



American Chemical Society  
Susquehanna Valley Section

## OCTOBER 2022 NEWSLETTER

The four hundred and sixty fourth meeting of the American Chemical Society, Susquehanna Valley Section will be the Wilkes University [Henry J. and Linda C. Pownall Lecture](#) on Wednesday the 19th of October at 7:00 p.m. in Stark Learning Center 105 (formerly room 101). The guest speaker is David Yaron, PhD, Professor of Chemistry at Carnegie Mellon University. The lecture will be preceded by a reception (5:00 p.m.) and dinner (5:30 p.m.) honoring Dr. Yaron at The Mary Stegmaier Mansion, 156 S. Franklin Street, Wilkes-Barre.

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### *“Using Machine Learning to Improve Quantum Chemistry and to Advance Student Learning”*

Dr. David Yaron  
Professor of Chemistry  
Department of Chemistry  
Carnegie Mellon University  
Pittsburgh, PA



This talk is on two quite distinct research areas that overlap primarily in their use of data science to address long-standing challenges in chemistry. In quantum chemistry, we are using the tools of deep machine learning, that are typically used to train neural networks, to develop low-cost quantum chemistry models. The form of these models dates back to the semiempirical quantum chemistry of the 1970's, when the parameters of the model were fit to a handful of experimental data. Advances in deep-learning frameworks now allow us to learn the model parameters from large sets of chemical data. This leads to models that are both computationally fast and accurate.

In student learning, our Open Learning Initiative (OLI) General Chemistry I and II courses gather millions of records each semester on how students learn chemistry. We are mining this data to discover how students learn and to find ways to improve the course materials.

## **BIOGRAPHY OF DR. YARON:**

David Yaron is a Professor in the Department of Chemistry at Carnegie Mellon University. He received a B.S. in chemistry from Wilkes College in 1983, a Ph.D. from Harvard in 1990, and did postdoctoral work at MIT before joining Carnegie Mellon in 1992. He develops quantum chemical methods for large systems, including especially organic materials for electronic and photophysical applications. Most recently, he has been working on ways to integrate machine learning into quantum chemical models and has developed a neural network that performs quantum chemical calculations within the network. He also develops and studies [educational materials](#) through his [ChemCollective](#) project and [Open Learning Initiative \(OLI\)](#) courseware. Dr. Yaron's dedication to, and excellence in, education has been recognized with a variety of awards including the Carnegie Mellon Teaching Innovation Award (2017) among others.

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## **DINNER:**

The lecture will be preceded by a reception (5:00 p.m.) and dinner (5:30 p.m.) honoring Dr. Yaron, held at [The Mary Stegmaier Mansion](#), 156 South Franklin Street, Wilkes-Barre, PA 18701. Dinner attendees may park on Wilkes University surface lots in addition to Mansion parking (see directions below). The reception will include Hors D'oeuvres and there will be a cash bar. Dinner will include Strawberry Field Salad, Rolls and Butter, Petite Dessert Display, and beverage service (Coffee, Tea, Iced Tea, Soda). Entrée choices include either Salmon a la Nage, Pork Tenderloin "1857", or Vegetarian Cheese Tortellini. As a result of the generosity of the Pownall's, our guests will be provided with dinner at no cost. However, dinner capacity is limited and reservations will be confirmed on a first-come, first-serve basis. Please RSVP for the event and dinner (noting your entree choice) to Gennie Singer ([genevieve.singer@wilkes.edu](mailto:genevieve.singer@wilkes.edu)) or 570.408.4750 by 3 p.m. Monday 10 Oct. 2022.

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## **DIRECTIONS TO WILKES UNIVERSITY:**

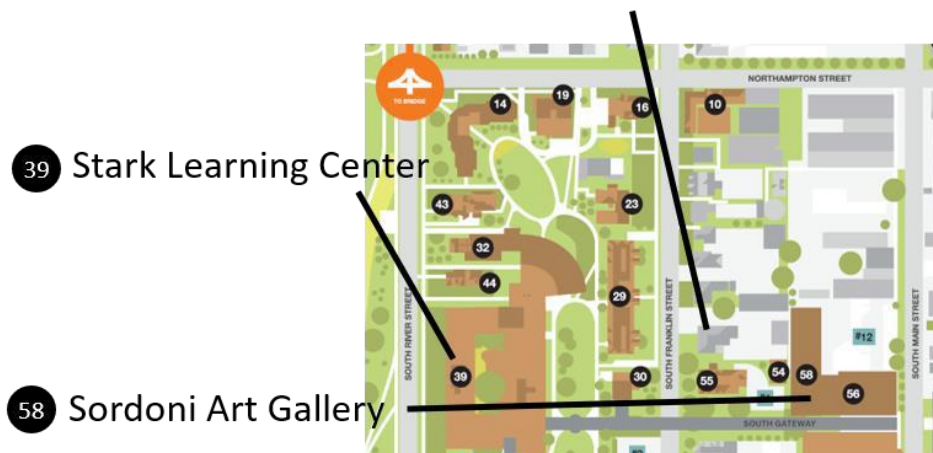
GPS: Wilkes University parking can be accessed at 141 S. Main St, Wilkes-Barre, PA 18702

Detailed directions can be found at:

<https://www.wilkes.edu/about-wilkes/planning-your-visit/directions-to-campus.aspx>

Take Exit 3 (River Street Exit), from PA Route 309N then make a left at traffic light. You are now on River Street. Immediately after turning left onto River Street, you will encounter the first of 8 traffic lights. Continue on River Street to the 8th light where you will turn left (east) onto W. Northampton Street. Continue on Northampton until you reach Main St. and turn right. You can park in the Parking #12 (141 S. Main St. next to the Karambelas Media and Communication Center/Sordoni Art Gallery). Additional parking can be found in Parking #8 (169 S. Main Street behind University Center on Main (UCOM) with entrance on W. South Street) and Parking #5 (84 W. South Street behind the Henry Student Center with entrances on S. River Street and S. Franklin Street).

## The Mary Stegmaier Mansion



detailed campus map (<https://wilkes.university-tour.com/map.php>)

parking (<https://www.wilkes.edu/about-wilkes/planning-your-visit/parking-locations.aspx>)

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### LOCAL SECTION NEWS:

#### 2022 LOCAL SECTION ELECTIONS:

Nominations are due for the position of Chair-elect. If interested, please contact any [section officer](#).

#### POSTPONEMENT OF SEPTEMBER SECTION MEETING:

The September meeting was postponed, and plans are being made to have [Dr. Freedman](#) present at Bucknell University at a later date. The SVS is planning on having two meetings in a single month to accommodate the rescheduled meeting. Please check the SVS website and forthcoming section newsletters for more information.

#### NATIONAL CHEMISTRY WEEK:



NCW will be celebrated October 16-22, 2022, with the theme, “Fabulous Fibers: The Chemistry of Fabrics” The Susquehanna Valley Section is once again collecting posters for this year’s event. If you know of a student in K-12 who would like to participate, please contact Karen Castle at [kcastle@bucknell.edu](mailto:kcastle@bucknell.edu). The deadline for submissions is Wednesday, October 12. For further details, see the [website](#).

#### OPEN POSITIONS IN THE LOCAL SECTION:

Do you want to use your talents to help other chemists in the Susquehanna Valley section? Listed below are examples of positions that need to be filled by willing individuals along with websites that give organizing ideas:

- SVS Chair-Elect

*This two-year position is the usual office taken on by local chemists who want to begin to become more involved in the local section.*

- [Chemistry Olympiad](#) Chair  
*Administer Local Chemistry Olympiad Competitions in coordination with the National Chemistry Olympiad.*
- WCC ([Woman Chemists Committee](#)) Chair  
*Help attract, retain, develop, promote, and advocate for women to positively impact diversity, equity and inclusion in the Society and the profession*
- CMA ([Committee on Minority Affairs](#)) Chair  
*Help increase the number & participation of racially & ethnically underrepresented scientists in the Society and its governance*
- Project SEED ([Summer Experiences for the Economically Disadvantaged](#)) Coordinator  
*Coordinators are responsible for establishing programs, identifying mentors, recruiting students, fundraising, and organizing activities such as field trips*
- CH&S ([Chemical Health and Safety](#)) Committee Chair  
*Help provide authoritative technical resources and mentorship in chemical health and safety for all*
- SCC ([Senior Chemists Committee](#)) Chair  
*Help improve communication among senior chemists, increase the number of senior chemists' groups and the level of their engagement within local sections, and encourage the involvement of senior chemists in programs focused on K-12 education, undergraduate networking, and mentoring*
- CCEW ([Chemists Celebrate Earth Week](#)) Coordinator  
*Help promote the positive role that chemistry plays in the protecting our planet (recyclable plastics, cleaner-burning fuels, phosphate-free detergents, environmental monitoring, and green chemistry initiatives).*

If you are interested, contact the section Chair (Allison Saunders, [saundersa@lycoming.edu](mailto:saundersa@lycoming.edu)), Secretary (Ronald Supkowski, [ronaldsupkowski@kings.edu](mailto:ronaldsupkowski@kings.edu)) or any member of the Susquehanna Valley Section leadership team ([executive committee](#), [committee chairs](#), [liaisons](#)).

#### LOCAL STEM COMPETITIONS:



A list of all STEM competitions for high school students is posted on our [website](#). If you have any questions about the contests or have suggestions for others, please contact either the person indicated on the site or the section webmaster, Ron Supkowski at [ronaldsupkowski@kings.edu](mailto:ronaldsupkowski@kings.edu) or 570-208-5900 x5733

#### NATIONAL ACS NEWS:

##### COVID-19

ACS is committed to helping combat the global COVID-19 pandemic with initiatives and free resources. Learn More at their website [acs.org/content/acs/en/covid-19](https://acs.org/content/acs/en/covid-19)

## ACS LEGISLATIVE ACTION NETWORK:

Legislation that may impact the chemical enterprise comes before Congress on a regular basis, and the ACS is committed to keeping its members informed and encouraging them to weigh in on high-priority issues. To see the position of the ACS on many legislative issues visit the ACS LAN website:

<https://www.acs.org/content/acs/en/policy.html>

To find out how to become more active in ACS advocacy activities, see the website:

<https://www.acs.org/content/acs/en/policy/memberadvocacy/advocacy-tools.html>

To join ACS' grassroots legislative advocacy network, ACT4CHEMISTRY, which will allow you to stay up to date on policy issues and contact legislators on behalf of chemistry and chemists, go to their website, follow the [Act4Chemistry Twitter](#) account, or email [advocacy@acs.org](mailto:advocacy@acs.org).

*Act4Chemistry Advocacy Issues. To take action go to the website*

[acs.org/content/acs/en/policy/memberadvocacy/issues.html#/takeaction](https://www.acs.org/content/acs/en/policy/memberadvocacy/issues.html#/takeaction)

### **Ask Congress to support climate change legislation**

With the growing climate crisis, the American Chemical Society recently endorsed a package of legislation to help address climate change, both to reduce greenhouse gas emissions, improve the sustainability of our energy and transportation sectors, and adapt to a changing world. ACS believes these steps are only part of addressing our changing climate, but it is a step towards leaving a better planet to our children and grandchildren. We ask you to raise these important issues to your Representative and Senators as they consider their legislative activities and priorities.

### **Ask the Senate to confirm science nominees for key positions & consider a chemist for the Chemical Safety Board**

In 2021, the Biden Administration nominated three chemists for three important roles at the Department of Energy (DOE) and the Department of Commerce National Institute of Standards and Technology (NIST). Dr. Geri Richmond and Dr. Laurie Locascio have been confirmed as DOE's Under Secretary for Science and Energy and the Under Secretary of Commerce for Standards and Technology, respectively. Dr. Asmeret Berhe has been nominated as the Director of the DOE Office of Science. ACS asks the Senate to vote on her nomination as quickly as possible. ACS is also asking Congress to encourage the nomination of someone with experience and a background in chemistry for one of the two remaining vacancies on the U.S. Chemical Safety and Hazard Investigation Board (CSB).

### **Ask Congress to support the Research Investment to Spark the Economy (RISE) Act**

We encourage you to ask that your members of Congress cosponsor and support the Research Investment to Spark the Economy (RISE) Act, [H.R. 869](#) and [S. 289](#). These bipartisan bills would authorize supplemental funding for a variety of research agencies.

### Support the Chemical Safety Board

The CSB is an independent federal agency that saves companies, universities, and local communities billions of dollars and countless lives by helping them prevent catastrophic incidents. Despite its great value, the administration has called for \$9.4 million for FY 2019 to be allocated to CSB, specifically for its elimination. Join us in asking appropriators and other members of Congress for their continued support of the CSB and its mission to protect workers and the public.

### Keep Science Funding Strong

Congress and the White House are working to complete the appropriations process for fiscal year 2021. Join us in asking appropriators for a strong and predictable boost in federal funding for scientific research.

### Congressional Chemistry Caucus

The Caucus' mission is to educate Members of Congress, their staff, and the public on the benefits of chemistry in today's society and its economic impact on our country. If you do not see your Representative or Senators represented in the Chemistry Caucus ask them to join.

### JOIN THE ACS:

If you know of anyone who would benefit from being a member of the American Chemical Society, please direct them to the membership website:

<https://www.acs.org/content/acs/en/membership.html>

### NATIONAL MEETINGS:



### *Spring 2023 ACS National Meeting*

The spring 2023 national meeting, “Crossroads of Chemistry” will be a hybrid event. The meeting will be held March 26-30, and the in-person event will take place in Indianapolis, IN. [Abstracts](#) are now being accepted, with a deadline of October 17. See the [website](#) for more information.

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Susquehanna Valley Section Web Page: <http://departments.kings.edu/SusquehannaValleyACS>  
Please send any comments about the monthly newsletter to Ron Supkowski, Section Secretary  
King's College 131 N River St Wilkes-Barre PA 18711 [ronaldsupkowski@kings.edu](mailto:ronaldsupkowski@kings.edu)

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