NJIT New Jersey Institute of Technology

Chemistry & Environmental Science Newsletter

Winter 2024 Vol. 5

Welcome To The Newsletter for the Department of Chemistry and Environmental Sciences!

Welcome to the Winter 2023/2024 issue of the CES Newsletter. Discover our latest news, including spotlighting our largest incoming class of graduate students, NJIT's attends the world's largest and oldest Forensic Science Association, Annual Research Day, Excursion of Forensic Anthropology class to the NYC Chief Medical Examiner's Office, research awards, recognitions, and upcoming events. Thank you for being an integral part of the CES community. The CES Newsletter is posted on the Department website: **https://chemistry.njit.edu/ces-newsletter**

CES Holds Its Annual Research Day

On Nov 7, 2023, the CES department celebrated its 2nd annual Research Day in the Agile Strategy Lab. The event combined a keynote lecture and a poster session followed by a reception. Dr. Thomas F. Miller, former Professor of Chemistry at Caltech, and Co-founder/CEO of Iambic Therapeutic was the keynote speaker for the event. Dr. Miller is a scientist and entrepreneur with a focus on the nexus of Artificial Intelligence (AI), chemistry, and biology. In 2020, he co-founded and became CEO of Iambic Therapeutics, a technology-driven biopharma that is disrupting the therapeutics landscape with its generative AI drug discovery platform. Dr. Miller delivered a lecture on "How generative AI solved the 1000-fold selectivity grand challenge in HER2 cancer drug discovery" which was well-received by an audience of more than 200 graduate and undergraduate students.

The poster session featured presentations by the research-active faculty and their graduate students which was exceptionally well attended. This event was designed as a social event in addition to research recruitment, and it succeeded at both. More than 150 undergraduate students interacted with the faculty, listened to the presentations by graduate students, and gained knowledge about the graduate program of the CES department. The event was organized by Assistant Professors Farnaz A. Shakib and Pier Alexander Champagne and would not have been possible without the great efforts of all CES faculties and their students. The success of the CES research day was crucially dependent on the involvement of University Lecturers (in particular but not only Christopher DeSantis, Mieke Peels, and Bhavani Balasubramanian) in tirelessly encouraging their students to attend this event. The CES department acknowledges funding from the Office of Graduate Studies and the support of Prof. Sotirios Ziavras, Vice Provost for Graduate Studies.

CES Chair Omowunmi Sadik Has Big Year As She Is Named a Fellow of the Academy of Inventors and The American Chemical Society.

Dr. Omowunmi Sadik, a Distinguished Professor and Chair of CES was awarded serval honors this year due to her outstanding research and community outreach record. Dr. Sadik was awarded a fellowship in both the American Chemical Society (ACS) and the Academy of Inventors (NAI).

Both awards are granted to individuals who have not only had academic success, but have also contributed to the wider community. According to the ACS, "the Fellow of the American Chemical Society (ACSF) designation is awarded to a member who, in some capacity, has made exceptional contributions to the science or profession and has provided excellent volunteer service to the ACS community." According to the NAI webcite, "The NAI Fellows Program was established to highlight academic inventors who have demonstrated a prolific spirit of innovation in creating or facilitating outstanding inventions that have made a tangible impact on quality of life, economic development and the welfare of society."

Dr. Sadik did not stop there, she was also awarded the 2023 University of Wollongong Alumni Award for Research & Scholarship. To cap things off, Dr. Sadik was asked to do an interview for Chemistry World, a publication of the Royal Society of Chemistry and to give a lecture at Pittcon 2024. The interview can be found here, and the information about the Pittcon lecture can be found**here**. Congratulations Dr. Sadik!

CES Meet & Greet

CES held its “Meet & Greet” Event on September 29, 2023, to welcome its new and returning students with warm and genuine smiles. The event, which was organized by the Undergraduate Program Advisor, Dr. Balasubramanian, had a friendly and welcoming tone with food and drinks and was attended by over 50 attendees, including faculty, staff, and students. Participants include the largest class of 2023/2024 PhD students, representing National Science Foundation Fellow, Fulbright scholar, and NIH Diversity Fellow. Presidents of the ACS Club, FRSC, and Environmental Science advisors introduced themselves and presented different opportunities to participate in the various club activities.

NJIT at the world’s largest and oldest Forensic Science Association

The International Association for Identification is the world’s largest and oldest forensic association. Each year they hold an educational conference that brings together forensic science practitioners from around the world for lectures on the latest technology, techniques, and research; workshops to practice basic to advanced skills; meetings; panel discussions; and an opportunity to collaborate with peers.

On Wednesday August 23rd, Dr. Kevin Parmelee from the NJIT Forensic Science Program presented a lecture titled *CSI Videography Revisited*. This presentation provided a new methodology for capturing sequential still images and video footage with a single device. The results of a feasibility study and review of current standards, technology, and best practices were provided to support the effectiveness and ease for implementing this new methodology.

On Thursday August 24th, Dr. Parmelee collaborated on a workshop with Lisa Ragaza, from the Connecticut State Forensic Laboratory, and Corey Bartoe, from the Virginia Department of Forensic Science. All three instructors are Footwear/Tire-tread examiners and provided a workshop on basic tire tread collection, processing, and preparation of materials for subsequent analysis of the evidence.

On Friday August 25th, Dr. Parmelee and Nolan O’Connor (pictured), an NJIT master’s student with the Department of Informatics, presented the lecture *Forensic XR: Digitizing a Forensic Lab*. This lecture described the collaborative work being performed at NJIT to utilize XR technology to aid forensic science learning options. This focused on the development of a flexible and accessible environment to teach tasks related to crime scene investigations.

In addition to these presentations, there was a robust lineup of lectures, workshops, and other events attended throughout the week. This conference provided an excellent forum to highlight the work and collaboration being

performed at NJIT.

Inside the Forensic Anthropology Unit of the New York City Office of Chief Medical Examiner

On Thursday, November 16, 2023, and thanks to the support of the CSLA Dean's Office, students from the forensic anthropology class had the opportunity to visit the Forensic Anthropology Unit from the New York City Office of Chief Medical Examiner (NYC-OCME) in Manhattan.

The tour was guided by Dr. Angela Soler, Assistant Director of the lab, who explained to the students the variety of cases sent to the Unit. Apart from the identification of human remains, the lab helps the forensic pathologists to determine the type of trauma to the bone and the weapon. The students had the chance to see examples of these determinations. At the time of the visit, the Unit was busy with two cold cases and a recent case for identification. The students demonstrated the knowledge acquired in the forensic anthropology class by correctly assigning the biological sex of the remains and estimated the age-at-death. The visit concluded with an explanation of the valuable role of facial approximation on the identification of human remains. Thanks to this visit the students had the opportunity to see first-hand the application of what they learnt in class to real forensic cases, and to gain a better understanding of the important role of forensic anthropology in different forensic scenarios.

NJIT and North Jersey Section of the ACS announces: The 36th Chemistry Olympics.

The 2024 NJCO will take place on **May 16, 2024**. If you're interested in participating or want to learn more about it, visit https://www.njchemistryolympics.com/. The webpage provides all the information about the eight events that make up this year's Chemistry Olympics. It's a great opportunity to showcase your chemistry skills and compete with talented individuals!

Dr. Carlos Pacheco and Dr. Mieke Peels have assumed the roles of on-site Directors. The previous director, Dr. Miriam Gulotta, is still helping as this event in a collaboration between NJIT and the North Jersey section of the ACS. Mr. John Krane and Ms. Genti Price have been collaborating with the Directors on various aspects of the website and logistics for this event.

We look forward to seeing you at NJIT on May 16th and hope everyone is having a wonderful school year!

Asieh Mahmoodi Wins Best Presentation at Graduate Research Day.

Asieh Mahmoodie (picured far left) has won the top prize for her presenation entitled **"Evolution in a Test Tube: Rescuing the Earth from Plastic Pollution"** at the Graduate Research Day held for NJIT students. Asieh, a 3rd year PhD student in Chemistry, is from Fars, Shiraz, Iran. Her advisor is Dr. Edgardo Farinas. Her research studies the biodegradation of plastic by genetically evolved enzyme through directed evolution. Her advice to her fellow students: "When you enjoy what you do, work becomes play."

Congratulations!

CES Continues to Expand Capabilities of NMR Lab

The 500-MHz instrument underwent the installation of a Sample Changer at the beginning of January '24. The device fully automates the system from sample insertion through all steps of the well-known data acquisition. The procedure for using

it is detailed in the step-by-step guide in front of the 500-MHz monitor (2-page) or through the webpage: https://research.njit.edu/nmrl/training.
The carousel can accommodate up to 24 samples.

We acknowledge the work of Dean Belfield in funding this device. It substantially increases data throughput, enabling us to make better laboratory plans in the future.

Shakib Theory Group Receives Grant From the NSF To Design Next Generation Batteries

Shakib Theory Group from the CES department has received a $240,000 grant from the National Science Foundation (NSF) to design new Lithium-sulfur batteries (LSBs) with a cathode consisting of electrically conductive metal-organic frameworks (EC-MOFs). Assistant Professor of Chemistry, Farnaz A. Shakib, leads the project "Computational Exploration of Electrically Conductive Metal-Organic Frameworks as Cathode Materials in Lithium-Sulfur Batteries" which is a collaboration with the University of Missouri-Kansas City. The Directorate of Engineering of NSF has awarded $360,000 in total for the completion of the project by the two institutions.

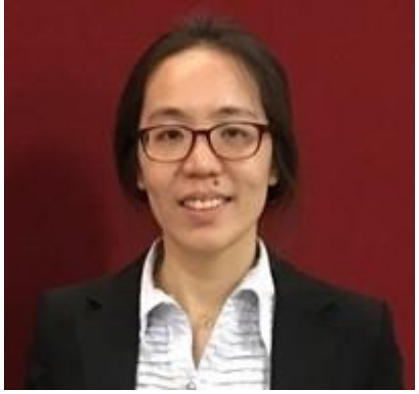
The researchers say that despite intensive research on LSBs, finding a porous cathode material with a high electrical conductivity that can prevent sulfur shuttling to the anode is still a pressing challenge. The project will address the unique structural and electronic properties of stacked layered 2D EC-MOFs as optimal cathode materials in LSBs. Apart from the apparent advantage of electrical conductivity, the layered architecture of EC-MOFs can endure extreme deformations without mechanical collapse. At the same time, their porous nature allows for efficient encapsulation of the active sulfur material in the cathode providing enhanced resistance toward its dissolution into the electrolyte solution (the shuttling effect).

The primary goal of this project is to probe the virtually unlimited chemical space of EC-MOFs to introduce ideal candidates as cathode materials. Since a case-by-case analysis of thousands of EC-MOFs as potential cathode materials is impractical, this research was designed to follow two main objectives: (i) creating a comprehensive and expandable database of EC-MOFs with an automated crystal structure creation tool followed by high-throughput screening discovery of EC-MOFs with desired structural and electrical properties; and (ii) investigating sulfur (S8) and its lithium-polysulfide derivatives encapsulation and possible transport at the electrode-electrolyte interface from advanced molecular dynamics simulations.

The first objective is already realized by the release of the EC-MOF/Phase I database by Shakib Theory Group, available at: **https://ec-mof.njit.edu/**. This database contains 1057 computationally ready bulk and mono-layer crystal structures where the users can visualize and download the cif/XYZ/POSCAR files of the desired EC-MOF. Upon the choice of desired metal nodes and organic linkers, the periodic DFT-level calculated properties of the optimized EC-MOF are also displayed at the bottom of the page. The completion of this database was a huge undertaking by the PhD student Zeyu Zhang in the Shakib group who successfully defended his PhD in July 2023 and is now pursuing his research as a postdoc scholar at the University of Michigan-Shanghai Jiao Tong University Joint Institute. Details of this research and the method/software developments entailed are published **here**.

Professor Lijie Zhang Wins Grant To Study Ways To Clean Up Our Water Ways

Assistant professor Lijie Zhang's group received a two-year $75,000 grant from the USEPA People, Prosperity and the



Planet (P3) Student Design Competition to advance technology for phosphorus management in waste streams. The team is developing a new technology by utilizing naturally benign minerals coupled with nanobubbles for the removal, recovery, and reuse of phosphorus from reverse osmosis concentrate.

Alexei Khalizov and Gennady Gor Receive NSF Award.

Gennady Gor (PI) and Alexei Khalizov (co-PI) received a new 3-year NSF Award "Elastic Properties of Confined Fluids and their Role for Wave Propagation in Nanoporous Media" from NSF CBET. This project connects the very different length scales - nanometers (molecular) to hundreds of meters (geophysical). While the applications are centered on hydrocarbons (shale gas and oil in particular), the fundamental questions that will be answered will be important for other fields, such as energy storage devices based on nanoporous solids.

The project is a collaboration between a theoretician Gor (NCE) and an experimentalist Khalizov (CSLA), and it is their 3rd NSF grant together within the last 3 years. It started from a joint NJIT Faculty Seed grant and an EAGER grant (which is an NSF seed grant). Notably, the prototype setup was built and the preliminary results were obtained by an undergraduate student Jason Ogbebor (a Chemical Engineering major and Chemistry minor) who has started his Ph.D. studies at MIT in fall 2023 (story **here**). Two other undergraduates who have been involved in this project are Filip Niemiec (Computer Engineering major) and Zayd Shaikh (Electrical Engineering major). Filip is now an Embedded Systems Engineer at the Naval Nuclear Laboratory, NY.

The abstract of the award can be found **here**.

CES https://chemistry.njit.edu/

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New Jersey Institute of Technology | 151 Warren Street, Dept. of Chemistry & Environmental Science, Newark, NJ 07102