

THE CAPITAL CHEMIST

A Publication of the Chemical Society of Washington Section of the American Chemical Society

March 14, 2024, CSW Dinner Meeting – featuring presentation of the Hillebrand Prize, Gordon Award, and College Chemistry Achievement Awards

Meeting Logistics

Date: Thursday, March 14, 2024

Time: 6:00 p.m. Check-in/Social Hour
6:30 p.m. Dinner
7:00 p.m. Speaker Presentation, Dr. Christopher Cahill

Location: ACS Headquarters – Othmer Hall
1155 16th Street, N.W., Washington, DC

Note: The building is undergoing renovations at the main entrance. Enter around the side of the building (on M Street)

Menu: Meal will be catered by Everfresh Catering and will feature slow-roasted prime rib served with red wine mushroom au jus, chargrilled salmon filet with Dijon tarragon caper sauce, pan-sauteed tofu topped with artichoke, pepper, tomato tossed over Mediterranean spice, with quinoa salad. Includes salad and rolls. Beverages will be provided.

Cost: \$30 per person (half price for students)

Note: An RSVP is required for dinner so we can plan appropriate seating and meals.

Register for the virtual option via Zoom: <http://tinyurl.com/5974ywws>

RSVP by noon (ET) Tuesday, March 12, to csw@acs.org. Please provide the names in your party as well as your contact information when you RSVP. The public is invited to attend. You may attend the talk only at no charge, but reservations are appreciated. If you need any further information or would like to make a reservation, please contact the CSW office by email at csw@acs.org.

Parking: Parking is available in nearby commercial parking garages. Please be aware that garage closing times vary. Parking is also available on the street after 6:30 pm, but be aware that most parking meters are in effect until 10:00 pm and may be limited to 2 hours. You should check the individual meters for details and payment methods as some are no longer coin-operated.

Metro: Blue/Orange/Silver Line: McPherson Square or Farragut West.
Red Line: Farragut North

Volume 74, Number 3
March 2024

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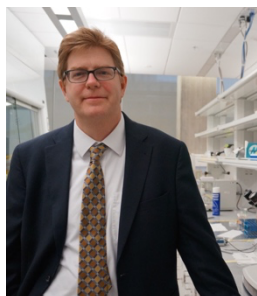
- Join us for two dinner meetings in March!
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- Attend WCC events at the Spring ACS meeting

Section News

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2023 Hillebrand Prize

Dr. Christopher L. Cahill

Department Chair, Professor of Chemistry and International Affairs
The George Washington University

Recipient of the 2023 Hillebrand Prize for illuminating research in condensed phase actinide chemistry and crystal engineering harnessing organic-actinide interactions, which inform efforts in environmental remediation, separations, and nuclear forensics.



2023 Gordon Award

Dr. Allison A. Aldridge

Recipient of the 2023 Gordon Award in recognition of exemplary service by a CSW member to the profession of chemistry, to the science of chemistry, and/or to the Chemical Society of Washington.

College Chemistry Achievement Awards

View List of Awardees: <https://tinyurl.com/2s4zz4ts>

Recipients of the College Chemistry Achievement Award are presented to outstanding seniors majoring in chemistry and biochemistry who have demonstrated excellence in chemistry based on a combination of (in order of importance) research experience, coursework, and a desire to pursue chemistry associated careers from each of the area four-year colleges and universities.

Speaker Bio

Christopher Cahill was born in Huntington, NY and grew up on an apple orchard in nearby Fort Salonga. His education includes a BS in Geochemistry from the State University of New York (SUNY) at Fredonia (1993) and a PhD in Chemistry from SUNY-Stony Brook (1999). He joined the faculty of GW in 2000 after a one-year post-doctoral position in the Environmental Mineralogy group at the University of Notre Dame. He is an expert in solid-state and materials chemistry, with a particular emphasis on X-ray crystallography and structure-property relationships in hybrid materials of relevance to the nuclear fuel cycle. He has published over 165 peer-reviewed papers in a range of areas related to the synthesis and structural characterization of materials and minerals. Current research areas include exploring the behavior of uranium and transuranic species under environmentally relevant conditions, as well as the synthesis of lanthanide containing sensor materials for nuclear forensics applications. Chris is the first physical scientist at GW to hold a joint appointment in the Elliott School of International Affairs, where he develops and delivers technical curricula targeting non-technical nuclear policy professionals. He is a recipient of the prestigious NSF CAREER Award (2004), a Bender Teaching Award (2005), a Fulbright Scholarship (2008), the Trachtenberg Prize for Teaching (2013), the Graduate Mentorship Award from the Vice President for Research at GW (2021), and was elected a Fellow of the American Association for the Advancement of Science (2021). He is a past President of the American Crystallographic Association (2014-2016), a member of the Cosmos Club, and has held visiting researcher positions at the Carnegie Institution of Washington and Argonne National Laboratory. During 2015-2016, he spent a sabbatical as the American Institute of Physics State Department Science Fellow at the US State Department's Office of Weapons of Mass Destruction Terrorism on the Nuclear Forensics Team. Chris served

as Acting Director of the Institute for International Science and Technology Policy at GW (2018) and has been the Chair of the Chemistry Department since 2019.

Abstract

Prof. Christopher Cahill will present some highlights of his research career from the past 24 years at GW. This will include his keen interests in establishing structure property relationships in (for example) lanthanide and actinide materials as relevant to the nuclear fuel cycle, as well as *p* and *d* block compounds with applications in radiation detection and solar cells. A common theme across these diverse compositions is the use of non-covalent interactions such as hydrogen- or halogen-bonding to 1. direct assembly of desired architectures in the solid state and 2. influence the electronic properties thereof. Examples of the latter include manipulating fluorescence signatures in uranium bearing materials, and molecular orbital constructs in Sb and Te halide perovskites. Moreover, he will touch on his interests in science policy and reflect on his year at the US Department of State as a member of Nuclear Forensics team within the Bureau of International Security and Nonproliferation.

March 21, 2024, CSW Dinner Meeting - featuring PANIC, a local NMR group

	
Frank Delaglio Principal Investigator National Institute of Standards and Technology	Ryan Nieuwendaal - Chair, PANIC 2025 Staff Scientist in the Functional Polymers Group National Institute of Standards and Technology
"Characterization of Biotherapeutics by NMR Spectroscopy Using Chemometrics and Machine Learning"	"Don't PANIC! It's an NMR Conference"
	
Join us in person* or virtually on March 21, 2024, at 6:00 P.M. ET *Dinner is served in person, requires registration and payment	
ACS Headquarters, Marvel Hall - 1155 16 th St., NW, Washington, DC	

Meeting Logistics

Date: Thursday, March 21, 2024

Time: 6:00 p.m. Check-in/Social Hour
6:30 p.m. Dinner
7:00 p.m. Speaker Presentation

Location: ACS Headquarters – Marvel Hall / Othmar Hall
1155 16th St., N.W., Washington, DC

Note: The building is undergoing renovations at the main entrance. Enter around the side of the building (on M Street)

Menu: Meal will be catered by Everfresh Catering and will feature Asian Stir Fry with chicken and beef. Vegetarian Option features vegan tofu vegetable stirfry. Sides include vegetable fried rice, steamed vegetables, salad and cookies and brownies. Beverages will be provided.

Cost: \$22 per person (half price for students)

Note: An RSVP is required for dinner so we can plan appropriate seating and meals.

Register for the virtual option via Zoom: <http://tinyurl.com/2p93vsys>

RSVP by noon (ET) Tuesday, March 19, to csw@acs.org. Please provide the names in your party as well as your contact information when you RSVP. The public is invited to attend. You may attend the talk only at no charge, but reservations are appreciated. If you need any further information or would like to make a reservation, please contact the CSW office by email at csw@acs.org.

Parking: Parking is available in nearby commercial parking garages. Please be aware that garage closing times vary. Parking is also available on the street after 6:30 pm, but be aware that most parking meters are in effect until 10:00 pm and may be limited to 2 hours. You should check the individual meters for details and payment methods as some are no longer coin-operated.

Metro: Blue/Orange/Silver Line: McPherson Square or Farragut West.
Red Line: Farragut North

Speaker Bios

Ryan Nieuwendaal is a Staff Scientist in the Functional Polymers Group at the National Institute of Standards and Technology, the metrology lab of the United States Federal Government. Working in the Department of Commerce, he performs solid state nuclear magnetic resonance (NMR) experiments towards understanding the local packing structures and molecular dynamics that occur in materials of industrial relevance, ultimately to establish structure-property relationships. Nanoscopic details such as atomic connectivity, interfacial structure, and mesophase order can be obtained from ^1H spin diffusion and discrete internuclear dipolar couplings (i.e., REDOR), even in the absence of long-range order. Hence, nanoscale models can be reliably developed for heterogeneous systems like semi-crystalline polymers, polymer blends, and polymer networks; all of which are utilized in commercially relevant materials. Over the course of his career, he has published articles mainly involving solid-state NMR of materials.

Frank Delaglio is a Principal Investigator at the National Institute of Standards and Technology, developing computational methods for Nuclear Magnetic Resonance (NMR) data to support development and manufacturing of drugs and vaccines, and to support basic research in structural biology. Frank's current focus is development of approaches for characterization of monoclonal antibody drugs and live cell therapies, so that these important therapeutics can continue to be safe and effective, and become more accessible and affordable. His interests include multidimensional spectral processing and analysis, chemometrics and machine learning, and data visualization. In the NMR community, Frank is best known for developing the *NMRPipe* software system while on the staff at the US National Institutes of Health. The software has been cited over 15,000 times in peer-reviewed literature and has been used to help generate over 40% of protein structures ever measured by NMR. Frank's career includes commercial software development, extensive pharma consulting, and regular participation as an advanced course instructor for the European Molecular Biology Organization. Frank earned a BA in Chemistry from Syracuse University, and a PhD from the Osaka University Graduate Department of Pharmaceutical Sciences.

Speaker Abstracts

Ryan Nieuwendaal

Having just celebrated its 10th annual conference, the Practical Applications of NMR in Industry Conference (PANIC) has served as a place for industrial, regulatory, government and academic scientists to share day-to-day aspects of NMR-related research. As a conference that is dedicated solely to the practical aspects of NMR, attendees regularly share details that are rarely discussed at other NMR meetings, making PANIC a rare opportunity to broaden knowledge, exchange ideas of the latest NMR developments, and discuss the nitty-gritty details of how to get NMR experiments to work. In this brief introduction to PANIC, I will highlight a few

vignettes from previous PANIC conferences, discuss what PANIC has coming up this year, and share details of our next in-person conference in 2025. Hopefully, everyone will see how fun (and practical!) NMR can actually be!

Frank Delaglio

Protein therapeutics are vitally important clinically and commercially, with monoclonal antibody (mAb) therapeutic sales alone accounting for \$180 billion in revenue for 2022. In order for these therapies to be safe and effective, their protein components must maintain their three dimensional fold and not aggregate. Nuclear magnetic resonance spectroscopy (NMR) is powerful and diverse tool to characterize this higher order structure of protein therapeutics, because NMR spectra are sensitive to molecular shape and intermolecular interactions as well as chemical structure, and NMR can reproducibly probe this information at atomic resolution. Furthermore, NMR has the advantage that it can be applied non-destructively to protein therapeutics as-formulated, with little or no sample preparation. Intriguingly, since NMR can also be applied to quantify the small molecule mixtures comprising the metabolome, NMR has the potential to characterize the growth metabolomics of the cells used in large scale to manufacture mAbs, and also the cells manufactured in small scale for personalized live cell therapies such as CAR-T cancer treatment. Exploiting NMR for these biomanufacturing needs leads to a series of computational challenges which we review, including metrics of spectral similarity, data handling for applications of principal component analysis (PCA), spectral analysis of mixtures, and identification of spectral features by computer vision and machine learning.

Women Chemists Committee Awards and Spring 2024 Events



The Women Chemists Committee (WCC) started the year with an announcement of its new 2024 chair, Lorena Tribe, a Professor of Chemistry at Penn State Berks. WCC will be presenting a new award during the ACS Spring 2024 meeting, the Pfizer Emergent Leader Award. The winners of the WCC Rising Star Award and the Eli Lilly Travel Award will also be recognized at the Spring 2024 meeting.

Here are the other events WCC will be hosting at the Spring 2024 ACS Meeting:

March 18

- Women in the Chemical Enterprise Breakfast featuring Amy Prieto, Professor of Chemistry at Colorado State University and the Founder & Chief Technical Officer of Prieto Battery,
- Women Chemists of Color “Sweet Treats” networking event featuring Raychelle Burks, Associate Professor of Analytical Chemistry at American University, Science Communicator, and recipient of the 2020 ACS Grady-Stack Award for Interpreting Chemistry for the Public

March 19

- WCC Luncheon, featuring the 2024 Garvan-Olin Medal Winner, Donna Huryn.

All events will be held at the Hilton New Orleans Riverside Hotel. The WCC breakfast and luncheon are ticketed events. Update your meeting registration (<https://xpressreg.net/register/acsa0324/xpresstoolkit/login.asp>) to attend. See you in New Orleans!

Carissa Hunters Reflects on ACS Leadership Institute

Carissa Hunter, Committee on Minority Affairs Co-chair, attended the ACS Leadership Institute in Atlanta, GA from January 26-28th. She represented our local section, where she was able to enhance her leadership skills. At the Institute, Carissa fostered new peer networks, learned more about the operations and structure of ACS, developed new leadership and management skills, and was able to identify new key support contacts. The sessions she attended brought about great ideas on motivating and engaging volunteers, grants our section should apply for, and ideas on types of events to best support our community and members. The experience was truly amazing, and she hopes to use what she has learned to help our local section.

Each local section presented a poster about the exciting things happening. Carissa was able to share about the ChemLuminary Award we won in 2023.



2024 Board Meeting Calendar

CSW's Board of Managers (BOM) meets quarterly to discuss CSW business and to have open floor discussion of new business. This includes all officers and reports of committee chairs. Meetings are open to CSW membership. Dates of the board meetings for 2024 are as follows:

- March 11
- May 20
- September 16
- November 21

Our meetings are always from 7pm - 9pm and are hybrid (both in-person at the ACS headquarters and on Zoom). To attend, please email csw@acs.org one week prior to the meeting to be put on the visitor registration for ACS Marvel Hall or to request a Zoom link if attending virtually.

ACS Division of Analytical Chemistry YCC Travel Award

The ACS Division of Analytical Chemistry is offering travel awards for Younger Chemists (under age 35) to travel to a meeting to present the results of their research. Individuals who may not have previously been able to participate in professional meetings are particularly encouraged to apply. Applications are due Nov 1st for winter and spring meetings and May 1st for summer and fall meetings. More information is available on the Division website at <https://acsanalytical.org/ycctravel/>. The application forms will be available when the application period is open.

CSW Member Publication Submission

We would like to highlight the work of CSW Members' accomplishments in terms of publications, book chapters, op-eds, reports, and presentations at local/national/international meetings. If you have such contributions, please complete the Google form using the link below.

Google

Form: <https://forms.gle/zRhFLkRWMdPXoLXNA>

Note that submission does not imply that your work is guaranteed to end up in the newsletter or website. We reserve the right to remove submissions that may be controversial or upsetting to others.



View the full list of submitted publications on the *Capital Chemist* website at <https://capitalchemist.org/2023/01/csw-recent-publications>.

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*A Publication of the Chemical Society of
Washington Section of the American
Chemical Society*

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The **Chemical Society of Washington (CSW)** is the
local ACS Chapter for the Washington, DC area
and serves approximately 3,500 members.

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CSW Calendar of Events

- March 11: CSW Board Meeting
- March 14: CSW Dinner Meeting
- March 21: CSW Dinner Meeting
- May 1: YCC Travel Award Deadline
- May 20: CSW Board Meeting
- September 16: CSW Board Meeting
- November 21: CSW Board Meeting