15, 1899, with 83 Charter members. The first Section meeting was held on May 17, 1899 in Room 207, John Harrison Laboratory of Chemistry, University of Pennsylvania. The first issue of *the Catalyst* was published in February 1916. A milestone noted in the Section’s history for 1917, was the appointment of the first standing committee on Public Relations which established an Employment Bureau. One hundred years later in 2017, we are still concerned with public relations and employment issues. Some things probably will never change.

Other interesting items noted in our history include the institution and sponsorship in 1915 of two social meetings a year, “Smoker” and Ladies Night.” A Women’s Committee was appointed in 1919. In 1928 the Chemical Education Committee sponsored the first continuing education courses. Section Service Awards were authorized in 1949, Annual Scholastic Achievement Awards were instituted in 1951, the Philadelphia Section Award was authorized in 1961, annual Awards in Pre-College Teaching were instituted in 1991, the Ulliot Lectureship Program was inaugurated in 1990, and the Ulliot Award for Meritorious Service was initiated in 1992. Charter flights to Europe were organized in 1963, 1965, 1967, 1969, 1971 and 1973. Our Section has had a colorful and creative history.

This month on March 23rd, we celebrate the Edgar Fahs Smith Memorial Lecture which was established in 1929 in honor of Edgar Fahs Smith. He was considered the first modern chemist at the University of Pennsylvania. Dr. Smith was a former Provost of the University and President of the American Chemical Society. Dr. Smith was awarded the second Priestley Medal in 1926. The lectureship is the oldest lectureship in the country jointly sponsored by a university and a local ACS section. The list of past awardees reads like a who’s who in chemistry. This year’s speaker is Dr. Peter J. Rossky, Dean of the Weiss School of Natural Sciences and Henry C. & Olga K. Weiss Professor of Chemistry and Biomolecular Engineering at Rice University, Houston, Texas.

I hope you will join us to honor Dr. Rossky and to listen to his lecture which will be followed by a dinner at Penne.

Respectfully, Deborah Cook

NEWS ATOMS—*Alan Warren*

Robert G. W. Anderson was named president and CEO of the Chemical Heritage Foundation. He had been serving as interim president since July 2016, and was former vice chair of the board of directors. He has broad experience in the history of science and museum leadership.

Anderson was director of the British Museum and Keeper of Chemistry at London's Science Museum, and served as director of the National Museums of Scotland. Among various honors he received the ACS Dexter award for the history of chemistry in 1986.

2017

Delaware Valley Science Fairs - Greater Philadelphia Expo Center in Oaks, PA

April 4th to April 6th

Judging Day - Wednesday, April 5, 2017

***ResMed: Residential School on Medicinal
Chemistry and Biology in Drug Discovery***
June 12-16, 2017
Drew University, Madison, NJ

This graduate level course concentrates on the fundamentals that are useful in drug discovery spanning initial target assay evaluation through clinical development. Several case histories of recent successful drug development programs will also be presented. The five-day program covers:

Principles of Med Chem	DMPK
Cheminformatics	Toxicophores
Lead ID & Optimization	GPCRs
Epigenetics	Kinase Inhibitors
Fragment-based Drug Design	Ion Channels
Structure-based Drug Design	Enzyme Inhibitors
Drug-like Properties	Bioisosteres
Plasma Protein Binding	Preclinical Tox
Molecular Modeling	Clinical Dev
Protein-Protein Interactions	Case Histories
Antibody-Drug Conjugates	

W. Greenlee, V. Gullo and R. Doll –Co-organizers

Attendees will be staying at The Madison Hotel
www.drew.edu/resmed
e-mail: resmed@drew.edu
phone: 973/408-3787; fax: 973/408-3504

MARCH MEETING

Board of Directors Meeting

4:00 PM - 5:00 PM

University of Pennsylvania, Chemistry Building
Room 117 (first floor Faculty Conference Room)
Department of Chemistry, University of Pennsylvania

and

Edgar Fahs Smith Lecture and Award

Presenter: Dr. Peter J. Rossky, Rice University

*Relaxation Photo-excited States in Complex Systems:
Two Stories of Harmony Between Theory and Experiment*

Thursday, March 23, 2017

5:00 PM - 6:00 PM Reception

Nobel Hall

Department of Chemistry, University of Pennsylvania
231 S. 34th Street, Philadelphia, PA 19104

6:00 PM - 7:15 PM Lecture

Carolyn Hoff Lynch Auditorium

Department of Chemistry, University of Pennsylvania
231 S. 34th Street, Philadelphia, PA 19104

7:30 PM Dinner

Penne Restaurant and Wine Bar at The Inn at Penn
3611 Walnut Street, Philadelphia, PA 19104

****Tickets for dinner are \$45 for members, \$22.50 for students****

Register at

<https://www.eventbrite.com/e/edgar-fahs-smith-lecture-dinner-tickets-31541343006>

Or by contacting the Section Office

PhilaACS@gmail.com

(215)-382-1589

SPEAKER'S ABSTRACT AND BIOGRAPHY

Dr. Peter J. Rossky

Harry C. and Olga K. Wiess Chair in Natural Sciences, Professor of Chemistry, Professor of Chemical and Biomolecular Engineering, and Dean of the Wiess School of Natural Sciences
Rice University

Relaxation Photo-excited States in Complex Systems: Two Stories of Harmony Between Theory and Experiment

Abstract: This presentation will focus on progress in our ability to understand, at the level of atoms and on the time scale of femtoseconds, the molecular rearrangements and time-dependent processes that occur following electronic excitation by light when these changes take place in liquid solutions or in unstructured solid materials, including those occurring in biological and synthetic polymeric materials. Computational models and experiments are increasingly able to simultaneously describe these processes, greatly enhancing the information that can be learned about chemistry from the combined theoretical and experimental analysis. In this presentation, two example cases will be discussed with focus on how time-dependent simulations of quantum phenomena can directly inform on mechanisms.

The first case is one where both the complex system and electronic process are relatively “simple:” we study the electronic excited state relaxation of photoexcited anionic water clusters to understand the measured cluster size dependence of the ground state recovery rate and how those values come about. In the second, we study far more complex molecular systems based on a simple semiempirical electronic structure method. Analysis of the evolution of electronic excited states in representative conjugated molecular systems, particularly relevant to the function of plastic solar cells, will be discussed, including the processes underlying exciton migration and exciton dissociation, including the impact of interfacial structure and of extrinsic electric fields.

Biography: Dr. Peter J. Rossky received his undergraduate degree in Chemistry *summa cum laude* from Cornell University and his PhD in Chemical Physics from Harvard. After postgraduate research as an NSF National Needs Postdoctoral Fellow at SUNY, Stony Brook, he joined the faculty at the University of Texas at Austin in the Department of Chemistry. There he held the Marvin K. Collie-Welch Regents Chair in Chemistry in the Department of Chemistry, as well as an appointment as Professor of Chemical Engineering. At Austin, he served as the Director of the Institute for Theoretical Chemistry, and then the Center for Computational Molecular Sciences in the Institute for Computational Engineering and Sciences. He also served as the Director of the Department of Energy-funded Energy Frontier Research Center on Charge Separation and Transfer in Energy Materials.

In 2014, he joined the faculty at Rice University as the Harry C. and Olga K. Wiess Chair in Natural Sciences, Professor of Chemistry, Professor of Chemical and Biomolecular Engineering, and Dean of the Wiess School of Natural Sciences.

His theoretical research program has pursued the elucidation of structure and dynamics associated with chemical processes in the condensed phase, with a focus on liquids, solutions, and photoactive molecular materials. Dr. Rossky has published more than 250 papers in the field. His work has emphasized realistic atomistic descriptions of complex molecular systems studied using classical and quantum statistical physics as well as quantum chemistry. His group has been a pioneer in the development of an understanding of the impact of an aqueous environment on the structure and function of biomolecular systems. His laboratory has also developed a number of new algorithms that underlie our ability to effectively study both the statistical properties and the dynamics of condensed phase molecular quantum systems using computer simulation. His lab currently focuses on the photo-induced dynamics in organic molecular systems, including both synthetic materials and biomolecules.

Dr. Rossky has served in a number of editorial positions including Senior Editor for the *Journal of Physical Chemistry* and as a member of the editorial advisory boards for the *Journal of Chemical Theory and Computation*, *Accounts of Chemical Research*, *The Journal of Chemical Physics*, *Chemical Physics Letters*. He is currently a member of the Editorial Board of *Proceedings of the National Academy of Sciences*. He has also served as the Chair of the Gordon Research Conference on Water and Aqueous Solutions as well that on the Physics and Chemistry of Liquids.

He has received a number of major recognitions for his contributions, including receipt of the American Chemical Society Physical Division Award in Theoretical Chemistry and the American Chemical Society Hildebrand Award in the Experimental and Theoretical Chemistry of Liquids. He has been selected as an Alfred P. Sloan Foundation Fellow, an NSF Presidential Young Investigator, a Dreyfus Foundation Teacher-Scholar, a John Simon Guggenheim Foundation Fellow, and has been elected as a Fellow of the American Physical Society, and a Fellow of the American Association for the Advancement of Sciences. He is a member of the American Academy of Arts and Sciences and the US National Academy of Sciences.



NOMINATIONS INVITED

FOR THE 2017 PHILADELPHIA SECTION, AMERICAN CHEMICAL SOCIETY AWARD

The Philadelphia Section invites its members and regional and topical groups to consider recommending candidate(s) for the Philadelphia Section Award.

This Award recognizes an individual, “who, by conspicuous scientific achievement through research, has made important contributions to man’s knowledge and thereby aided the public appreciation of the profession.” Any member of the American Chemical Society, Philadelphia Section, may be nominated for this award. Recent awardees include: Donna Huryn (University of Pittsburgh), Feng Gai (University of Pennsylvania), Ahmed Abdel-Magid (Therachem Research Medilab), and Marisa Kozlowski (University of Pennsylvania).

INSTRUCTIONS FOR SUBMITTING NOMINATION

- (1) The nominator should provide detailed biographical data of the nominee, showing educational and employment data, a list of publications and a record of other accomplishments pertinent to consideration for this award.
- (2) One or two seconding letters (at least one of which should be from a person in an organization other than that of the nominee) should be requested in support of the nomination.
- (3) Nominators and seconders should be identified with addresses and telephone numbers so that they can be contacted, if necessary, for additional information.
- (4) Unsuccessful nominees from previous years may be renominated. In fairness to the nominee, however, re-nominations must be accompanied by an updating of the nominee’s biographical data and list of accomplishments in order to make the nomination competitive. Unsuccessful nominees who have been considered three years in a row should not be renominated for the fourth year in succession without prior consultation by the nominator with the chair of the Awards Committee.

Nomination forms are available from the Section Office. Contact the Administrative Secretary, Ms. Krista Leary at:

Philadelphia Section, ACS
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323
(215) 382-1589; email PhilaACS@gmail.com

The completed packet of nomination materials may be emailed to PhilaAcs@gmail.com or mailed By **April 1** to Elizabeth Wagoner, Chair, Awards Committee, at the Section Office address above.

CHEMICAL CONSULTANTS NETWORK MARCH 8, 2017 MEETING

What the ACS Philadelphia Section & the Chemical Consultants Network Can Do for You!

DATE & TIME: Wednesday, March 8, 2017, 4:30 PM at Avenue Kitchen
(Near Villanova University)

[Click here to register](#)

Open network event - Find out how the ACS Philadelphia section and the Chemical Consultants Network can provide great career benefits and networks, as well as a FREE resource for institutions seeking cost-effective, experienced chemical, pharma and biotech consultants. This is also a great opportunity for younger scientists to network with folks who've worked in many areas of the chemical and pharma enterprises.

Agenda:

4:30 - Event opens

5:00 - Description and ongoing mission of the Philadelphia section ACS, and its benefits to members.

Speaker: Deborah Cook (Chair, Philadelphia Section ACS)

5:20 - Description and ongoing mission of the Chemical Consultants Network, and its benefits to members and partnering institutions (many ways for our members to engage!).

Speaker: Keith D. Wing (Chair-Elect, Chemical Consultants Network)

5:40 - Open networking

Philadelphia Section of the American Chemical Society: The American Chemical Society (ACS) is the world's largest scientific society and one of the world's leading sources of authoritative scientific information, and is the premier professional home for all engaged in the chemical enterprise. The Philadelphia Section is one of the oldest and largest in the ACS, founded in 1899 by 83 chemists, and today has over 4000 members.

<http://philadelphia.sites.acs.org/>

Chemical Consultants Network: The Chemical Consultants Network (CCN) is an organization of almost 200 chemists and chemical engineers who work as consultants. We hold monthly meetings on topics of interest to consultants and inform potential clients about our areas of expertise through our search-friendly web site. CCN is a topical group of the Philadelphia Section of the ACS and is supported by the National AIChE

<http://chemconsultants.org/>

Location: Avenue Kitchen (side room to your left as you enter restaurant), 789 Lancaster Ave, Villanova, PA 19085. **Directions:** Use "Directions" button on [MAP](#) link.

RESERVATION IS REQUIRED FOR ATTENDANCE:

Click here to register to attend the event, or e-mail CCNReservations@aol.com or call the CCN phone number at (877) 326-2959 and leave a message. Fee, including appetizers, is \$10. CASH BAR. Reservation/cancellation deadline: **Saturday, March 4th**. If notice received as email, do not reply; use above reservation links only, or CCN phone.



Philadelphia Area Girls Enjoying Science™ (PAGES™) Volunteers Needed

You are invited to participate in the Spring 2017 session of the Philadelphia Area Girls Enjoying Science™ (PAGES™) mini-conference for 6th grade girls which Chestnut Hill College will be hosting on Saturday, April 22, 2017.

A sign-up form for you to fill out and return via mail, FAX, or e-mail (preferred) is located at <http://pagesprogram.org/events/wcc-pages-invitation-4-22-17-2/>. Please return the form by April 6, 2017. **If you do not get a prompt reply to your sign-up, please email Dr. Kathy Thrush Shaginaw at KATT@verizon.net. Please provide emergency contact information** – this was very important before the fall 2012 session, when Superstorm Sandy made communications more difficult and volunteers were not necessarily at their workplaces the week before the event.

Don't forget to check out our web site at <http://www.PAGESprogram.org> and a nice article at <http://connections.chc.edu/article/female-scientists-future-get-started-chc>.

As a scientist volunteer, you bring an experiment to share with three small groups of girls (4 – 7 students each). The program provides the girls with safety glasses, aprons, paper towels, gloves, and bench covers. Safety is our number one priority, so keep the experiments as safe as possible. It is better to focus on a couple of concepts, rather than overwhelm the girls with a lot of information. The girls love to take something home with them, so please provide them with a hand-out if you can.

Some of you have a favorite experiment that you like to do with the girls. There is no reason why you cannot continue to do this experiment – girls are not allowed to come twice. The National Chemistry Week (NCW) 2017 theme is "**Chemistry Rocks!**" exploring the chemistry of rocks and minerals. It would be great if you could share an experiment exploring the forensics with the girls. There are books and other resources available to you to design your experiments. In addition, if there are some supplies that you need, let us know as soon as possible, so that I can try to get them from one of our sponsors.

We always welcome new volunteers to the program, so feel free to invite a co-worker or one of your students to attend.

Information about this event and other National Chemistry events can be found at: <http://philadelphia.sites.acs.org/>, just click on the National Chemistry Week link or go to <http://www.PAGESprogram.org>.

If you have any questions, feel free to me at (215) 736-9285. Thank you for your support of this worthy program.

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Contact the Section Office at
PhilACS@gmail.com or (215)
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Put "Volunteer" in the subject line or
leave a message including contact in-
formation.

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ACS	47
Drew University	40
Micron Inc.	47
NuMega Resonance Labs, Inc.	47
Robertson Microlit Labs	47
Tyger Scientific, Inc.	47

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PHILADELPHIA SECTION, ACS
CURRENT CALENDAR OF ACTIVITIES

Date and Time	Event	Location
Wednesday, March 8 4:30-7:00 PM	Chemical Consultants Network: <i>What The ACS Philadelphia Section & The Chemical Consultants Network Can Do for You!</i> Speaker: Dr. Deborah Cook, Chair, Philadelphia Section ACS; and Speaker: Keith D. Wing, Chair-Elect, Chemical Consultants Network	Avenue Kitchen 789 Lancaster Ave. Villanova, PA 19085 Click here to register to attend the event , or e-mail CCNReservations@aol.com
Thursday, March 16 11:30 AM-2:00 PM	Joseph Priestley Society; Presenter: Rachel King, CEO, GlycoMimetics. <i>Reflections on Building a Biotech Company: The Story (so far!) of GlycoMimetics</i>	Chemical Heritage Foundation 315 Chestnut Street Philadelphia, PA 19106 https://www.chemheritage.org/event/joseph-priestley-society-rachel-king
Thursday, March 16 8:00 PM	Philadelphia Organic Chemists Club Industrial Award; Presenter: Dr. Spencer D. Dreher, Merck: <i>Enabling Modern Catalysis in Drug Discovery and Development: From Collaboration to Chemo-informatics</i>	University of Pennsylvania Department of Chemistry Carolyn Hoff Lynch Hall http://www.pocclub.org/
Thursday, March 23 5:00 PM Reception 6:00 PM Lecture 7:30 PM Dinner	Edgar Fahs Smith Lecture and Award; Presenter: Dr. Peter J. Ros-sky, Rice University: <i>Relaxa-tion Photo-excited States in Complex Systems: Two Stories of Harmony Between Theory and Experiment</i>	University of Pennsylvania Department of Chemistry Carolyn Hoff Lynch Hall Philadelphia, PA https://www.eventbrite.com/e/edgar-fahs-smith-lecture-dinner-tickets-31541343006
Monday, March 27 6:00-9:00 PM (snowdate, March 29)	YCC Poster Session and Grad School/Career Fair	University of the Sciences Athletic Recreation Center 720 S. 43 rd Street Philadelphia, PA 19104 https://www.eventbrite.com/e/acs-ycc-poster-session-and-grad-schoolcareer-fair-tickets-31393954162
April 2-April 6	253 rd American Chemical Society National Meeting and Exposition: <i>Advanced Materials, Technologies, Systems and Processes</i>	San Francisco, CA https://www.acs.org/content/acs/en/meetings/spring-2017.html?cid=home_meetings
Thursday, April 13 11:30 AM-2:00 PM	Joseph Priestley Society; Noah Clay, Director, Quattrone Nanofabrication Facility, School of Engineering and Applied Science, University of Pennsylvania: JPS Symposium, <i>Emerging Companies Based on Inventions at the Singh Center for Nanotechnology of the University of Pennsylvania</i>	Chemical Heritage Foundation 315 Chestnut Street Philadelphia, PA 19106 https://www.chemheritage.org/event/joseph-priestley-society-noah-clay

Thursday, April 13 8:00 PM	Philadelphia Organic Chemists Club Sigma-Aldrich Student Choice Lecture; Presenter: Dr. David A. Nicewicz, University of North Carolina at Chapel Hill: <i>New Avenues in Synthesis via Organic Photoredox Catalysis</i>	University of Pennsylvania Department of Chemistry Carolyn Hoff Lynch Hall Philadelphia, PA http://www.pocclub.org/
Thursday, April 20 5:00 PM	Philadelphia ACS Section Event; Speaker: Mary Virginia Orna, Professor, The College of New Rochelle: <i>Lost Elements</i>; and Student Scholastic Achievement Awards	McCall Conference Center Lynn Blvd. Upper Darby, PA http://www.maryvirginiaorna.net/
Saturday, April 22 9:00 AM–1:30 PM	The Philadelphia Area Girls Enjoying Science™ (PAGES) Mini-Conference for 6 th Grade Girls	Chestnut Hill College Philadelphia, PA 19118 www.PAGESprogram.org
Thursday, May 18 6:00 PM	Philadelphia ACS Section Event; Speaker: Sam Kean, Science Writer: <i>The Disappearing Spoon</i>; and Excellence in Teaching Awards	McNeil Science and Technology Center University of the Sciences Philadelphia, PA
Thursday, May 25 8:00 PM	The Teva Lecture at Philadelphia Organic Chemists Club; Presenter: Dr. Sean P. Brown, Amgen: <i>Interdiction at a Protein-Protein Interface: Structure-Based Design of Mcl-1 Inhibitors</i>	University of Pennsylvania Department of Chemistry, Carolyn Hoff Lynch Hall Philadelphia, PA http://www.pocclub.org/
June 4-June 6	2017 Mid Atlantic Regional Meeting (MARM 2017): <i>Elements of Transition</i> ; Co-organized by the Lehigh Valley and Susquehanna Sections of the ACS	Hershey, PA http://marm2017.sites.acs.org/
August 20-24	254 th American Chemical Society National Meeting and Exposition: <i>Chemistry's Impact on the Global Economy</i>	Washington, DC https://www.acs.org/content/acs/en/meetings.html?cid=home-meetings
Thursday September 28 5:00-8:00 PM	Philadelphia ACS Section Event: Tour of the PA Biotechnology Center	Pennsylvania Drug Discovery Institute At the Pennsylvania Biotechnology Institute 3805 Old Easton Rd Doylestown, PA 18902