

A Publication of the Southern California Section of
the American Chemical Society

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JANUARY/FEBRUARY 2025

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2025

Happy New Year!



ACS
Chemistry for Life®

SCALACS

A Publication of the Southern California Section of the
American Chemical Society

Volume LXXX

JANUARY/FEBRUARY 2025

Number 1

SOUTHERN CALIFORNIA SECTION 2025 OFFICERS

Chair:

Veronica Jaramillo

Chair-Elect:

Edye Udell

Secretary/Treasurer:

Barbara Belmont

Executive Committee Members at Large:

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Sunhwa (Clarita) Joung

Krishna Kallury

Benjamin Ku

Eric Kuenstner

Jessica Lu

Aaron Moment

Lucky Morales

Sahar Roshandel

Councilors:

Brian Brady

Robert de Groot

Veronica Jaramillo

Eleanor Siebert

Barbara Sitzman

Alternate Councilors:

Elham Fazelpour

Krishna Kallury

Thomas Mathew

Michael Morgan

Alexandros Oxyzolou

Immediate Past Chair:

Richard Kidd

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CHAIR'S MESSAGE



Dear SCALACS members,

As a new year unfolds, I find myself reflecting on the remarkable journey of the Southern California Local Section of the American Chemical Society (SCALACS) over the past year. We have accomplished so much, from engaging the broader community through impactful outreach programs to fostering intellectual growth within our membership through thought-provoking seminars.

Our outreach efforts have been truly inspiring. We have reached out to many students, igniting their curiosity about chemistry through interactive demonstrations and engaging workshops. The impact of these initiatives has been deeply rewarding, as we inspire the next generation of scientists.

The SCALACS seminar series has consistently provided a platform for insightful discussions and valuable knowledge sharing. A particular highlight is mentioned in this newsletter, "Science at Schrödinger" by Dr. Katherine Bay which highlighted the uses of AI in STEM education.

Beyond scientific pursuits, we have also cultivated a strong sense of community among our members. Our visit to the Getty Museum, for instance, provided a unique opportunity for members to connect on a personal level and explore the fascinating interplay between art and science.

Looking ahead, we have an exciting array of events planned. We will be participating in the City of STEM + LA Maker Faire on March 29, where we will showcase the wonders of chemistry to the public. We are also thrilled to partner with the LA Zoo on April 12 for a special program designed to "Engage Girls in STEM" through interactive exhibits and engaging activities. Furthermore, we are planning a series of networking events to foster meaningful connections among our members, providing valuable opportunities for professional growth and collaboration.

Two significant national initiatives will also be celebrated this year. Chemists Celebrate Earth Week (CCEW), from April 20-26, will focus on the captivating theme of "Glaciers: Hot Topic, Cool Chemistry." And during National Chemistry Week (NCW), from October 19-25, we will delve into the fascinating "Hidden Life of Spices."

To ensure that SCALACS continues to thrive and effectively serve the needs of our members, we are organizing a strategic planning workshop this spring. Your valuable input is crucial as we collectively chart the course for the future of our organization.

I encourage each and every member to actively participate in the vibrant life of SCALACS. Share your ideas, volunteer your time, and help us build a thriving community of chemists. Stay connected with SCALACS through our website and social media channels.

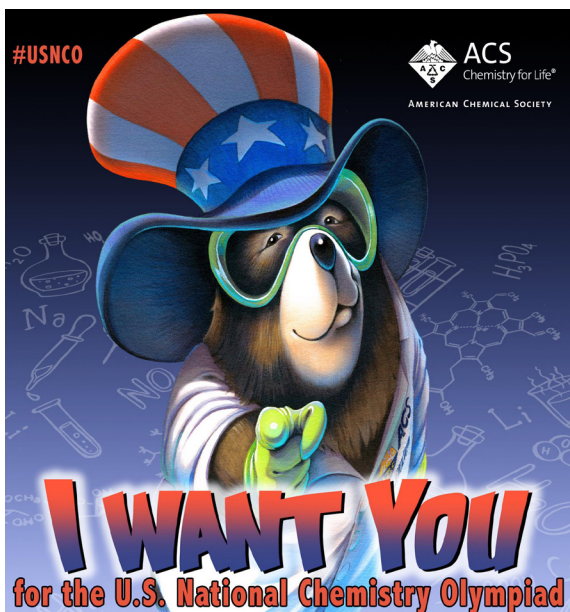
Sincerely,

Veronica I. Jaramillo, Ph. D.

Dean of Natural Sciences

Fellow of the American Chemical Society

SCALACS 2025 Chair



2025 US NATIONAL CHEMISTRY OLYMPIAD

Teachers, the **online registration form** for the 2025 US National Chemistry Olympiad on the ACS website is open now. Deadline for registration is **January 17, 2025**. Registration after this date will not be accepted by USNCO.

Only **parents or guardians of students CAN register** a participating student at the ACS website via the link below. **Teachers will not be allowed** to register students and **students will not be allowed** to register themselves. **If parents or guardians do not register their student with USNCO by the January 17, 2025 deadline, the student will not be able to participate in the local exam.**

Teachers, please copy and send this link to your students for their parents or guardians to register: <https://www.acs.org/education/olympiad.html>

Once registration closes, an **\$11 exam fee** per student is required. The SCALACS office will send the parents of the participating students a payment link via email. Payment must be received by **February 14, 2025**.

KEY DATES FOR 2025 USNCO EXAM

*Schedule is subject to change. All changes will be posted on the USNCO website:
<https://www.acs.org/education/olympiad.html>*

November 15, 2024	Online Registration opened
January 17, 2025	Student Registration closes
February 14, 2025	Payment Deadline
March 19-20, 2025	Local Section Exam for SCALACS
April 5-13, 2025	National Exam
June 1-14, 2025	Study Camp
July 5-14, 2025	2025 International Chemistry Olympiad

Any questions, please contact our SCALACS administrator, e-mail office@scalacs.org or call 310-327-1216.

2025 SCALACS GOVERNANCE ELECTION RESULTS

Our Election for 2025 SCALACS Governance has concluded. This election was processed by ElectionBuddy.com. We thank all other members who submitted their votes. The SCALACS Elected Governance for 2025 is as follows:

ELECTED OFFICERS:

CHAIR: Veronica Jaramillo

CHAIR-ELECT: Edye Udell

SECRETARY/TREASURER: Barbara Belmont

EXECUTIVE COMMITTEE MEMBERS AT LARGE:

David Hanna (Jan. 2023 – Dec. 2025)

Sunhwa (Clarita) Joung (Jan. 2025 – Dec. 2027)

Krishna Kallury (Jan. 2025 – Dec. 2027)

Benjamin Ku (Jan. 2023 – Dec. 2025)

Eric Kuenstner (Jan. 2025 – Dec. 2027)

Jessica Lu (Jan. 2024 – Dec. 2026)

Aaron Moment (Jan. 2024 – Dec. 2026)

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Sahar Roshandel (Jan. 2023 – Dec. 2025)

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Robert de Groot (Jan. 2025 – Dec. 2027)

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Eleanor Siebert (Jan. 2025 – Dec. 2027)

Barbara Sitzman (Jan. 2023 – Dec. 2025)

ALTERNATE COUNCILORS:

Elham Fazelpour (Jan. 2025 – Dec. 2027)

Krishna Kallury (Jan. 2023 – Dec. 2025)

Thomas Mathew (Jan. 2025 – Dec. 2027)

Michael Morgan (Jan. 2025 – Dec. 2025)

Alexandros Oxyzolou (Jan. 2024 – Dec. 2026)

IMMEDIATE PAST CHAIR:

Richard Kidd

Election Dates: October 16 - November 24, 2024

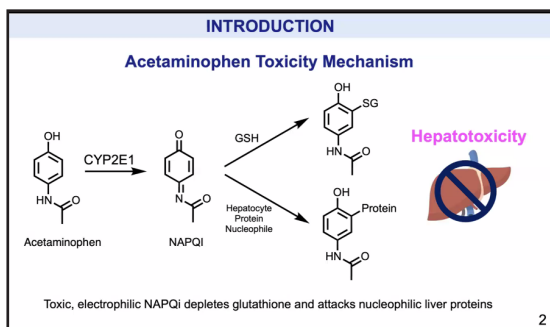
Election Vendor: ElectionBuddy.com

Submitted by and certified by Barbara Belmont, SCALACS Secretary/Treasurer

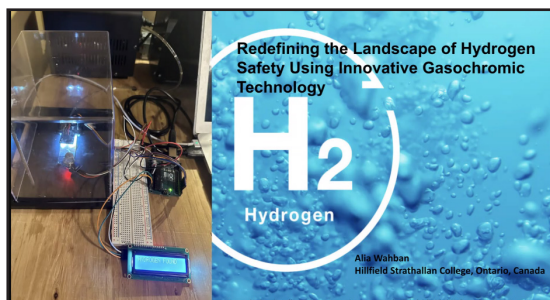
HIGH SCHOOL STUDENTS RESEARCH SYMPOSIUM

LIST OF TOP TEN PRESENTERS

The Virtual High School Students Research Symposium, held on November 2, 2024, featured 22 talented high school students from the U.S. and Canada, each presenting their impressive research. This event was made possible through the support of the ACS LSAC-Innovative Projects Grant (IPG). Below are the top ten presenters, who were awarded a \$100 gift card for their outstanding presentations.



CHLOE LEE (Texas)
 IB World School at
 Plano East Senior High School
 Title: Chemical Modification of
 Acetaminophen to Decrease Liver Toxicity
 and Enhance Drug Efficacy



ALIA WAHBAN (Canada)
 Hillfield Strathallan College,
 Hamilton, Ontario
 Title: Redefining the Landscape of Hydrogen
 Safety using Innovative Gasochromic
 Technology

Introduction

- Skin cancer is the most prevalent cancer worldwide.
- **8 million** incidences and **120,000** deaths annually¹.
- 5-year survival rate of Melanoma is just **15%** if detected late²; it can become **deadly in 6 weeks**².
- Early detection is critical in preventing cancer development and lethality.

Current Diagnostics

- 1. Primary care visual inspection**
 - 40% Misdiagnosis rate³
- 2. Specialist visual dermoscopy**
 - 20% Misdiagnosis rate⁴
 - Low specificity⁴
 - Long referral wait times
 - Specialized training shortage
- 3. Skin biopsy**
 - Highly invasive
 - Expensive: \$100-\$400⁵
 - 55% unnecessary benign cases⁵
 - 5 million U.S. biopsies yearly⁶

5,000,000 x 55% x \$200
= **\$550,000,000 wasted annually.**

Anthony EFthimiadis

ANTHONY EFTHIMIADIS (Canada)
 Oakville Trafalgar High School
 Title: Rapid Screening for Major Skin
 Cancers with Interpretable CNN-Transformer
 Hybrid Networks, Lesion Evolution Tracking,
 Trait Identification, and Color Constancy
 for Improved Generalization in Diverse
 Populations

1 | Introduction

1) Lactational Mastitis:
 A breast infection that happens in lactating women. Mastitis can enter through a crack in the nipple's skin or a milk duct opening. There are two types of mastitis: Clinical and Subclinical [1]

3) Characterized by hardening of the breast and the breast's color turning to red, with associated burning pain

The mothers physiological state (food, medication, immunity, hormones, etc.) are transferred to the infant through breast milk.

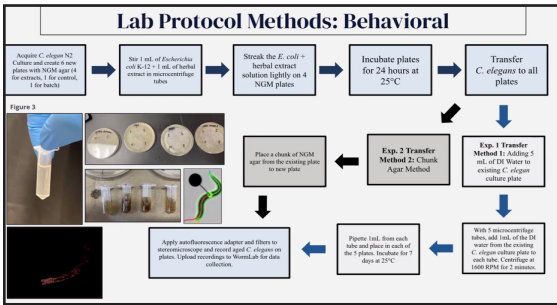
Fig 1 illustrates how elements of the mother's physiological state (such as mastitis) pass to the infant via breast milk.

2) 7-10% of U.S. women experience lactational mastitis [2]

4) Cause:
 Hyper-lactation
 Excessive pressure on the breast
 Stress / fatigue

USC Viterbi School of Engineering 8-22-2024 Center [1]Hewitt, C. (2016). Acute, subclinical, and subacute mastitis: Definitions, etiology, and clinical management. Clinical Lactation, 7(2), 1-9. [2]Hewitt, C. (2016). Lactational mastitis: Occurrence and medical management. Breastfeeding medicine: An Official Journal of the International Board of Lactation Consultant Examiners

ABDARHMAN SHEER (California)
 Francisco Bravo Medical
 Magnet High School
 Title: Laser-Induced Graphene-Based
 Sensor for Detection of Subclinical Mastitis



RAMIN SARKAR (Georgia)
 Gwinnett School of Mathematics,
 Science and Technology
 Title: Treatment Analysis for Alzheimer's
 Using Caenorhabditis elegans as a Model

Targeting NF- κ B in Acute Myeloid Leukemia via Oligonucleotide Therapeutics

Hriday Meka
 North Hollywood High School, Los Angeles,
 California

HRIDAY MEKA (California)
 North Hollywood High School
 Title: Targeting NF- κ B in Acute
 Myeloid Leukemia via Oligonucleotide
 Therapeutics"

METHODS

Independent Variables	Dependent Variable	Hypothesis
<p>Treatments:</p> <p>Industry Standard Control: Oxytetracycline (1.5 g dissolved in 98.5 mL) as approved by EPA</p> <p><i>Murraya koenigii</i> extract concentrations:</p> <ul style="list-style-type: none"> • 10% Concentration (LR) • 20% Concentration (MR) • 30% Concentration (HR) <p>Untreated Control: Plants not receiving any treatment</p>	<ul style="list-style-type: none"> • Control/Management of <i>Candidatus Liberibacter asiaticus</i> as reflected by qPCR, disease severity, chlorophyll content, plant vigor, and stomatal conductance <p>Constants</p> <ul style="list-style-type: none"> • Water • Sunlight • Fertilizer • Temperature <p>*Experiment was replicated 10 times. (5 treatments x 10 replications)</p>	<p>Hypothesis: If the novel bactericide derived from curry leaf extract is delivered through trunk injection, it will exhibit high efficacy in managing the <i>Candidatus Liberibacter asiaticus</i> bacterial population, improving citrus physiological processes, and holistically managing the disease severity.</p>

TANISHKA AGLAVE (Florida)
 Strawberry Crest High School IB
 Title: Advancing Sustainable Citrus
 Greening Disease Management: A
 comprehensive eco-friendly approach
 for the management of candidatus
 liberibacter asiaticus using trunk injection
 of murraya koenigii derived biological
 extract and its validation through
 precision agriculture tools

Prediction of Hippocampal Morphology During Aging

Lucia Ortega
 Grade 12
 Francisco Bravo Medical Magnet High School

LUCIA ORTEGA (California)
 Francisco Bravo Medical
 Magnet High School
 Title: Prediction of Hippocampal
 Morphology During Aging

BCHM018

Breastmilk: Nature's Vaccine Against COVID-19

Human Milk Immune Complexes Isolated Following
 Pregnancies Complicated by COVID-19 Infection Contain
 SARS-CoV-2 Nsp13 Helicase and Biologically Active Factors

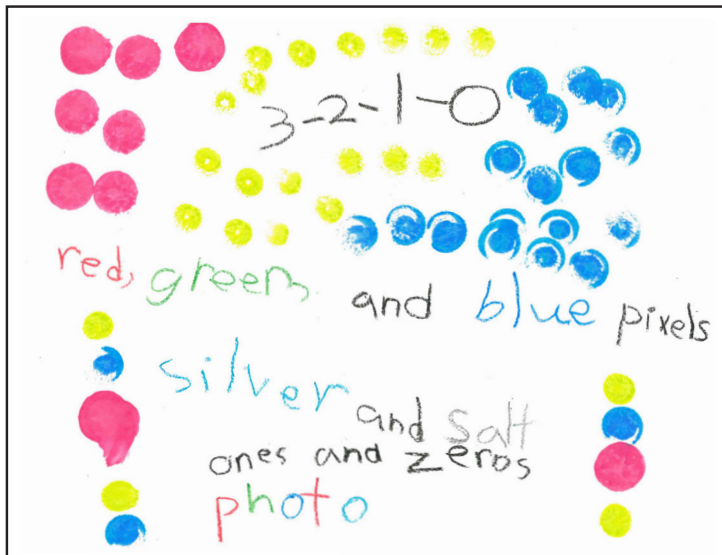
Vaishnavi Kolluru
 Dougherty Valley High School
 San Ramon, CA, USA

Unless otherwise specified, all visuals were either hand-drawn and assembled by
 Vaishnavi Kolluru, or created by Vaishnavi Kolluru using Excel.

VAISHNAVI KOLLURU (California)
 Dougherty Valley High School
 Title: Human Milk Immune Complexes
 Isolated Following Pregnancies
 Complicated by COVID-19 Infection
 Contain SARS-CoV-2 Nsp13 Helicase
 and Biologically Active Factors

(Continued on page 10.)

2024 SCALACS NCW POEM CONTEST WINNERS



As part of NCW 2024, students from grades K-12 were invited to share their interpretation of this year's theme, "Picture Perfect Chemistry", in the form of illustrated poems. Winners at the local section level qualified for the national contest.

Congratulations to these two winners of our local section.

Winner for K-2 category:

RALPHAEL HEBIE

GRADE 2

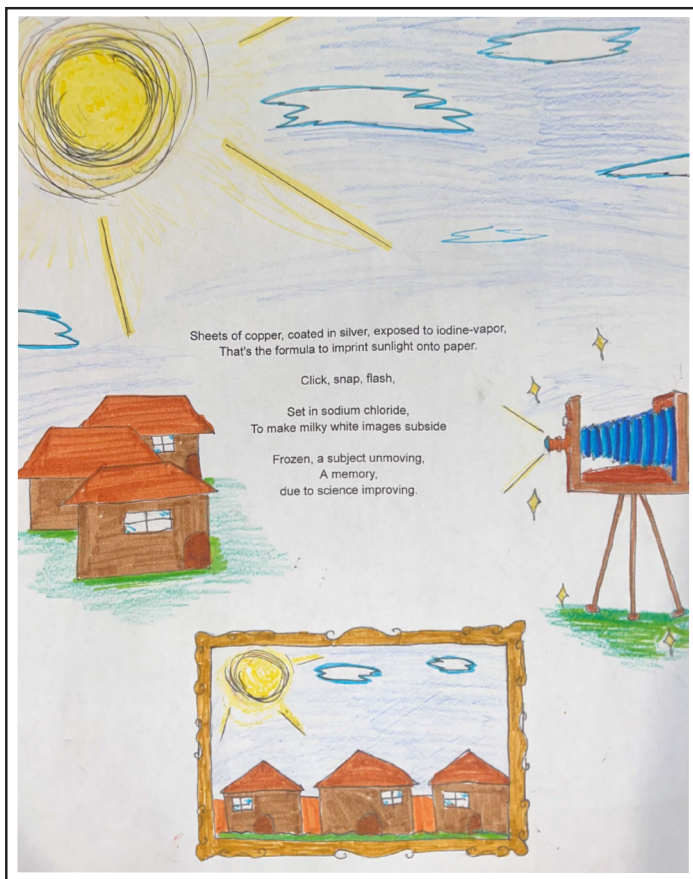
LOS OLIVOS ELEMENTARY SCHOOL

Winner for 9-12 category:

SOPHIE DADIKOZIAN

GRADE 12

CLARK MAGNET HIGH SCHOOL

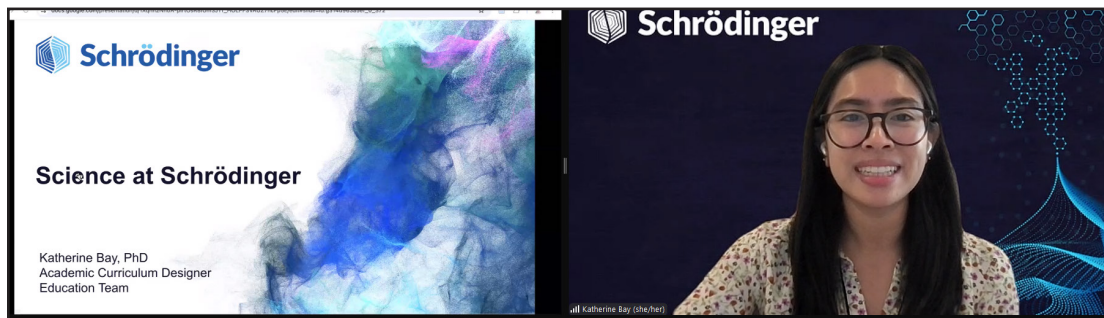


Check out the national winners here:

<https://www.acs.org/education/national-chemistry-week/plan-an-event/illustrated-poem-contest/winners.html>

SUMMARY OF THE "SCIENCE AT SCHRÖDINGER" SEMINAR

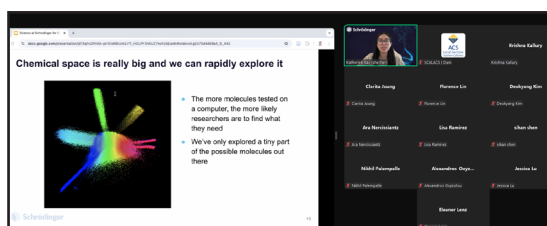
Presented by Dr. Katherine Bay, Senior Scientist at Schrödinger on
November 15, 2024



The seminar was organized in fulfillment of one of the project goals of the LSAC grant proposal awarded to SCALACS in early 2024, viz. "The Utility of Artificial Intelligence (AI) in STEM Education & Research". The speaker, Dr. Katherine Bay, is a specialist in the applications of AI as an educational tool and in drug discovery research. She works as a Senior Scientist at Schrödinger leading the "Teaching with Schrödinger" program and developing academic curricula that integrate Schrödinger's molecular modeling tools in the classroom.

Schrödinger, Inc. is an international scientific software and biotechnology company that specializes in developing computational tools and software for drug discovery and materials science. Their software is used by pharmaceutical companies, biotech firms, and academic researchers to simulate and model the behavior of molecules at the atomic level. This accelerates the design and development of new drugs and materials more efficiently, reducing the time and cost of bringing them to market. The company's software tools include molecular dynamics simulations, free energy calculations, quantum mechanics calculations, and virtual screening tools. The company also offers consulting services and collaborates with partners in the industry to advance the field of computational chemistry and drug discovery.

At the outset, Dr. Bay introduced herself as a former student at Artesia High School, then graduated from Univ. of La Verne, and later obtained her Ph.D. at UCLA. After a brief period of teaching at La Verne, she joined Schrödinger. She commenced her seminar explaining how tedious and expensive the drug discovery process has been. It takes 10-15 years and



several billion dollars to commercialize a drug. Computing tools help in simplifying the process by integrating machine learning with computing to optimize the physical parameters. Schrödinger's "Rapid Discovery" Program cuts down the drug development timeframe from seven years to around 10 months.

She explained how computing the physical properties of a molecule (properties shown in parentheses in the following examples) provides solutions to investigational screenings. Examples: How much dosage? (Potency, Bioavailability), How long a drug will stay in the body? (Clearance), Will other medicines interfere? (Drug-Drug Interactions), Will the drug reach the targeted site? (Permeability and Selectivity), Will there be side effects? (Selectivity), Can we make it? (Synthesizability), and Will it make the person sick? (Toxicity).

By extending the principle of the historic Schrödinger equation, quantum mechanics and molecular dynamics through computational studies enable us to check target validation, lead



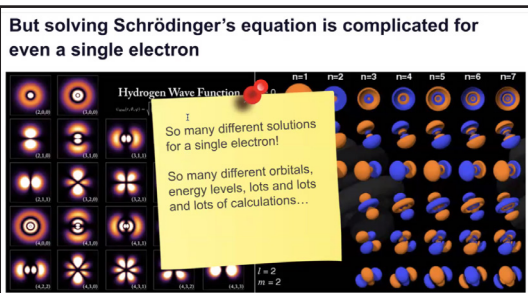
Students of Ms. Clarita (Sunhwa) Jung, Science Teacher at Pacifica Christian School joined the virtual presentation of Science at Schrödinger by Dr. Katherine Bay.

optimization, hit identification and preclinical development. Dr. Bay illustrated these check marks with the example of predicting how a drug molecule binds to a protein.

Dr. Bay described Schrödinger's contribution to an investigational drug SGR-1505, a mucosa associated lymphoid tissue lymphoma translocation protein 1 (MALT1) inhibitor. The FDA gave clearance for an NDA (New Drug Application) for SGR-1505 and it is in clinical trial now. Schrödinger leveraged their physics-based computational platform to rapidly identify novel MALT1 allosteric inhibitors with high potency, high specificity and other important drug-like properties. Multiple tumor models confirmed the potent anti-tumor activity of SGR-1505 as a monotherapy and in combination with standard care agents for the treatment of B cell malignancies.

She concluded her presentation by describing Schrödinger's Certification Courses, which include:

- (1) Introduction to molecular modeling in drug design,
- (2) Introduction to computational antibody engineering,
- (3) PyMol 3.0 (latest advancement in 3D molecular visualization and animation software),
- (4) Organic electronics,
- (5) Homogeneous catalysis and reactivity,
- (6) Surface chemistry,

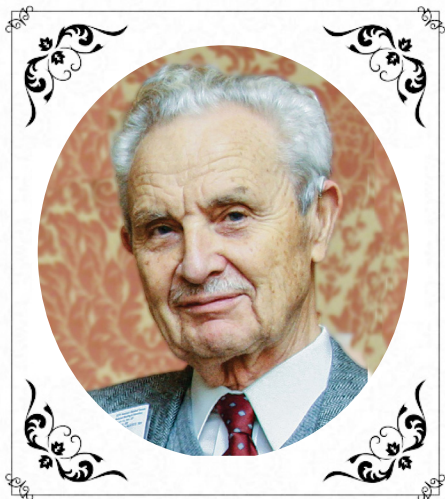


- (7) High throughput virtual screening for hit finding and evaluation,
- (8) Free energy calculations for drug design with FEP Plus,
- (9) Pharmaceutical formulations,
- (10) Battery materials,
- (11) Polymeric materials, and
- (12) Consumer packaged goods.

Schrödinger also offers educational lessons for chemistry courses in general, organic, advanced organic and medicinal/biochemistry areas. Their website <http://www.schrodinger.com/teaching-with-schrodinger> gives more information.

Dr. Bay also answered a number of questions from the student and regular audiences in attendance. The seminar generated tremendous enthusiasm among science teachers and their students.

All summaries for SCALACS virtual seminars and symposia are written by Krishna Kallury.



In Memoriam

CELEBRATING THE ACHIEVEMENTS OF ATTILA E. PAVLATH (1930-2024)

By Krishna Kallury

(Member of the National Senior Chemists Committee & Chair, Senior Chemists Committee/Professional Relations, Southern California Local Section)

I had the pleasure of working with Dr. Pavlath on the National Senior Chemists Committee (SCC) for the past two years (2023-24) and got to know his dedication to chemistry firsthand. Dr. Pavlath was the Chair of the SCC Sub-Committee on ACS Fellows and a member of the SCC In-reach National Meetings Planning Sub-Committee and the Partnerships to expand work with the Office of Philanthropy. He helped in the set up and presentation of our SCALACS posters at the 2023 ACS Fall Meeting in San Francisco and the 2024 Fall Meeting in Denver. These posters highlighted the collaborative efforts of SCC/SCALACS and SCC/National ACS which were supported by Dr. Pavlath.

Attila Pavlath functioned as Senior Emeritus Scientist at the U.S. Department of Agriculture (USDA) until his last days. He received his education in Budapest, Hungary. After his stint as an assistant professor at the Technical University of Budapest, he left Hungary in 1956 and joined McGill University, Canada, as a research fellow. In 1958, he joined Stauffer Chemical Company, California, to lead a research group on agriculture-related problems. In 1967, he joined the USDA, where he headed several research projects at the Western Regional Research Center, Albany, California, and was involved in research until his passing. Dr. Pavlath published more than 130 research papers, authored 10 books and numerous chapters, and held 25 patents. In 1997, he received the Pioneer of the Year award from the American Institute of Chemists. In 1999, he was elected President of the American Chemical Society and in 2004, he was elected to the Hungarian Academy of Sciences. In 2018, he was awarded Charles Lathrop Parsons Award by the ACS Board of Directors for outstanding

public service in advancing the impact of chemistry on society.

During his research at the US Department of Agriculture (USDA) Western Regional Research Center in Albany, California, Dr. Pavlath met many challenges, not the least of which were the shifting research priorities at the USDA that compelled him to move into new areas.

An article in *Vortex* 2023, Volume 85 (issue 1) of California Local ACS Section Newsletter describes his contributions when the USDA shifted its concerns from fabrics and biofuels to preserving produce, keeping dairy cattle healthy, and finding substitutes for petroleum-based wrapping materials. The following excerpt is quoted from this article.

"The skin of an apple keeps it fresh by preventing it from losing moisture and protecting it from oxygen in the air. If you cut an apple open, the exposed surface oxidizes and turns brown in a matter of minutes, and the fruit dries out as water escapes into the atmosphere. Consequently, if you want to make a fruit salad that includes apple slices, you need to prepare the apples immediately before serving. The same applies to many other fruits and vegetables with a protective skin. Refrigeration can slow the deterioration, but only for a few hours. This creates problems for food preparation in industrial, hospital, and school cafeterias, where the cleaning, paring, coring, and slicing of fruits and vegetables is very labor-intensive if done on-site.

Yet today, you can go to the supermarket and buy refrigerated apple slices, fruits, and vegetables that remain fresh, nutritious, and tasty for as long as two weeks. Institutions can now provide more fresh fruits and vegetables

in their cafeterias because these items, like the salads you buy in the supermarket, can be processed at a central location and shipped to the site without spoilage. All of this is a direct result of Dr. Pavlath's work on edible films at the USDA."

Dr. Pavlath's challenge was to find a replacement for the fruit's natural protective skin that would keep oxygen out, keep moisture in, and be indistinguishable from fresh fruit in taste, aroma, and appearance. Studies had shown that human taste buds could detect anything above 0.2% added to the food, so the amount of preservative had to be below that threshold.

For safety, the coating had to adhere to the FDA's strict requirements for food additives. For example, Dr. Pavlath did not investigate using chitosan, an organic carbohydrate found in the skin of shrimp and lobsters. You consume chitosan when you eat shrimp, but the FDA forbids its use as a food additive when extracted from seafood. Eventually, Dr. Pavlath came up with a preservative that consisted of water, calcium ions, and ascorbate ions, where the ratio of calcium ions to ascorbate ions ranges from 1.5:1 to 2.5:1. When dipped into a solution of this preservative, an edible coating forms on the fruit. The coated fruit can be stored at

temperatures from -7° C to room temperature (20° C), with an optimum temperature range of 2° C to 5° C.

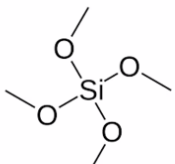
Dr. Pavlath's discovery started an entire industry of edible films. The first companies to use this technology paid the USDA millions in royalties through the 17-year life of the patent. Dr. Pavlath recalls, "The USDA in its kind heartedness, gave me a very small percentage of the royalty — a couple thousand. I didn't do it for money, but because it was a challenge. Like many other things in my life, when a problem appeared and I had to develop new ideas and new ways to solve the problem."

Dr. Pavlath also contributed significantly to fluorine chemistry (see American Chemical Society Monograph Series No. 155, "Aromatic Fluorine Compounds," 2013) and materials for solid fuels rockets in the Space Program (Christe, Karl O.; Guertin, Jacques P.; Pavlath, Attila E., Stauffer Chemical Co, Western Research Center, Richmond, CA, Submission to the US Defence Department, AD0481721 "High Energy Oxidizes").

SCALACS and its members salute the pioneering efforts of Attila Pavlath in advancing chemistry.

(Continued from page 5.)

Methodology



1. Synthesize & purify CsPbBr₃-SiO₂ nanoparticles using varying proportions of TMOS:FCA

- a. **Independent variable:** ratio of TMOS to FCA
- b. **Control group:** 0% TMOS / 100% FCA nanoparticles

2. Characterize nanoparticles to determine optimal synthesis conditions for optical yield and particle suspension

- a. Fluorescence photometry
- b. Dynamic light scattering
- c. Scanning Electron Microscopy
- d. Transmission Electron Microscopy
- i. **Dependent variables:** nanoparticle size, fluorescence spectra/intensity, and physical structure

Above: Chemical structure of tetramethylorthosilicate

KATHERINE LAM (Arizona)
University High School
Title: Novel TMOS-dependent
Synthesis of CsPbBr₃-SiO₂ Core-
Shell Nanoparticles for Biosensing
Applications

We had the honor of hearing from **GRACE SUN**, a 16-year-old junior from Lexington's Paul Laurence Dunbar High School who won the \$75,000 George D. Yancopoulos Innovator Award at the 2024 Regeneron International Science and Engineering Fair that took place in Los Angeles, CA last May. She shared with us her journey in pursuit of STEM education and research.

**My Journey Through
K-12 in Pursuit of
STEM Education and
Research**

Grace Sun
Lexington, Kentucky

Thank you to all the attendees, participants, and judges who were present at this event. We hope that event such as this will inspire more high students to be involved in not only STEM education but research as well.

SUMMARY OF THE 2024 UNDERGRADUATE & GRADUATE RESEARCH SYMPOSIUM

Friday, December 13, 2024 • 9:30 AM - 12:30 PM

The symposium was organized by SCALACS as part of the LSAC/DEIR Grant proposal funded in early 2024. The focus of the proposal was combating climate change and new directions in medicinal chemistry for treating diseases such as cancer. Twelve students were invited to participate, three of them are graduate students and the rest undergraduates. Five of them were from universities in California and the rest from other states. Dr. Thomas Mathew of USC and Dr. Katherine Bay and Emma Kuzcowski from Schrodinger, New York functioned as judges.

Linnea Shu (Undergraduate) and David Pe (Graduate) were the first two speakers, from Tolman award winner Prof. Sarah Tolbert's research group at UCLA. Linnea described her studies on the doping of 3-PHT with LiTFSi (Lithium bis-trifluorosulfonyl imide) in different solvents to increase the conductivity. David spoke about enhancing the power of Li-ion batteries by doping the electrodes with transition metals like tungsten or Niobium which enable batteries to charge faster. He

elaborated on phase transition studies and concluded that mixed solid solutions retain capacity better than separated. In this work, David combined operando synchrotron X-ray diffraction with electrochemical kinetics analyses to illustrate how nanoscale crystal size leads to suppression of first-order insertion-induced phase transitions and their negative kinetic effects in MoO₂, a tunnel structure host material.

Anticancer Activity in vitro: cell viability (IC50, 72h, Presto Blue)

Tissue of Origin	Breast	Ovarian	Bladder	Lung	Selectivity Index (SI)			
Cell line	MCF-7, MDA-MB-231	SKOV-3, A2780	5637, T24	A549, H1975				
Cisplatin	7.46 ± 0.62	3.84 ± 0.30	1.46 ± 0.31	3.21 ± 0.08	2.86 ± 0.36	2.72 ± 0.20	6.21 ± 0.08	2.7
Osiplatin	10.14 ± 0.89	42.6 ± 3.6	1.82 ± 0.02	8.21 ± 0.07	>100	15.8 ± 0.02	29.8 ± 1.3	1.9
Oxo-cisplatin	32.02 ± 0.08	38.5 ± 4.4	2.70 ± 0.40	33.1 ± 2.9	69.9 ± 4.8	67.8 ± 2.5	53.5 ± 4.0	0.7
Oxo-osiplatin	>100	>100	4.83 ± 0.12	>100	>100	>100	>100	N _A PH
Au-1	16.5 ± 1.0	49.0 ± 5.7	11.53 ± 1.0	45.7 ± 2.6	89.9 ± 7.8	24.9 ± 0.02	22.8 ± 5.5	0.9
PIAu-3	7.07 ± 0.51	14.52 ± 2.0	4.56 ± 0.68	5.0 ± 1.2	12.8 ± 1.8	15.0 ± 2.1	48.9 ± 5.5	3.2
PIAu-4	3.20 ± 0.01	7.9 ± 1.4	3.45 ± 0.12	3.21 ± 0.02	7.06 ± 0.48	10.25 ± 0.41	30.1 ± 0.89	2.9
PIAu-5	5.87 ± 0.01	2.99 ± 0.05	6.65 ± 0.90	3.01 ± 0.09	5.42 ± 1.1	12.85 ± 0.45	>100	>7.7

Presentation by Rebecca Turay.

Rebecca Turay from CUNY Brooklyn College described modification of Cisplatin analogs containing Pt(IV)-Gold(I) complexes with the same core. Based on results with Auranofin which showed reduced side effects with this metal combination, she is in the process of synthesizing compounds with cisplatin core with the same metals. Currently she is trying to improve the yields in the synthesis.

Yeshvi Tomar from USC explored the use of Iron electrode for grid energy storage with Selenium as additive. Three aspects were investigated: how does Iron selenide impact

Applications of semiconducting polymers

- Low cost
- Processible in solution
- Lightweight
- Flexible
- Biocompatible

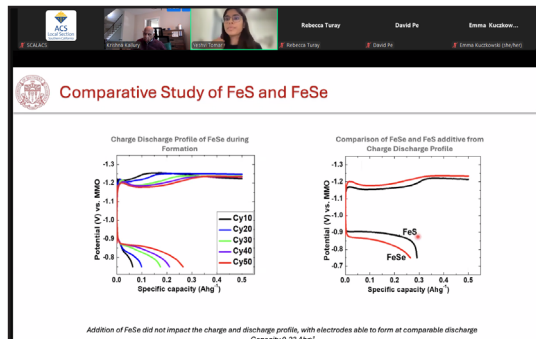
Presentation by Linnea Shu.

Working toward high power density batteries

Requires:

- Sufficient electrical conductivity
- High Li-mobility
- Unintrusive or suppressed phase transitions (PTs)

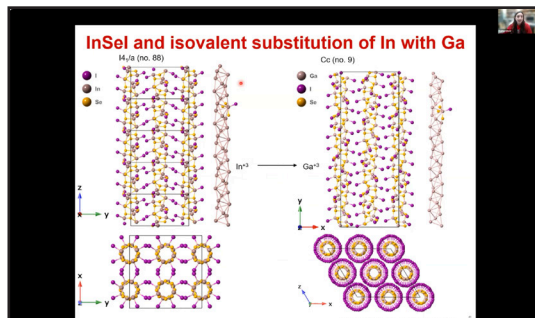
Presentation by David Pe.



Presentation by Yeshvi Tomar.

the Iron electrode, is Selenium reversible under battery operation and can Selenium improve the longevity of the electrode. The Se (2-) outperformed S (2-) in cells. Iron sulfide and selenide have comparable capacities.

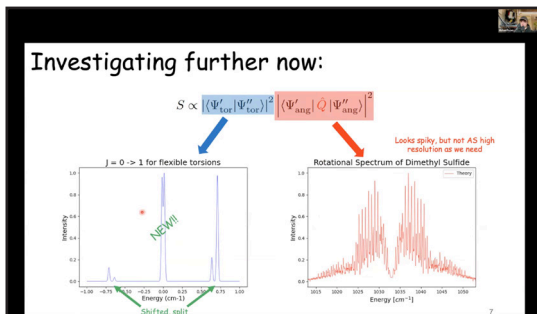
Carlos Garcia-Guerrero of UC Santa Cruz described his therapeutic targeting studies on *Saccharomyces cerevisiae* using splicing inhibitors in Humanoid Branch Point Binding Pocket. The RDS3 gene in yeast, a homolog to PHF5A in humans was used as a model. Therapeutic target splicing refers to a strategy in drug development where the goal is to manipulate the process of RNA splicing within a cell to treat diseases by correcting aberrant splicing patterns.



Presentation by Kaitlyn Dold.

Through single crystal X-ray diffraction (SC-XRD), high-resolution transmission electron microscopy (HRTEM), second-harmonic generation (SHG) imaging, and density functional theory (DFT), she established the structural helicity and the unusual “squircular” helix cross-section in this unprecedented structure. Her group elucidated the compositional dependence of the helicity and photophysical and nonlinear optical properties of GaSI compared to other III–VI–VII 1D vdW crystals.

Presentation by Carlos Garcia-Guerrero.



Presentation by Michael Rosen.

Michael Rosen from the University of Washington presented a theoretical study on the high resolution rotational vibrational spectra of HCl and DCl and of dimethyl sulfide. Rotational, Torsional and Coriolis-type Hamiltonians were studied in these computations.

Kaitlyn Dold from UC Irvine presented her research on all-inorganic III-VI-VII class of materials. She described the discovery and comprehensive characterization of GaSI, a wide-bandgap 1D vdW III–VI–VII crystal that displays a rare and unnatural helical motif.

Discrete Variable Representation (DVR)

$$I(v) \propto v |\langle \Psi_f | \hat{I} | \Psi_i \rangle|^2$$

- Need to write out Hamiltonian and Dipole Moment matrices
- Hamiltonian is kinetic plus potential energies ($H = T + V$)
- Performing linear algebra on Hamiltonian (diagonalization) returns eigenfunctions and their energies E (remember, $E = \hbar^{-1} v$)
- Choose to write the matrices in DVR basis
 - Rows and columns of matrices represent discrete positions in space

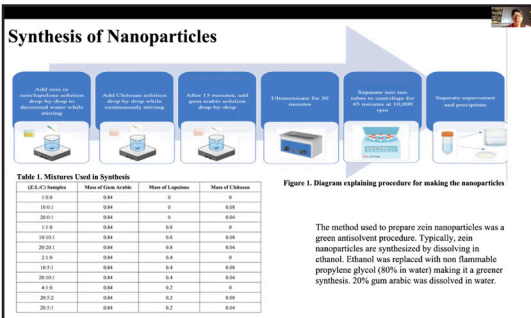
	x = -2	x = -1	x = 0	x = 1	x = 2
x = -2					
x = -1					
x = 0					
x = 1					
x = 2					

DVR Representation of Potential Energy Of Ball on Spring

Presentation by Dan Lotan.

Dan Lotan from University of Washington described his work on formic acid dimer using 2D-DVR. Formic acid dimer as the prototypical doubly hydrogen-bonded gas-phase species was studied from the perspective of the three translational and the three rotational degrees of freedom which are lost when two formic acid molecules form a stable complex. He described the associated fundamental vibrations, their combinations, and their thermal shifts by different electronic structure calculations and vibrational models.

The next speaker was Antonio Ocampo from Fairleigh Dickinson University, New Jersey. Prolonged skin exposure to UV radiation may result in sunburn, with possible inflammatory and oxidative stress to the



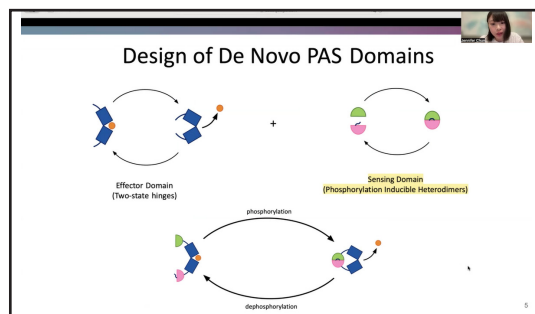
Presentation by Antonio Ocampo.

skin, skin photoaging, photocarcinogenesis, even DNA damage, and apoptosis if sunscreen protection is not used. Due to the advantages that they offer, such as high encapsulation capability, increased stability of encapsulated bioactive agents, and release control, nanoparticulate materials have been used in sunscreens despite the hazard they present: their capacity to penetrate the skin causing toxic side effects (especially the chemical sunscreens). Antonio's study reports the preparation of nanoparticulate composites containing only GRAS (generally recognized as safe) substances and using an eco-friendly, inexpensive procedure. The ingredients used have properties that are beneficial to the skin. Zein (Z), a prolamin-rich protein from corn, is biodegradable and biocompatible, is a moisture attractor, and shows effective absorption by cells. Lupulone, extracted from hops, is an antibacterial and antioxidant agent that has a stimulating effect on the collagen production in the body due to its content of phytohormones. Gum arabic (GA) is a natural glycoprotein used in beverages and cosmetics as an emulsifier/ stabilizer. Composite matrices containing Z/GA/L were prepared using a simple method (antisolvent), which replaces the flammable solvent ethanol with aqueous propylene glycol. Their biological activity was investigated as well. The zein-based nanoparticles showed antioxidant and antimicrobial effects and modulatory activity on the matrix metalloproteinase MMP-1.

The last speaker, Jennifer Meehyun Chun from University of Washington, described her work on De Novo design of phosphorylation inducible heterodimers. A protein heterodimer is a complex formed by two different protein subunits and phosphorylation is a post-translational modification where a

phosphate group is added to a protein. This can significantly impact the function of a heterodimer by altering its structure, stability and binding affinity, leading to activation or inhibition of its cellular signaling pathway. In computational chemistry, de novo structure prediction refers to an algorithmic process by which protein tertiary structure is predicted from its amino acid primary sequence. Jennifer used Rosetta and Fast Relax to study Ser, Tyr and Thr amino acid phosphorylation-dephosphorylation. She used PyMoL to study H-bonding in the heterodimers. She is planning to do experimental studies with ELISA, SPR and Fluorescence polarization.

One student was absent during the symposium scheduled time and another had problems with his microphone and had to withdraw his presentation.



Presentation by Jennifer Chun.

Listed below are the **five top winners of the Symposium**, each of whom was awarded a \$100 gift card for their outstanding presentations:

UNDERGRADUATE STUDENTS

- Meehyun Jennifer Chun, University of Washington
- Michael Rosen, University of Washington
- Linnea Shu, UCLA

GRADUATE STUDENTS

- Kaitlyn Dold, University of California Irvine
- David Pe, UCLA

Congratulations to the winners and thank you to all presenters and judges who took their time to be part of this symposium. Join us for the virtual 2025 New York ACS Project SEED Research Symposium on Saturday, February 8, 2025; 10 AM - 1 PM PST. See event information on page 14.

You're Cordially Invited to the 2025 New York ACS Project SEED Research Symposium

*A Virtual Celebration of Innovation and
Student Excellence in STEM*

*Co-sponsored by the New York and Southern California ACS
Local Sections, supported by the LSAC DEIR Grant*

When: Saturday, February 8, 2025
1–4 PM EST | 10 AM –1PM PST

Where: Online (Virtual Event)

Cost: FREE (Registration required)

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BY

HAROLD GOLDWHITE
California State University, Los Angeles
hgoldwh@calstatela.edu



In this column I wish to discuss one of the most influential books published in the twentieth century affecting the history not just of chemistry but of all science, namely "The Structure of Scientific Revolutions" by Thomas S. Kuhn. I quote from the author's Preface: "The essay that follows is the first full-published report on a project originally conceived almost fifteen years ago. At that time I was a graduate student in theoretical physics already within sight of the end of my dissertation. A fortunate involvement with an experimental college course treating physical science for the non-scientist provided my first exposure to the history of science. To my complete surprise, that exposure to out-of-date scientific theory and practice radically undermined some of my basic conceptions about the nature of science and the reasons for its special success." The essay was first published in 1962 and a slightly enlarged version appeared in 1970.

Chapter titles give a quite clear guide to Kuhn's thinking about how science progresses. In his "Introduction, A Role for History", the author argues that the classics of science and science textbooks imply that they embody the content of science uniquely and that the techniques embodied therein are the ones that will advance their particular branch of science. Kuhn asserts that this is what most scientists do, and calls that "Normal Science". He equates normal science to puzzle-solving and suggests that it leads to the formulation of paradigms that are the views accepted by the majority of the scientific community of particular segments of their sciences.

And then along comes anomaly – the emergence of phenomena or data that cannot be explained by the current paradigms. An example might be the failure of classical physics, in the hands of such able practitioners as Kelvin and Jeans, to explain "black-body radiation". The explanation of

this particular anomaly led to a far-reaching scientific revolution (hence the title of the book) namely the invention of quantum theory by Max Planck, a physicist whose work had previously been mainly in thermodynamics, and who devised quantum theory as a formalism to explain the phenomena without at first realizing its revolutionary implications. An article by Einstein a few years later explaining the photo-electric effect was influential in leading scientists to accept quantum theory.

So anomaly may lead to a state of crisis in scientific theory, and the answer to anomaly may be a scientific revolution and the emergence of new paradigms. The implications of these new paradigms lead to new pursuits of normal science and textbooks are rewritten to embody the new views – until the next anomaly and the next revolution.

Kuhn concludes with a discussion of what constitutes progress in a field of study. Why does science apparently, and uniquely, move steadily ahead whereas areas such as art or political theory do not? This may be solely semantics. We label areas that do progress in the way described: "sciences". As the author puts it: "Does a field make progress because it is a science, or is it a science because it makes progress?"

Kuhn's essay has had, and continues to have, a considerable impact on historians of science, with both supporters and detractors. It has affected my own teaching of history of chemistry and I use Kuhn's approach to discuss, among other topics, Lavoisier's oxygen theory of combustion, and Dalton's atomic theory. The concepts of paradigm and revolution have, thanks to Kuhn, become essential tools in thinking about the history of science.

Happy New Year!

UPCOMING 2025 EVENTS

January (TBD)	SCALACS Virtual Seminar on "Science and Culture"
February 8	Virtual Project SEED Students Symposium
March 19 & 20	USNCO Local Section Exam for SCALACS
March 23 - 27	ACS Spring 2025, San Diego
March 29	LA County Office of Education's Engaging Girls in STEM at the LA Zoo, Los Angeles
April 12	City of STEM + LA Maker Faire, Exposition Park, Los Angeles
April 20 - 26	Chemists Celebrate Earth Week (CCEW) <i>Glaciers: Hot Topic, Cool Chemistry!</i>
April 22	SCALACS 55th Anniversary of Earth Day Virtual Seminar on "Biosensors in monitoring & treatment of ailments/diseases"
May 10 - 16	2025 Regeneron International Science and Engineering Fair (ISEF), Columbus, Ohio
May (TBD)	SCALACS Virtual Seminar on "Wearable Biosensors"
June (TBD)	SCALACS Students Research Poster Session on "Nutritional contributions of natural materials in health promotion"
July 5 - 14	International Chemistry Olympiad, United Arab Emirates
August 17 - 21	ACS Fall 2025, Washington, DC
September	SCALACS Science Fair at a local school promoting contributions of food constituents from various cultures towards chemistry/STEM
October (TBD)	SCALACS Hispanic Heritage Celebration Virtual Seminar on "Analytical components of biosensors"
October 19 - 25	National Chemistry Week (NCW) <i>Hidden Life of Spices</i>
October 23	Mole Day
November (TBD)	SCALACS High School Students Research Symposium
December (TBD)	SCALACS Undergraduate/Graduate Research Symposium

*Actual event dates and titles to be announced. Events are subject to change.
For most up-to-date information, visit www.scalacs.org.*

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For more information or to find events, visit www.scalacs.org



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