ACS of Western New York

Double Bond

The Newsletter of the Western New York Section of the American Chemical Society

Volume 96 ***October 2024***

THE JACOB F. SCHOELLKOPF MEDAL

The Western New York Section of the
American Chemical Society
invites you to be present
for the presentation of the
Jacob F. Schoellkopf Medal
TO

Eva Zurek
for 2023

AND TO

Timothy Gregg
for 2024

Wednesday evening, the sixteenth of October
two thousand twenty-four

Cash bar with cold and hot hors d'oeuvres at six o'clock
Dinner at seven o'clock

Presentations to follow dinner

The Hotel at the Lafayette
391 Washington St. | Buffalo, NY 14203

For dinner reservations, please use this link:
https://schoellkopfmedalwn.wixsite.com/wnyacsevents
or
contact the Schoellkopf Chair, Luis Velarde

OFFICER CANDIDATE BIOGRAPHIES

The following slate of candidates for 2025 WNYACS Executive positions has been established. In accordance with our bylaws, an election ballot will be circulated. Look for a separate email with an election link to our provider, **ElectionBuddy.com**. You need the Access Key and Password that are included in the notification email from ElectionBuddy.com in order to vote. Brief biographies of the officer candidates are presented below.

Chair (2025): Chris Li
Chair-Elect (2025): Jason Benedict
Vice-Chair (2025):
Secretary (2025-2026): Caitlyn Montross
Councilor (2025-2027): David Nalewajek
Member at Large (2024-2025): Matthew Crawley

Other officers currently serving in various roles are listed on page 4. Anyone interested in getting involved with the local section is encouraged to contact these folks, as we are always looking for new people interested in contributing ideas or in helping to organize events.

For Chair (2025):

Chris Li is currently an Assistant Professor at the University at Buffalo, SUNY. Chris received his undergraduate degree at the University of California, Davis in Chemical Engineering and he subsequently worked as an R&D engineer in chemical industries for three years. Chris received his Ph.D. degree in Chemistry at Pennsylvania State University with Prof. Tom Mallouk working on CO_2 reduction and electrochemical system design. From 2018 to 2020, Chris joined Prof. Ted Sargent's group as a postdoctoral scholar at the University of Toronto. At the University at Buffalo, SUNY, Chris' research group focus on developing electroanalytical techniques to study chemical mechanisms in electrocatalysis reactions, and reactor design for energy storage and environmental applications.

For Chair-Elect (2025):

Jason Benedict is a Professor in the Department of Chemistry at the University at Buffalo. His research seeks to understand and ultimately control the interaction of light and matter in crystalline materials. From photo-responsive metal-organic frameworks to low-flux upconversion materials, his research is focused on the design and synthesis of next-generation smart 'materials by design'. Jason is also active in outreach programs; he recently chaired and organized the 7th annual Western New York Undergraduate Research Symposium and the U.S. Crystal Growing Competition – a fun STEM activity for students in grades K-12.

Jason received his B.S. in Chemistry from Arizona State University. He received his Ph.D. from the University of Washington with Bart Kahr. Jason worked as a postdoctoral researcher with Philip Coppens at UB before joining the faculty in 2011.

For Secretary (2025-2026):

Caitlyn Montross is an Associate Professor in the Natural Sciences department at Daemen University. She teaches primarily Organic, Bioorganic, and Medicinal chemistry courses to undergraduate students. She is actively involved in undergraduate research spanning topics from designing fouling-release coatings for the deterring of zebra mussels to the detection of PFAS in soil and snow melt samples on ski hills to the generation of active learning assignments suitable for lecture or lab to increase student engagement and comprehension of chemical concepts. She received her Ph.D. from the University at Buffalo in 2017.

For Councilor (2025-2027):

David Nalewajek is currently an ACS Fellow and recently retired Research Fellow at Honeywell. He received his B.S. in chemistry from Canisius College in 1974 and his Ph.D. from UB in 1978. His postdoctoral was spent at AT&T Bell Laboratories where he researched the design and synthesis of multidimensional superconductors. His current research interests remain in the development of environmentally acceptable CFC replacements and fluorine based polymers for use in electronic and membrane separation technologies. He currently holds 95 U.S. Patents. Dave has been active in community outreach activities since 1980, serving as lecturer/demonstrator at the Buffalo Museum of Science and at local elementary schools. Within the WNYACS organization, he has held positions of member-at-large, vice-chair, chair-elect and chair. He has served as councilor for this Section since 1992. In addition, Dave has served three terms as chair of the Schoellkopf committee and was the recipient of the Schoellkopf award in 2003. In 2013, Dave was recognized as ACS Volunteer of the Year for the WNY Section. In 2015, he was elected as Fellow of the American Chemical Society for his work on CFC replacements and promotion of STEM initiatives in the WNY community. Dave also serves as chair for National Chemistry Week where he has served as chair/co-chair since its inception.

For Member at Large (2024-2025):

Matthew R. Crawley was born and raised in Wilson, NY. He attended the University at Buffalo, where he completed his B.S. in Chemistry, graduating summa cum laude. Initially working as an undergraduate researcher in Sarbajit Banerjee's lab, and later in Timothy Cook's lab. Matt went on to earn his Ph.D. in chemistry under the tutelage of Timothy Cook working on multinuclear catalysts for energy-relevant small molecule activations. Currently, he continues his work in the Cook Lab as a postdoctoral researcher. In addition to postdoctoral research, Matt has lectured several courses including general chemistry. Matt's research interests focus on structure elucidation and physical inorganic chemistry, of particular interest are high-resolution X-ray crystallography and heteronuclear and 2D-NMR techniques.

WNYACS SCHOELLKOPF MEDAL DINNER

Oct 16, 2024, 6:00 PM – 10:00 PM

For 94 consecutive years the WNY Section of the American Chemical Society has recognized the work of its peers' accomplishments, continuing service, and achievements

Dinner Selections:

Filet Mignon

Herb Roasted Salmon

Eggplant Parmesan

Wine served with meal

Tappo at the Lafayette,
391 Washington St, Buffalo, NY

$50.00 per person ($25.00 per student)

Business casual to cocktail attire is welcome

Please RSVP by October 7, 2024

For tickets, please use the link to the registration site:
schoellkopfmedalwn.wixsite.com/wnyacsevents

For questions or cash payment arrangements email Luis Velarde (lvelarde@buffalo.edu) or Luis De Jesús Báez (ldjesus@buffalo.edu)

THE SCHOELLKOPF MEDAL RECIPIENT

2023

The award jury has selected Eva Zurek, Professor in the Department of Chemistry at the University at Buffalo, SUNY, to receive the 2023 Jacob F. Schoellkopf Medal

in recognition of pioneering contributions to the fields of superconductivity, high pressure science and technology, and superhard materials chemistry through the development of computational methods for a priori prediction of the structures of solids, emergent properties of materials under high pressure, and the way molecules orient and organize on surfaces and within nanoscale architectures.

Eva Zurek was born in Kraków, Poland, coming to Canada at age 5. Eva received a BSc and an MSc from the University of Calgary. In Calgary she conducted computational chemistry research, with Tom Ziegler, on methylaluminoxane, one of the most industrially important activators for alkene polymerization. Here, Eva met her future husband Jochen, who was a postdoctoral fellow in Tom Ziegler's group.

Eva accepted a Ph.D. fellowship from the *Max Planck Research School for Advanced Materials* in Stuttgart, Germany, where she worked with Ole Krogh Andersen and Arndt Simon, combining their experience in computational physics and inorganic synthesis. Eva received her Ph.D. from the University of Stuttgart in 2006, and stayed on in Andersen's group for another year as a postdoctoral fellow. In her research she applied techniques of computational chemistry and band structure methods to a wide variety of topics including nanotubes and fullerenes, developing methods to calculate Wannier functions in solids, and studying the electronic structure of solids under high pressure.

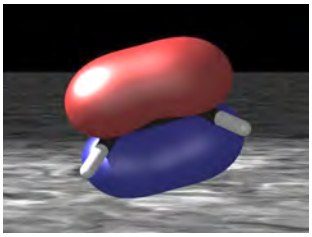
In 2008 and 2009, Eva was a postdoctoral associate at Cornell University with Nobel Laureate Roald Hoffmann. At Cornell, she used computations to study the species that might comprise metal-ammonia solutions (in collaboration with Peter Edwards, professor of Inorganic Chemistry at Oxford University) and hydrogen-rich compounds under pressure (in collaboration with eminent physicist Neil Ashcroft). On the weekends she visited Jochen in Buffalo.

In 2009 the two-body problem was solved, and Eva became an Assistant Professor at UB, where she was promoted to Full Professor in 2016. Since then, Eva received the *Alfred P Sloan Fellowship* (2013), *The Minerals, Metals and Materials Society Young Leader Award* (2014), *UB Exceptional Scholar Young Investigator Award* (2014), *Quantum Systems in Chemistry and Physics Promising Young Scientist Award* (2014), the *APT Teaching Award* from UB (2016), a *SUNY Chancellor's Award for Excellence in Scholarship* (2021), and became a *SUNY Distinguished Professor* (2024). In 2024 Eva was selected as a *Physical Science Finalist* by the *Falling Walls Foundation*, and in 2021 she was named a fellow of the *American Physical Society (APS)*.

Currently, Eva serves as an editorial board member of *Physical Review Materials*, and she is Chair for the APS's *Division of Computational Physics*. She has served on numerous APS committees, and was key in establishing the *Neil Ashcroft Early Career Award for Studies of Matter at Extreme High Pressure Conditions*. Eva has been interviewed by *Scientific American*, NPR's *Science Friday*, CBC's *Quirks and Quarks,* the *New York Times*, *C&EN News*, *Chemistry World* and other venues on breakthroughs in materials discovery.

At UB Eva's research has been geared towards studying the electronic structure, properties and reactivity of a wide variety of materials using first-principles calculations. She is interested in high pressure science, superhard, superconducting, quantum and planetary materials, catalysis, as well as solvated electrons and electrides. Her group, comprised of chemists, physicists and materials scientists and chemical engineers, develops algorithms for the *a priori* prediction of the structures of crystals, interfaces them with machine learning models, and applies them in materials discovery. As of 2024, Eva had published or submitted around 200 original research articles and book chapters, and given over 150 invited conference, seminar, or workshop talks and presentations.

When Eva had time she used to enjoy photography, hiking, skiing and scuba diving. Now, she enjoys everyday adventures with her children, Adrian (9), Isabella (7) and Julian (almost 5), and her husband Jochen.



THE SCHOELLKOPF MEDAL RECIPIENT

2024

The award jury has selected Dr. Timothy M. Gregg, Associate Professor in the Department of Chemistry and Biochemistry at Canisius University, to receive the 2024 Jacob F. Schoellkopf Medal

> *in recognition of his outstanding dedication to teaching and mentoring and his selfless service to the Western New York Section of the American Chemical Society.*

Tim grew up on Cape Cod, Massachusetts, where he was inspired by his high school chemistry teacher who introduced organic chemistry to the class after running out of the usual high school chemistry topics. Tim studied medieval studies and chemistry at Brown University, deciding ultimately to pursue the more marketable of these interests. There, he worked with Prof. David E. Cane on organic synthesis directed toward terpene biosynthesis mechanism studies, and received his AB degree in 1989. His interests took him to The University of Arizona, where he studied organic synthesis with Prof. Eugene A. Mash. This work included methodology studies on selective reactions of conformationally flexible cyclic substrates, as well as synthesis of putative metabolites of environmental contaminants. He received his PhD in 1995.

At that point, Tim and his wife, Tracy, a geologist, also with a newly minted PhD, pursued postdoctoral positions, and with luck and hard work settled in eastern Massachusetts. Tim joined Prof. Robert Abeles' lab at Brandeis University, synthesizing novel mechanism-based enzyme inhibitors, while Tracy studied submarine lava flows at Woods Hole Oceanographic Institution. In 1998, they moved to Buffalo where Tracy started her appointment as the first woman ever hired as an Assistant Professor in the UB Department of Geology, and Tim began postdoctoral studies at UB with Prof. Huw Davies in the Department of Chemistry.

At UB, Tim received an NIH Postdoctoral Fellowship, and later helped secure an NIH synthesis core facility contract for Davies' group, providing investigational compounds to the National Institute on Drug Addiction. He was involved in rhodium carbenoid cyclopropanation and C-H insertion research, including computational investigations into carbenoid reaction mechanisms. He was appointed as a Research Assistant Professor at UB in 2002. In 2005, Tim started as an Assistant Professor in the Department of Chemistry and Biochemistry at Canisius College.

In the 20 years he has been at Canisius, Tim has taught chemistry at all levels, retaining a soft spot for organic spectroscopy, especially the clean lines of a well-shimmed NMR. Over 25 undergraduate researchers have spent summers immersed in projects in his lab, with 15 continuing on to earn MD and PhD degrees. Though he cannot claim too much of the credit for their ultimate successes, Tim takes pride that his students are now physicians in a variety of specialties, or are research scientists at institutions including Roswell Park, Honeywell, Pfizer, Merck, Johnson & Johnson, and PPG Industries.

Through all the teaching and mentoring at Canisius, Tim has also steadfastly supported the Western New York Local Section of the American Chemical Society. He has been WNYACS newsletter editor, and web site developer for 20 years. He has helped to organize elections, speakers, and the popular Undergraduate Research Symposium.

When not immersed in classes and labs, Tim enjoys growing daylilies and tinkering with the design and construction of model sailboats. He is also the forge master for the Niagara region of the New York State Designer Blacksmiths. While vacations with a volcanologist in the family are interesting, Tim and Tracy and their 2 children, Robert and Edith, are happy to have western New York to call home.

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