Chair’s Message

By Dr. Wunmi Sadik, Distinguished Professor and Chair

We have just completed another successful academic year! One theme that seemed to dominate the year is re-emergence! For almost two years, as the world battled the global pandemic, the power of the human spirit to rebound was put on full display. We returned to face-to-face instructions with a better appreciation of the power of human connection. Chemistry and Environmental Science department re-emerged with several firsts: we held our first Annual Graduate Students’ Award Ceremony to celebrate the achievements of our students in research, teaching, and community service. We received our first NSF REU (Research Experience for Undergraduates) site (PIs: Wunmi Sadik and Dean Belfield). CES faculty, Assistant Professors Pier Alexandre Champagne and Farnaz Shakib, organized the first computational chemistry workshop for NJIT students. Finally, for the first time since its inception, we welcome three full-time faculty members to our Forensic Science Program: David Fisher (returning as Senior University Lecturer), Kevin Parmelee (Professor of Practice), and Sara Casado-Zapico (Assistant Professor).

Congratulation to the Class of 2022. Our graduates received multiple accolades: Dr. Qi Wang, working with Professor Hao Chen, received the Eastern Analytical Symposium (EAS) Outstanding Graduate Student Award. He also won the International Student Best Paper Award 2021. Simone Bishara, a CES Biochemistry major, received a 2022 Goldwater Scholarship—the most prestigious national undergraduate scholarship in the natural sciences, engineering, and mathematics. In addition, one of our biochemistry students was accepted to the Harvard Medical School program. Our enrollment numbers have continued on an upward trajectory. Compared to the CES enrollment for Fall 2019 (150), Fall 2020 (170), and Fall 2021 (282), the Fall 2022 is set to break the admissions records of the previous years.

Ours is a department with appropriately high research expectations, commensurate with a PhD-granting Chemistry department aspiring to be among the top ranks of chemistry departments at R1 universities. External research funding is a typical and reasonable expectation of such a department and is consistent with the department's and college's vision. Several of our faculty members have received new grants, including Drs. Belfield & Sadik (NSF-Germination), Genoa Warner (NIH), (Continued on page 2)
Chair’s Message
(Continued from page 1)

Hao Chen and Edgardo Farinas (NSF), Mengyan Li (NSF), Yuanwei Zhang, and Mengyan Li (NJDEP). Our faculty received the NJIT Seed Grants, including Hao Chen, Sara Casado-Zapico, Lijie Zhang, Genoa Warner, Som Mitra, and Amir Varkouhi. In addition, Dean Belfield was named a Fellow of the Royal Society of Chemistry (FRSC)! RSC is the world’s oldest professional society of chemists. The society awards fellow status to distinguished chemists that have made outstanding contributions to the advancement of the chemical sciences. Dr. Mengyan Li was also named a Senior Member of the National Academy of Inventors.

I want to acknowledge the continuing dedications of our faculty and staffs, particularly as we re-emerge from the pandemic—including our outreach committee’s efforts toward the 2022 Virtual New Jersey Chemistry Olympics and graduate recruitment.

Enjoy the newsletter!

Omwunmi “Wunmi” Sadik, Ph.D.
Distinguished Professor and Chair
Chemistry and Environmental Science

NSF REU BioSMART Site at NJIT

From the bottom to the top of the stairs. Joy Kuzman - NJIT, Joy Duan - University of Alabama at Birmingham, Hari Ramesh - Academy of Mathematics, Science and Engineering with County College of Morris, Ojasvita Reddy - NJIT, Nneka Arinseh - Harvard University, Steven Douglass - Rowan University, Darshman Danak - NJIT, Renallan Neckles - Indiana University of PA, Emad Sawaged - NJIT, Brandon Fiallos-Mejia - Saint Elizabeth University

CES has received its first NSF REU (Research Experience for Undergraduates) site (PIs: Wunmi Sadik and Dean Belfield—$403,732). The REU site for BioSensor Materials for Advanced Research & Technology (BioSMART) at the Environment/Biotechnology Nexus will provide a unique learning experience for UG in biosensors (https://centers.njit.edu/smart/about-biosmart-center/). This REU takes advantage of the biosensor research opportunities at NJIT in the Departments of Chemistry & Environmental Science, Biological Sciences (Federated with Rutgers), and Chemical Engineering & Material Science. The intellectual focus emphasizes: (i) biosensor materials, (ii) biorecognition and protein engineering, (iii) sensor designs and characterization, and (iv) field applications. Planned activities include one week of science boot camp, career development workshops with interactive workshops on equity and inclusion awareness, team building, Teaching the Art of Dissemination, extracurricular events, and responsible conduct of scientific research. BioSMART REU site award will support the training of 10 students for ten weeks during the summers of 2022-2024. It is anticipated that a total of 30 students, primarily from schools with limited research opportunities or from an under-represented groups, will be trained in the program. The minimum GPA requirement is 3.0. The program will draw students from sophomore through senior classes. Students participating in this project will receive a $6,000 ($600/week) stipend for the 10-weeks program, free accommodation, and a host of career development activities and industrial visits.

https://chemistry.njit.edu/
Molecular Dynamics in Condensed Phase Software Developed in CES

CES Assistant Professor, Dr. Farnaz A. Shakib, has developed and released a multi-faceted general-purpose molecular dynamics software package coined DL_POLY Quantum v1.0 based on DL_POLY Classic [1]. This highly-parallelized software is available for the use of the community through github (https://github.com/fashakib/DL_POLY-Quantum-v1.0) together with example cases in the “data” subdirectory including bulk water (TEST42 and TEST45), dry and hydrated 2-dimensional metal-organic framework Cu4(HHTP)2 (TEST43 and TEST46), and zeolitic-imidazolate framework ZIF-8 (TEST44).

Some of most significant modifications in DL_POLY quantum v1.0 are as following:

1. Implementing Nose-Hoover Chain (NHC) thermostat for classical simulations in canonical ensemble based on Suzuki-Yoshida scheme [2-4]. The thermodynamic control variables in the canonical ensemble are constant particle number N, constant volume V, and constant temperature T, which characterize a system in thermal contact with an infinite heat source [5].

2. Implementing Nose-Hoover Chain thermostat/barostat for isothermal-isobaric ensemble through Martyna-Tobias-Klein (MTK) algorithm [6,7] for classical MD simulations. Experiments are more commonly performed at conditions of constant pressure P, rather than constant volume, hence the NPT NHC ensemble is also implemented in DL_POLY quantum v1.0.

3. Implementing the four-site flexible quantum water potential model qiIP4P/δ [8], for both classical and path integral molecular dynamics (PIMD) simulations. It is a fixed-point charge model for liquid water in which the O–H stretches are described by Morse-type functions. Two positive charges of magnitude qM/2 are placed on the hydrogen atoms of each water molecule with a negative charge of −qM placed on a mass-less M-site located at point rM along the vector connecting the oxygen atom to the center of mass of the two hydrogens.

4. Implementing a 12-6 Lennard-Jones potential as external potential for confinement simulations.

References

NJIT JOINS EFFORT TO MAP OUT STRATEGIES FOR NOAA TO MITIGATE POLLUTION IMPACTS ON FRESHWATER SYSTEMS

By Dr. Zeyuan Qiu

Protection of coastal and marine resources starts from freshwater systems. Professor Zeyuan Qiu joined a multi-agency and multidisciplinary team that consists of New Jersey Sea Grant Consortium, Stevens Institute of Technology, New Jersey Institute of Technology and Montclair State University to do just that. The NOAA National Sea Grant Network awarded the project team a grant entitled “Optimizing green infrastructures and low impact developments to mitigate pollution impacts on freshwater systems” to conduct a scoping study to prioritize research needs, delineate the roles of the NOAA Sea Grant Network, identify strategies for the Sea Grant Network for deploying GI/LIDs to mitigate runoff and pollution impacts on freshwater systems, and administer a regional competitive grant program that implements some of the proposed strategies.

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NEWS FROM THE NMR LABORATORY
BY CARLOS POCHECO

In coordination with the Dean of CSLA and the Chair of CES, the acquisition of a broadband probe for the 500-MHz instrument in the NMR lab is under way. The probe configuration allows greater sensitivity for routine carbon-13 and proton NMR, and observation of any nucleus with frequencies within the Silver-109 to Phosphorus-31 range. Thus, one could regularly acquire Boron-11 NMR, Silicon-29 NMR, Nitrogen-15 NMR among several other accessible nuclei, including those not commonly observed, and thereby augmenting the latitude of research activity at NJIT. In addition, the probe is fitted with a device called Automatic Tune and Match (ATM) which allows all NMR users to automatically adjust the probe frequency for any combination of nucleus/solvent. Adding this feature removes the need for users to make any manual adjustments prior to analysis. Thus, the 500-MHz operation will be completely automated, enhancing its overall productivity. All NMR users may expect the enhanced capacity of the instrument by mid-Fall 2022.

From left to right: Kevin Belfield, Dean of the College of Science and Liberal Arts at NJIT, Luca Grisanti, Farnaz Shakib, Pier Alexandre Champagne

With the rise of computational chemistry as a powerful tool for the prediction and understanding of chemical behaviors, there is a recent push to introduce more chemistry students to the discipline. This is what two computational chemists from NJIT were hoping for when they organized the first computational chemistry workshop for NJIT students, which was held on Saturday April 30th, 2022.

Assistant professors Pier Alexandre Champagne, who specializes in computational organic chemistry, and Farnaz A. Shakib, specialized in quantum dynamics method development and materials simulations, teamed up with visiting professor Luca Grisanti from the Ruder Boškovic Institute in Croatia, to offer the attendees a pair of lectures interspersed with practical exercises. The lectures and hands-on practices related to electronic structure calculations of molecular systems as well as dynamics simulations of condensed-phase biological systems, covering the basics all the way to state-of-the-art applications.

Over 15 participants benefitted from this whole-day event, mostly graduate and undergraduate students (including visiting students from Italy and Croatia), in addition to interested faculty members from NJIT. With the success of this first edition, it is likely that this celebration of computational chemistry will continue to be offered every year, ensuring that computational tools meet the hands of as many researchers as possible.

by Pier Alexandre Champagne

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Interested in a degree offered by CES?

CES undergraduate programs include:
- B.S. Biochemistry
- B.S. Chemistry
- B.S. Environmental Science
- B.S. Forensic Science - Forensic Biology, Forensic Chemistry, and Digital Forensics concentrations

More information can be found at: https://catalog.njit.edu/undergraduate/science-liberal-arts/chemistry-environmental-science/

Professor Hao Chen’s lab receives grant from Colgate-Palmolive

Professor Hao Chen and his research group recently received a new grant of $30,000 from Colgate-Palmolive Company, to support the characterization of the package surface chemistry without dissolving the materials under coating surface, by high resolution mass spectrometry. This is a continued support from the Colgate-Palmolive Company. The new project aims to target on finding a novel and sustainable packaging material for toothpaste products.

Professor Zeyuan Qiu and Students help preserve New Jersey old-growth forests

Professor Zeyuan Qiu, Harleen Oza, Daniil Ivanov and PEC Commissioner Harrison Watson visit the Province Line Woods with Patricia Shanley in March.

Professor Zeyuan Qiu led a team of biochemistry students, including Daniil Ivanov and Harleen Oza, and conducted a quantitative study to estimate the economic value of ecosystem services provided by forest for two large forest parcels in Princeton Township. The ecosystem services refer to the benefits provided by forest to the community such as carbon sequestration, air purification, and stormwater mitigation. The analytical results helped local environmental organizations and Princeton Township to take action and preserved one of the forest parcels from urban development.

To learn more about their effort, read the article from the NJIT Newsroom with the link below: https://news.njit.edu/njit-students-and-faculty-help-save-new-jerseys-old-growth-forests

https://chemistry.njit.edu/
CES Students Find Success!

Check out the great achievements of students and alumni of CES programs!

Dr. Qi Wang Has Big Year: Wins Two Awards.

Dr. Qi Wang’s graduate research has earned two awards this year. First from the Eastern Analytical Symposium (EAS), which continues to actively support a Student Research Awards program to recognize students involved in research in the broad field of analytical chemistry. Nomination criteria include excellent grades, appraisals of how the students handle their investigations, their approach and how they resolve problems and publicly disseminate their work. PhD student in the Chen lab, Qi Wang, won the 2021 ESA Outstanding Graduate Student Award. Qi has been recently hired by Merck Co, a top pharmaceutical company in the world, as a senior scientist. During his PhD study at NJIT, Qi has published >10 peer-reviewed articles in high impact journals such as Water Research, Chemical Science, Journal of Organic Chemistry and Analytical Chemistry, etc.

Qi also won the international journal of mass spectrometry (IJMS) Best Student Paper Award 2021. The award was created to recognize young researchers in mass spectroscopy. Congrats to Dr. Qi Wang!

CES Kicks Off Its Annual Graduate Students’ Award Ceremony

By Prof. Farnaz Shakib

On April 25th, 2022, CES held its very first Outstanding Graduate Student Award Ceremony to celebrate the achievements of its body of students in research, teaching and service to the community. The graduate students had competed for these awards by submitting their application packages including research proposals and teaching statements to an award committee composed of five faculties including Dr. Farnaz A. Shakib, Dr. Genoa Warner, Dr. Michael Eberhart, Dr. Sara Casado Zapico and Dr. Lijie Zhang. After a careful evaluation of the application packages by the committee, four students were awarded by a certificate and prize money presented by the Department Chair, Dr. Sadik. Zeyu Zhang (Shakib group), Dung Ngoc Pham (Li group) and Indrani Gupta (Mitra group) were awarded the Outstanding Graduate Student Award in Research category while Ali Hasani (Khalizov group) was awarded in the Teaching category. The attendee enjoyed lunch, door prizes and online trivia to create a fun event for the whole department. This ceremony is intended to be held annually with more categories including awards for undergraduate and master’s students. So, make sure to apply next year!!!
CES Students Find Success!

Check out the great achievements of students and alumni of CES programs!

On April 2, 2022, Shaina Pearson (senior undergraduate student, Shakib Theory Group) represented the CES department at the 15th Annual Undergraduate Research Symposium in William Paterson University of New Jersey. Shina presented the results of her research on the application of Ring Polymer Surface Hopping method to study non-adiabatic dynamics in condensed phase which she has performed under the mentorship of Dr. Dil Limbu (postdoctoral research scholar, Shakib Theory Group). Shaina’s poster won the 1st place award in Materials & Polymer Chemistry Division. She is excited to continue her scientific journey as a PhD student at the CES department in the upcoming Fall 2022 semester.

Sumbel Yaqoob Wins Land Conservancy of New Jersey Environmental Scholarship

CES graduate student, Sumbel Yaqoob, was awarded with the Land Conservancy of New Jersey Environmental Scholarship of $7,500 toward her continued academic studies. This scholarship will support Sumbel’s research on biotransformation and biodefluorination of per- and polyfluoroalkyl substances (PFAAs), which are known as “forever chemicals” in water.

Forensic Majors Visit the US Customs and Border Protection Lab

By David Fisher, Director of Forensic Science Program

On Monday, February 7, forensic science majors taking Prof Fisher’s Forensic Microscopy (FRSC 480) class visited the US Customs and Border Protection (CBP) Lab located in Newark, NJ. The Laboratories and Scientific Services is the forensic and scientific arm of US CBP, providing forensic and scientific testing in the area of trade enforcement, weapons of mass destruction, intellectual property rights, and narcotics enforcement. US CBP Scientific Services coordinates technical and scientific support to all CBP trade and border protection activities. Students in NJIT’s FRSC program learned about this unique lab as well as employment in the federal government.

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CES Outreach: Getting Involved In the Community

Find out about the different ways CES is supporting the local community!

High School Students in CES Research Labs Earn Recognition For Their Research Efforts

Christopher Prainito, a local high school student who performed research in Professor Omowunmi Sadik's lab, was named a finalist in the Regeneron Science Talent Search (Regeneron STS) for his research involving development of a polymer-based paper sensor that changes color from blue to red upon detection of the COVID-19 spike protein in a saliva sample. The Regeneron STS is a very prestigious science competition for high school seniors which awards original research. Congratulations to Christopher!

Jeffrey Xu, a local high school student working with Professor Hao Chen, finished in 1st place in Chemistry at the New Jersey Science Fair for his summer research project on tryptic microdroplet digestion of proteins. His work was recently accepted into the Journal of American Chemical Society for Mass Spectrometry. Congratulations to Jeffrey!

The New Jersey Chemistry Olympics Triumphs in uncertain times; again!

Thursday May 26, 2022 was the closing date for the 3rd virtual New Jersey Chemistry Olympics (vNJCO); an event run by the Department of Chemistry and Environmental Science of the College of Liberal Arts and Science (CSLA) at the New Jersey Institute of Technology (NJIT) and the North Jersey Section of the American Chemical Society (NJACS). There were 34 in person Olympics prior to the pandemic. Fourteen coaches from 10 high schools led 134 students into battle during this year’s competition. Unlike previous virtual NJCOs, these students were almost always in person which greatly facilitated teamwork. Unfortunately, the onset of the Omicron variant in December and January forced presentations to the judges to be remote. This year only 4 events were offered so judging time was reduced to 2 days rather from 2 weeks used in 2021.

The 2022 theme was: The real news on face masks and lead contamination in water supplies.

The events of the 2022 vNJCO were:

- Environmental Research (ER): Face Masks (the Real news) where students investigated pathogen particle size vs. the shielding effectiveness of different masks. Judges: Dr. Alexei Khalizov, Ali Hasani, Na Mao.
- WebSite Design (Web): Chemistry and the Presence of Lead, where students created websites to explain the chemistry of lead and lead complexes, the water crisis at Flint Michigan (the Real news), and how much lead is too much. Judges: Dr. Sandra Keyser, Ms. Debra Sweet
- Debate (D): Should a clearly enforceable Maximum Contaminant Level (MCL) for lead in our water supplies be established under the Safe Drinking Water Act (SDWA)? This event is back after being well received during its pilot run in vNJCO 2021. Teams had to research both sides of the argument, design questions to ask the pro side if you are representing the con side and vice versa, and become knowledgeable enough to defend either side against students from another school on event day. Judges: Dr. Michael Bonchonsky, Ms. Emma Bitar.
- Chemical Nomenclature (Nom): a fast paced quiz that asks participants to name a given structure or give the structure based on the name. Participants have 10 minutes to answer 30 questions covering ionic compounds and ions, inorganic compounds, and basic organic compounds and ions. The questions are graded automatically in the Moodle Learning Management System.

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System. The NJCO thanks NJCO directors Drs. Kathleen Gilbert and Miriam Gulotta for creating the quiz and providing the questions. Both are university lecturers at NJIT. Drs. Kathleen Gilbert and Miriam Gulotta are also NJACS* executive board members.

7 of the 10 schools were awarded at least one medal. South Brunswick proved the most versatile winning 1 medal in each of the four events. Pascack Hills totally dominated the Nomenclature event taking home both the gold and one of the 2 silver medals in that event. Hunterdon County’s website score was off the charts! They provided users detailed structures of lead chelators and described in detail how the chelators bind to lead. The team also fully understood the lead crisis in Flint Michigan. The Woodbridge Academy (WA) greatly improved their preparedness for this, their second vNJCO. They doubled the number of medals and added a gold and a silver medal to the bronze medal they won in 2021.

The NJCO is designed to give high school students an opportunity to perform scientific investigations in a manner very different from what happens in a high school classroom. The steering committee that designs the events is composed of CSLA faculty and NJACS members (industrial scientists, faculty members in chemistry or related areas, high school teachers). The question “after 37 years is the NJCO still relevant?” is addressed every year. An interest poll goes out to previous coaches in the Fall and event planning proceeds from there. This year’s virtual competition gives us data on the interest of the student competitors. They weren’t on the NJIT campus with few outside distractions. They were home where sports, exams, proms, etc. all compete for their time. Yet they went above and beyond to compete in the NJCO. All for a cool T-shirt, team medals, and a small surprise gift.

Our warmest congratulations go to the students who participated and their coaches. Thanks to the professionals and graduate students who did the judging, to our event steering committee for designing the events, and to Genti Price for the certificates and her work behind the events. Our thanks to Dr. Onowummi Sadik, chair of the Department of Chemistry and Environment Science for her support and her presence at the award ceremony. Thanks to Dean Kevin Belfield for all his support whenever we need it, for getting us funding and for the informative talk he gave to the students at the awards ceremony. Lastly, thanks well beyond words to Dr. Kathleen Gilbert (NJIT, NJACS), and Ms. Diane Krone (NJACS), the other 2 directors whose responsibilities would fill up more would more than double the length this article and without whom there would be no NJCO.

Thanks to Merck Pharmaceuticals, NJIT CSLA, and the NJACS for financing the event.

I look forward to seeing many of the same faces in-person at the 2023 in person NJCO.

Respectfully submitted, Dr. Miriam Gulotta (NJIT, NJACS)

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Royal Society of Chemistry Awards Fellow Status to NJIT’s Kevin Belfield

Kevin Belfield, dean of NJIT’s College of Science and Liberal Arts, has been named fellow of the Royal Society of Chemistry (RSC).

RSC is the world’s oldest professional society of chemists, founded in 1841, and has grown to over 54,000 members around the world. The society awards fellow status to distinguished chemists that have served a minimum of five years in a senior position and have made an outstanding contribution to the advancement of the chemical sciences.

“It’s humbling to even be considered for this recognition, yet alone receive it, particularly considering the distinguished chemists and Nobel Laureates that currently are fellows,” said Belfield. “These include David MacMillan, M. Stanley Whittingham and Sir Gregory Winter, winners of the Nobel Prize in Chemistry in 2021, 2019 and 2018, respectively. It’s a thrill to be in such company.”

Highlighting a decorated research career spanning more than 30 years, Belfield is perhaps most noted as a trailblazer in the field of photochemistry — specifically creating two-photon (light-activated) processes to nondestructively image and cause optical changes in three dimensions within materials. His pioneering work has led to breakthroughs in the development of rewritable 3D optical data storage, as well as two-photon absorbing materials that are now commonly used in microfabrication and 3D printing today.

Belfield is also widely recognized in his field for his research developing novel fluorescence contrast agents, useful in bioimaging for tracking cancer progression and wound healing. Such work is also now being harnessed to study processes associated with early-stage Alzheimer’s disease. Belfield has published over 250 peer-reviewed journal articles, book chapters and conference proceedings that have been cited over 7,500 times.

He holds 15 patents and leads the Belfield Research Group, which is currently developing everything from light-activated cancer-fighting drugs, to probes for labeling biological samples and for advanced bioimaging, to novel lightweight high-strength polymers and plastics that can be used as artificial joints and cardiovascular implants, among other medical applications.

Belfield arrived at NJIT as CSLA Dean and Professor of Chemistry and Environmental Science in 2014, and has since assumed a leading role in student mentorship and education in chemistry, launching a number of vital initiatives and programs at the college including New Jersey’s first Forensic Science degree program and the Professional Science Masters in Cell and Gene Therapy Sciences within the Department of Chemistry and Environmental Science since 2018.

The latest honor from RSC follows several significant career achievements and honors, including being inducted into the National Commission of Cooperative Education Co-op Hall of Fame (2010), being elected a Fellow of the American Association for the Advancement of Science (2013) and being named Fellow of the American Chemical Society (2019).

Belfield is currently involved in research funded by the National Science Foundation, the National Institutes of Health and U.S. Department of Education.

Written by: Jesse Jenkins
Published: Monday, February 14, 2022 online

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