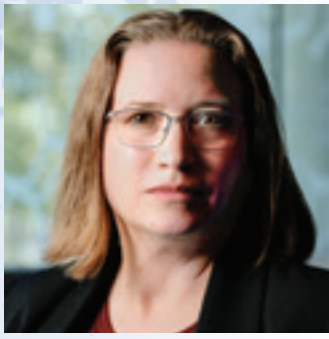
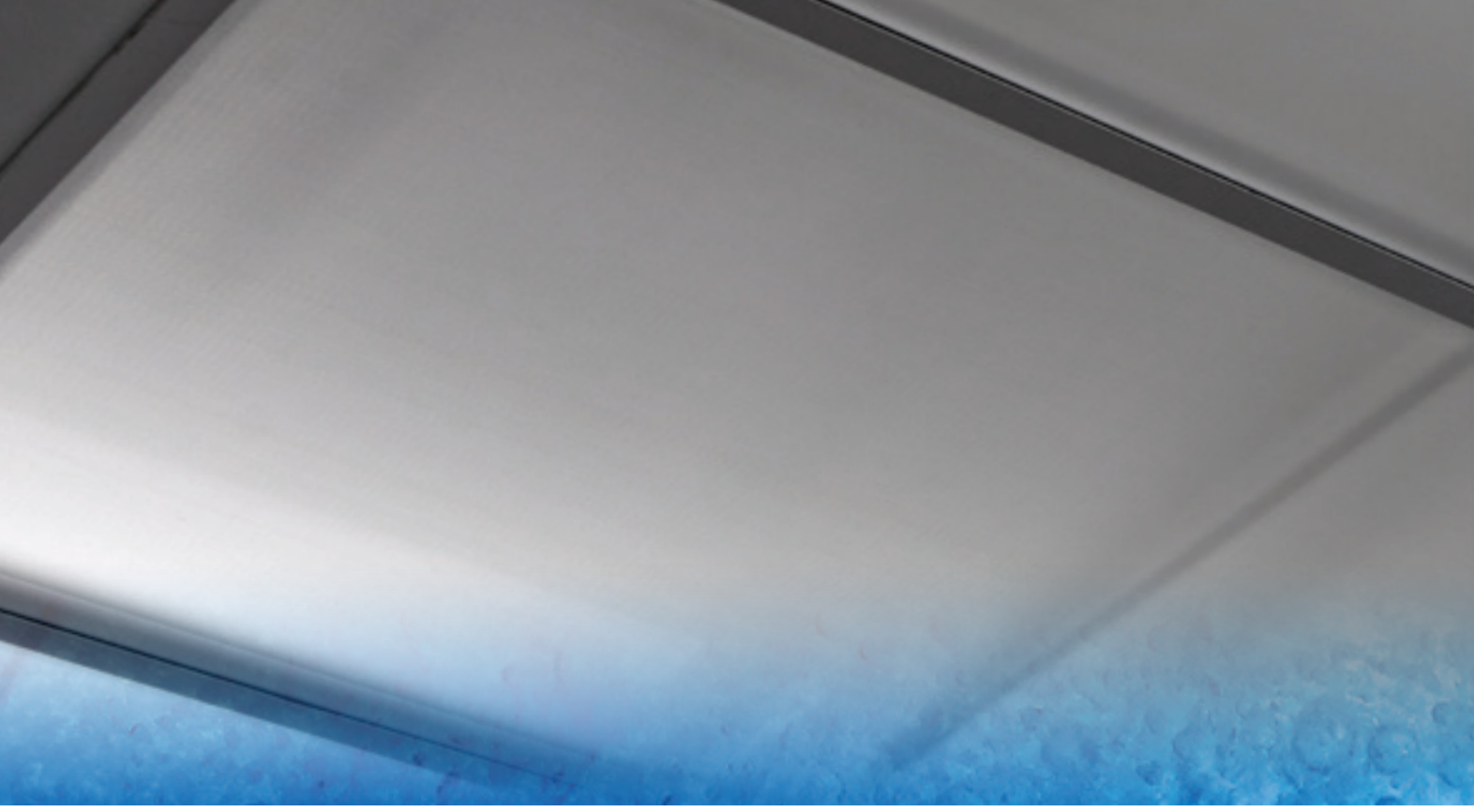
STRUCTURES

A PUBLICATION OF THE HAUPTMAN-WOODWARD INSTITUTE WINTER 2021





HWI SCIENTISTS LEAD NATIONAL RESEARCH EFFORTS FIGHTING COVID-19



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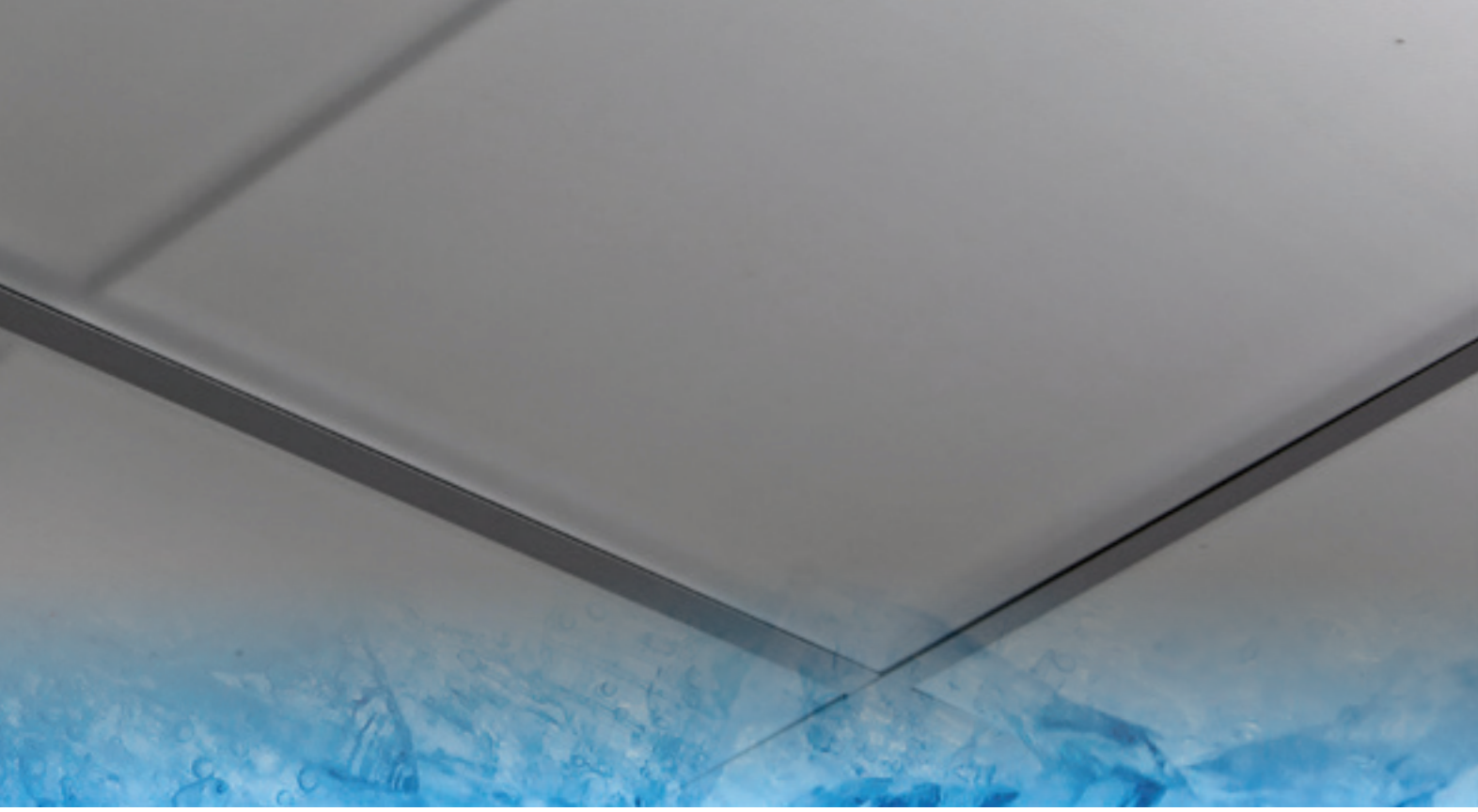

WORK

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The Cryo-EM Center at HWI is now open and ready to work on projects with academic and industry partners.

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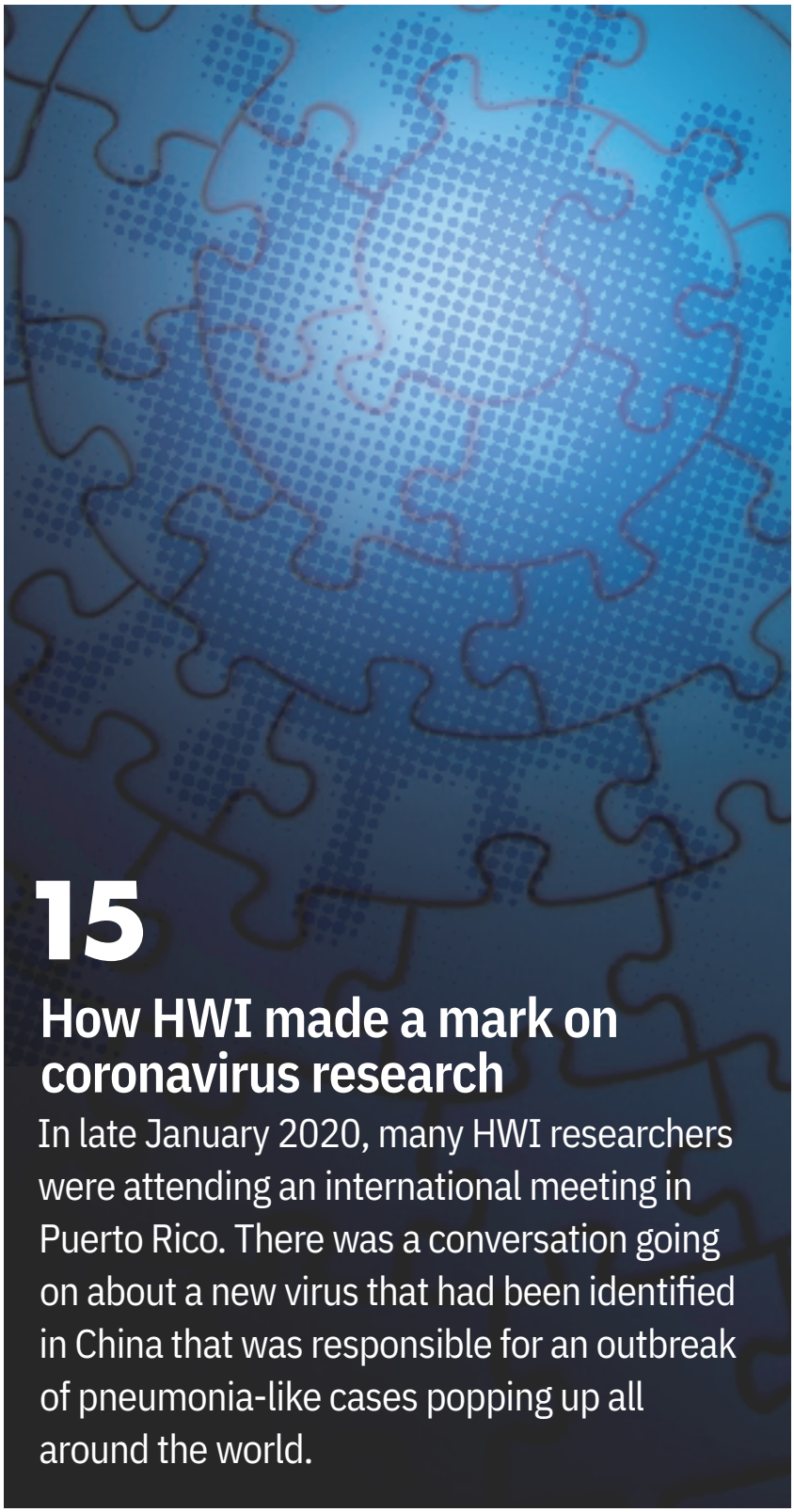
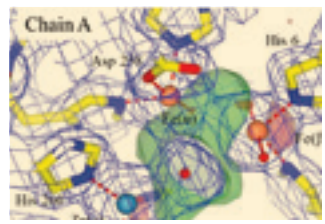
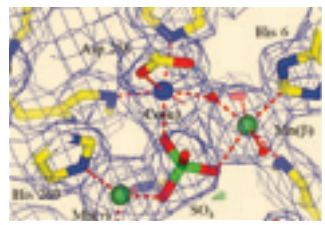


IMCA-CAT

Industrial Macromolecular Crystallography Association Collaborative Access Team

Accelerating research and drug development in partnership with IMCA-CAT—more on page 34

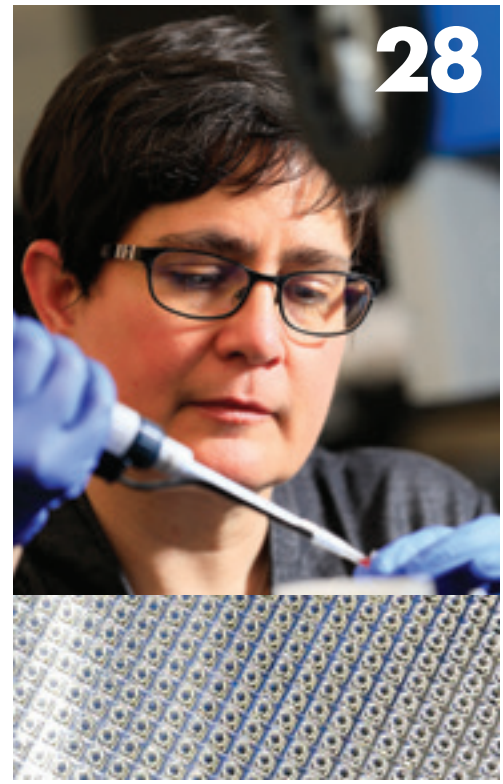




"We turned the numbers into a picture and hidden within the data was an explanation of how this molecular machine worked."

You too can make an impact in a multitude of ways and create your own legacy—page 32

SPOTLIGHT



Got Crystals?

Our Crystallization Center supports the fight against COVID-19 and was recently named the National Crystallization Center.

STRUCTURES

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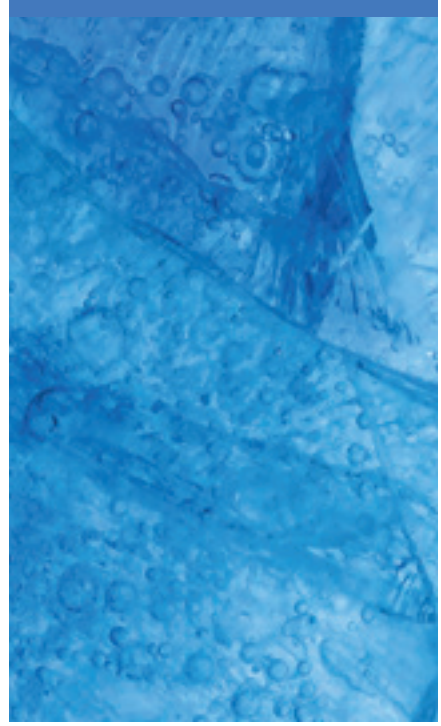
A MESSAGE FROM THE CEO

WELCOME TO THE WINTER 2021 ISSUE OF STRUCTURES, it's been over a year since our last issue, and what a year it has been. In our last issue, we talked about a new technology we were embracing, cryo-electron microscopy, and how that could accelerate the research we are doing. Amazingly, given the unexpected interference of a pandemic that has changed life as we knew it, at least for the moment, our Cryo-EM center is now operating and has recently produced the first data. A significant element of its success will be an effort by the board and local foundations to equip the Center with the most advanced detector available today. This was an amazing effort and an action that demonstrates the belief in the mission of the Institute to improve the health and well-being of humanity through Structural Biology.

The COVID-19 pandemic has been tragic for many. The scientific response worldwide has demonstrated what is possible when structural biology is applied to this kind of threat. The virus has been called the invisible enemy and the pictures that have been seen in the media are from what we do as a scientific discipline. We make the invisible visible. Never has the work that the Institute does been demonstrated so well. The pandemic significantly impacted our operations and continues to do so. We have many staff working from home. Despite this, we have played a major part in the fight against COVID-19. The Buffalo News had a front-page article on the Monday after the Super Bowl, which nicely explained our contributions. Our Crystallization Center has been working on over 60 different projects with laboratories across the nation and the director was asked to present the Center's work to a National COVID-19 working group that reports to the highest levels. Our staff in Chicago, running a facility for six of the top ten international pharmaceutical companies, have looked at thousands of potential drug candidates and have helped in the process of therapeutic development. We also have studies going on in Buffalo to look at how the drugs interact with the virus and to computationally understand how these viruses infect us. We have been busy.

EDWARD SNELL, PHD

President & CEO
Hauptman-Woodward
Medical Research Institute



The Institute is classed as an essential business during this period and our work on other diseases has continued. This would not have been possible without the work of many outside of the scientific efforts. Our building and facilities team have worked tirelessly to keep the Institute open and operational with creative ideas to keep us safe. Scientific staff are staggering their activities and are being adhered to mask and hand hygiene protocols. Administratively, we have embraced remote working, and the use of video conferencing has made connections with our team in Chicago closer than ever before.

During the pandemic, we have been working to integrate our research services, partly due to the new Cryo-EM Center, but also to leverage its capabilities with those we already provide to the structural biology community. Several articles describe this and introduce some of the new faces that are making this happen. There are a lot of exciting things happening and a lot to come.

Thank you for your support and for making much of what is described in this Structures issue happen.

THE INAUGURAL CRYO-EM CENTER LECTURE

Nobel Prize winner, Dr. Joachim Frank, presented an on-line lecture "Single-Particle Cryo-EM: Visualizing Biological Molecules In Their Native State" on Thursday, February 11 to celebrate the opening of the Hauptman-Woodward Medical Research Institute's new Cryo-Electron Microscopy (Cryo-EM) Center.

→ WELCOME

Dr. Frank is a Professor in the Department of Biochemistry and Molecular Biophysics and the Department of Biological Sciences at Columbia University and a Distinguished Professor of SUNY Albany. We are honored that Dr. Frank gave this inaugural lecture as he is one of the seminal figures in the history of Cryo-EM. He won the Nobel Prize for Chemistry in 2017 with Jacques Dubochet and Richard Henderson for developing Cryo-EM for the high-resolution structure determination of biomolecules in solution. The lecture was very well attended with over 600 people registered for the event from all over the world. HWI's CEO, Dr. Edward Snell, described the importance of adding Cryo-EM to ongoing activities at the Institute and he thanked the numerous foundations, corporations and community members for their generous donations that made the Center possible and ThermoFisher for sponsoring the lecture.

Dr. Frank gave an exciting overview of the development of Cryo-EM, interspersed with amusing anecdotes and recollections from his lengthy career. His contributions include developing general methods for reconstructing images into the shapes of particles and, in 1987, the first demonstration that these methods can be used for 3-D reconstruction by Cryo-EM single particle analysis. He presented a graphical timeline, adapted from his 2017 review in Nature Protocols, showing how his work laid the foundation for later technical advances to drive the limits of resolution for Cryo-EM to the atomic scale.

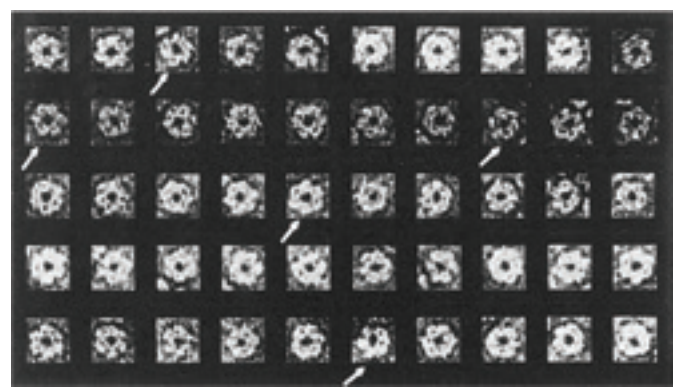
TO THE CLUB

Dr. Frank recalled visiting the Institute in June 1991 on an NIH site visit to evaluate a Research Program Project Grant proposal and again after the opening of the current HWI building in the early 2000's. He had fond memories of the Institute's Research Director and namesake, Dr. Herbert Hauptman, and he shared an image depicting Dr. Hauptman holding one of his glass geometric shapes (which are on display in the atrium of the Institute). This was part of Dr. Frank's talk titled "Medieval Iconography of Scientists", a series of paintings and photographs of famous scientists contemplating their life's work in their offices.

He described Dr. Hauptman as his 'real space companion,' alluding to the fact that both he and Dr. Hauptman were mathematicians who advanced the interpretation of raw structural biology data into usable images for structure analysis and determination, and they both won the Nobel Prize for Chemistry. As Dr. Jiang said in his introduction to the lecture, mathematics went a long way for both of them.

Dr. Frank ended his lecture by showing the real-world importance of Cryo-EM, illustrated by the role of Cryo-EM in combating various recent infectious disease outbreaks around the world, including particularly important contributions to understanding the current SARS-Cov2 or COVID-19 pandemic.

If you missed the lecture, a recording is available on our website **hwi.buffalo.edu/hwi-Cryo-EM-center-inaugural-lecture.**



Early images of a bacterial protein showing the power of electron microscopy to determine biomolecule structures (Frank et al., (1978) Ultramicroscopy, volume 3, pages 283-290).

HWI'S NEW CRYO-EM CENTER IS OFFICIALLY OPEN!

HWI is proud to add cryo-electron microscopy (Cryo-EM) to the range of its structural biology techniques. Cryo-EM has revolutionized high-resolution structure determination of biomolecules and was recognized in 2017 with a Nobel Prize in Chemistry to Joachim Frank, Richard Henderson, and Jacques Dubochet. The power of Cryo-EM single-particle analysis lies in the preservation of macromolecules in frozen-hydrated states through rapid vitrification, which enables the visualization of biological targets in their native state. Unlike X-ray crystallography, there is no requirement to crystallize the protein as structures are determined from single protein particles frozen in ice rather than from crystals which can be very challenging, if not impossible, to grow for many biomolecules. Single-particle analysis relies on observing a sample in multiple different orientations and can determine structures of macromolecular complexes that bear certain flexibility or heterogeneity that often prevents their crystallization. Over the past decade, technical and methodological improvements have enabled routine high-resolution Cryo-EM structures of well-behaving biological samples.

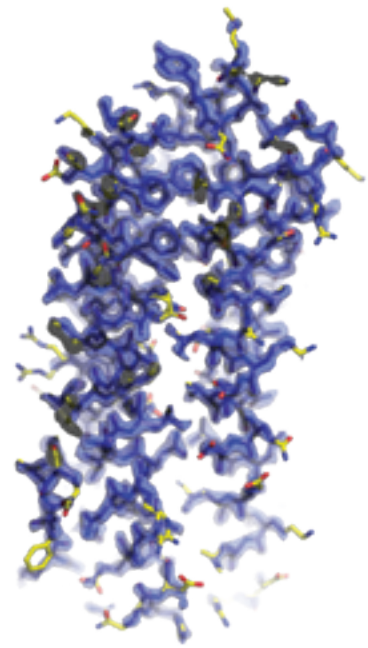
AFTER YEARS OF PLANNING AND DESIGN, MONTHS OF CONSTRUCTION, AND WEEKS OF MICROSCOPE CALIBRATION AND VALIDATION, THE WAIT IS OVER…

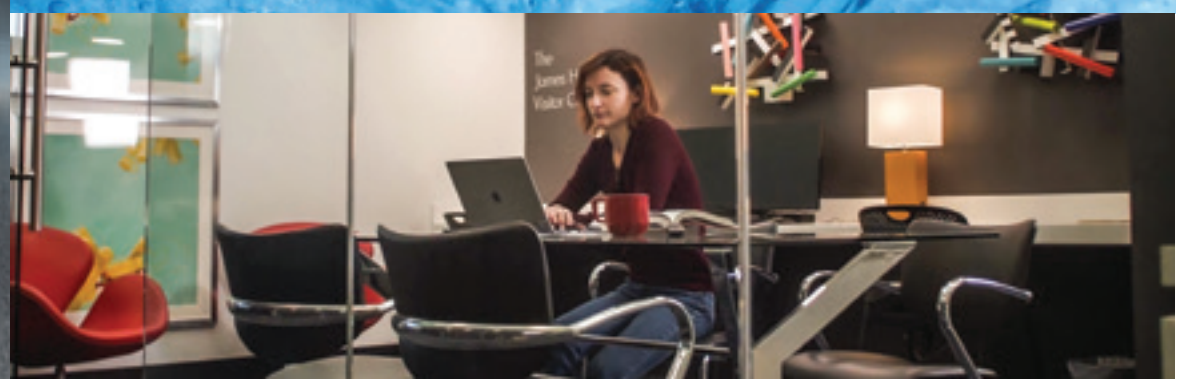
Planning for Cryo-EM began in early 2014 after a small meeting took place in England on complementary structural approaches where a paper was presented on Cryo-EM and how there had been impressive recent advances. HWI CEO, Dr. Edward Snell, was presenting work in the same meeting, heard the talk, and came back to HWI to spread the word to the scientific team. The potential was obviously there and as we looked at how to take advantage of it, results kept coming from this new approach. The excitement grew and the board learned this from the scientific team and were convinced about this new potential. We are grateful to our donors who supported the capital needs to construct a purpose-built center specifically designed for Cryo-EM and to purchase a state-of-the-art microscope and a high-end direct electron detector. Construction started in March, 2020, and was completed in December 2020, despite delays due to the coronavirus pandemic ThermoFisher Scientific installed the microscope at the end of 2020 through January 2021.

HWI reached out to many in the field and listened to their advice. The center was designed to provide a stable environment for optimal performance of a Cryo-EM instrument. The Cryo-EM Center is separate from the main part of the HWI building and has key card-controlled access to reduce foot traffic and noise. The floor is seismically stable and the walls of each microscope room are isolated from exterior walls to minimize mechanical vibrations. Room temperature in the scope room is finely controlled by a set of glycol cooling panels mounted on the walls of the microscope room to minimize temperature fluctuations. Even interference of the microscope by turbulent airflow is minimized by a unique double ceiling with membrane diffusing panels.

Currently at the HWI Cryo-EM Center, its first Cryo-EM system is made up of a ThermoFisher Glacios cryo-transmission electron microscope (TEM) equipped with a newly-released Falcon 4 Direct Electron Detector, which is geared for high-throughput grid screen and delivery of a large volume of high-resolution data in a short one-day working cycle. The main purposes are to enable the fast turnaround of Cryo-EM specimens from sample freezing to data collection and delivery. This new system is able to deliver truly atomic resolution recording approximately 250 movies/hour and has been benchmarked at 2.2-2.3 Å from an overnight data collection of only ~9 hours. It is thus highly suited for high-resolution single particle analysis. In addition, the hardware and software in the new Glacios allow for the collection of electron diffraction data from nano-meter-sized 3D crystals—a technique named micro-ED, which will enable the integration of some key techniques available in the three centers of HWI in order to achieve high-throughput crystal growth and screening, micro-ED data collection, structure determination and molecular modeling. The addition of Cryo-EM thus makes such integrated techniques a powerful weapon to address cutting-edge scientific questions and accelerate therapeutics development in the immediate future.

The layout and functionality have been designed to promote the highest quality scientific results. The Center is now producing results yielding astonishing levels of detail.

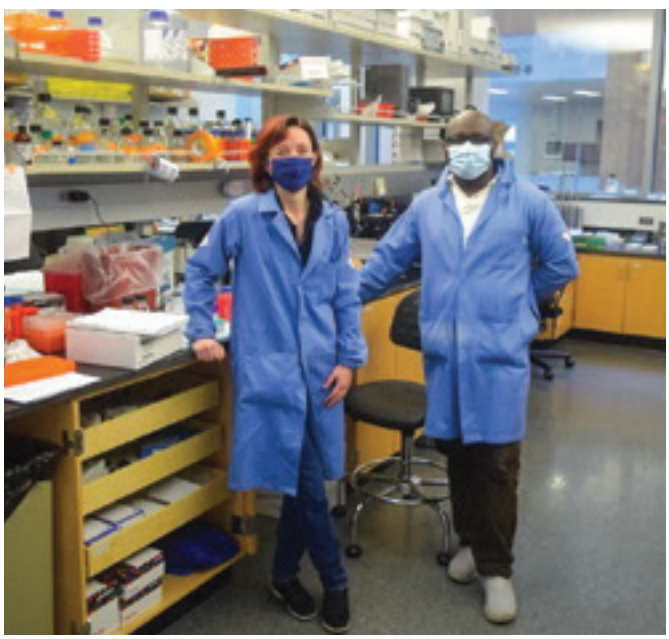




HWI has been at the forefront of protein crystallography for decades. X-ray crystallography has allowed us to visualize proteins in great detail, providing the necessary information for drug design. But thus far, mostly due to technological limitations, our study of proteins has been limited to observations at cryo-temperatures, where the proteins are frozen. But proteins are not static—on the contrary—they move through different shapes while functioning and these movements are as critical to their activity as the structure. Studying these dynamic behaviors has become possible very recently, thanks to the availability of stronger, brighter X-ray facilities and amazing advances in protein production and crystallization.

VISUALIZING PROTEINS AT WORK

A collaboration between Dr. Diana Monteiro at HWI and Profs. Wei Liu, Petra Fromme and Alexandra Ros at Arizona State University is working on making molecular movies of proteins while they function. These are stop-motion movies: snapshots of proteins changing shape while they carry out their function. The experiments make use of cutting-edge methods and instrumentation and require a broad range of expertise. The team comprises scientists with expertise ranging from synthetic chemistry to protein biology, through engineering and X-ray science. We are specifically looking at one class of proteins, called GPCRs, as they are the target of roughly 12% of all medications currently on the market. These proteins are present in cell membranes and are difficult to both obtain in large quantities and crystallize. Dr. Monteiro is providing the team with novel molecules that will be used to activate the proteins during the experiment.



These molecules are light-sensitive and are being designed and synthesized in the new synthetic chemistry laboratory established by Dr. Monteiro and Dr. Snell at HWI. The work is being supported through NIH and NSF (BioXFEL) grants and has provided funds for the expansion of the HWI team with the hiring of a new postdoctoral scholar, Dr. Emmanuel Amoah. Drs. Amoah and Monteiro are working hard to bridge the gap between chemistry and biology and develop new chemical tools that enable these complex structural biology experiments. The project was started in mid-2020 and the first prototypes of these synchronizing agents are already ready for initial tests.

The biological questions we try to address are becoming more and more complex, especially when the boundaries are torn down by the emergence of new technology. Scientific research is continuously becoming more and more collaborative and interdisciplinary, with experts pooling their knowledge to solve ever more complicated puzzles.

A big thank you to William J. Constantine

WILLIAM J. CONSTANTINE JOINED THE HWI BOARD IN 2018. During his tenure on the board Bill has been a driving force in development efforts. As Development Chair, Bill had the vision to start building a development department that included a full-time development person and increasing board participation in philanthropic giving.

Recently, thanks to Bill's leadership, the HWI Board and Community partners came together to help purchase a microscope upgrade for our new Cryo-EM Center. It was Bill's $100,000 challenge gift that helped raise the $400,000 needed for this upgrade in less than a months' time.

This upgrade will allow us to double or triple data delivery, enhance the quality of results, and allow users to view and judge data quality on the fly during data collection. All of these benefits will improve the Cryo-EM Center's performance, increase demand for use of the microscope, and augment revenue generation for HWI.

Bill's dedication to HWI pours into every event that the Institute hosts and programs it offers. We are fortunate to have a knowledgeable and strong leader like Bill as part of our family.


IT STARTED AS A

HOW HWI MADE A MARK ON CORONAVIRUS RESEARCH

CONVERSATION

In late January 2020, many HWI researchers were attending an international meeting in Puerto Rico. There was a conversation going on about a new virus that had been identified in China that was responsible for an outbreak of pneumonia-like cases popping up all around the world.

This virus would eventually be named SARS-CoV-2 (Severe Acute Respiratory Syndrome Coronavirus 2). One of our collaborators at the meeting was Dr. Brenda Hogue, a specialist on coronaviruses. On hearing the news of this new virus, she left the meeting early to return immediately to her lab to initiate work on the new virus.

Coronaviruses are named for the 'corona' which means crown. When you look at them, they have distinct spike structures coming out of them that look like the projections on a crown or rays of light that come from the sun. These spikes are the 'hooks' that catch cells in the human body and allow the virus to infect us.

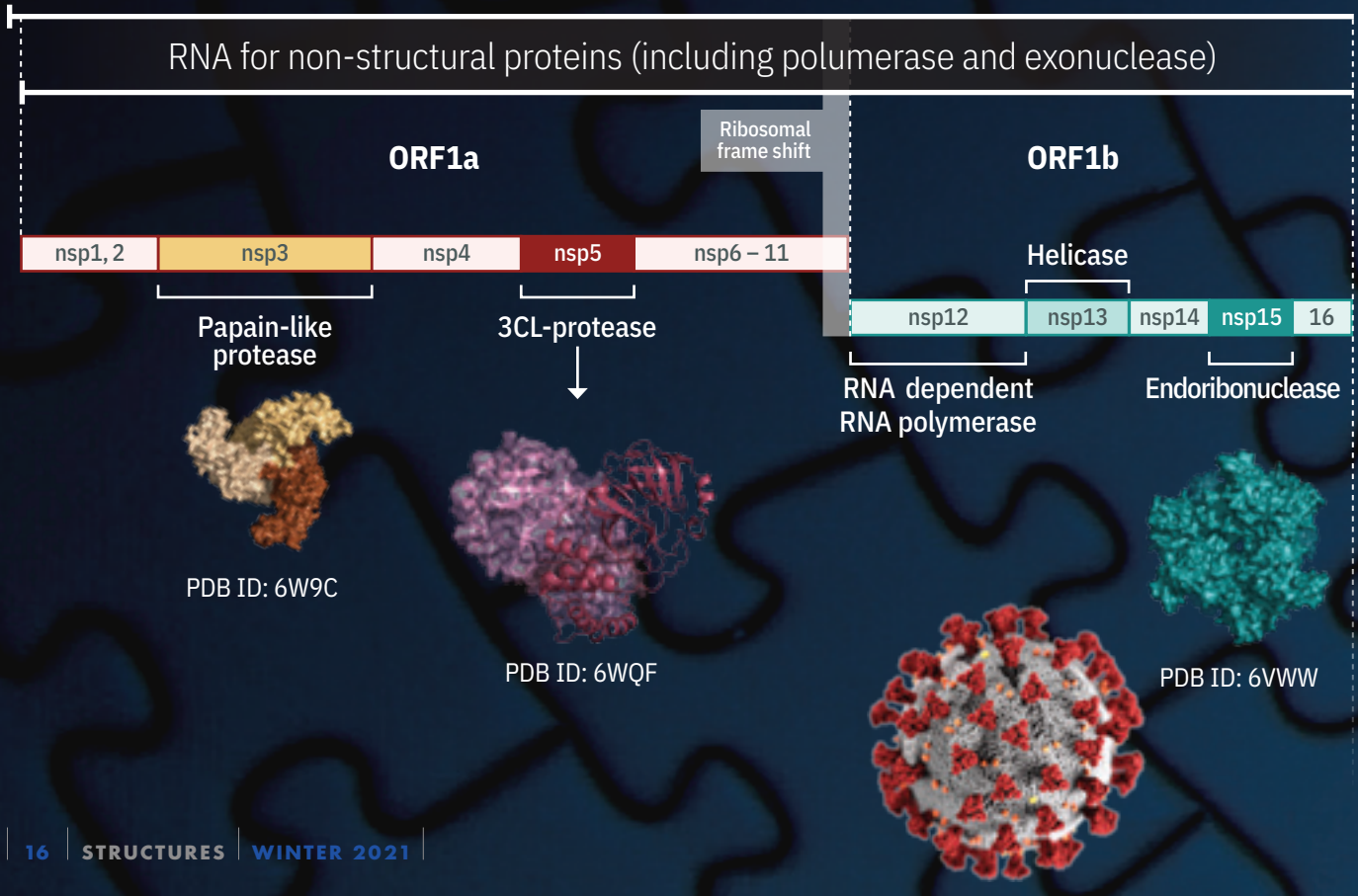
The virus has been called the invisible enemy, yet by now almost all of us have seen representations of what it looks like. The virus is over ten million times smaller than us and impossible to see with a standard laboratory microscope.

The virus itself is made up of multiple parts, and the process used to see those parts is called structural biology, which is the expertise of the Institute. In the weeks after the first report of the cluster of pneumonia cases in the initial outbreak, the first SARS-CoV-2 genome sequence was made publicly available. The genome is the blueprint for all the parts that make up the virus and is the code that enables the virus to reproduce in human cells. The urgency that drove Dr. Hogue back to her lab from the meeting in Puerto Rico impelled many researchers to pivot to studying this new viral threat. Structural biologists worldwide pivoted to focus on solving structures of the pieces and parts that make up the SARS-CoV-2 virus. In a matter of just two weeks, the first three-dimensional structure of one of the critical viral proteins, the main protease, was solved using X-ray crystallography. At HWI, we have been at the forefront of X-ray crystallography for decades. A picture of the spike protein emerged almost as quickly from cryo-electron microscopy, the technique we are bringing to Buffalo in our new Cryo-EM Center. We began to see our enemy.

On March 1st the first positive case of the COVID-19, the disease caused by the SARS-CoV-2 virus, was seen in New York State; just under 2 weeks later the first positive cases were seen in Erie County. Four days later in New York State, businesses were asked to reduce workforce density and all non-essential businesses were closed on March 22nd. The Institute was classified as essential for research we were doing to combat COVID-19. The Crystallization Center at HWI began working with other structural biologists on SARS-CoV-2 proteins on March 18th.

Multiple proteins make up the virus, like parts in the engine of a car. The SARS-CoV-2 virus has 29 proteins that make up its 'engine', each of which performs a specific role in how the virus works. Some of the parts are targets for new drugs for treatment after infection and some of the parts are targets for vaccine development to prevent infection. X-ray crystallography and Cryo-EM were used to determine structural information from these targets with the Institute being involved in over 60 studies from laboratories nationwide and helping support other collaborative research worldwide.

Therapeutics Targets

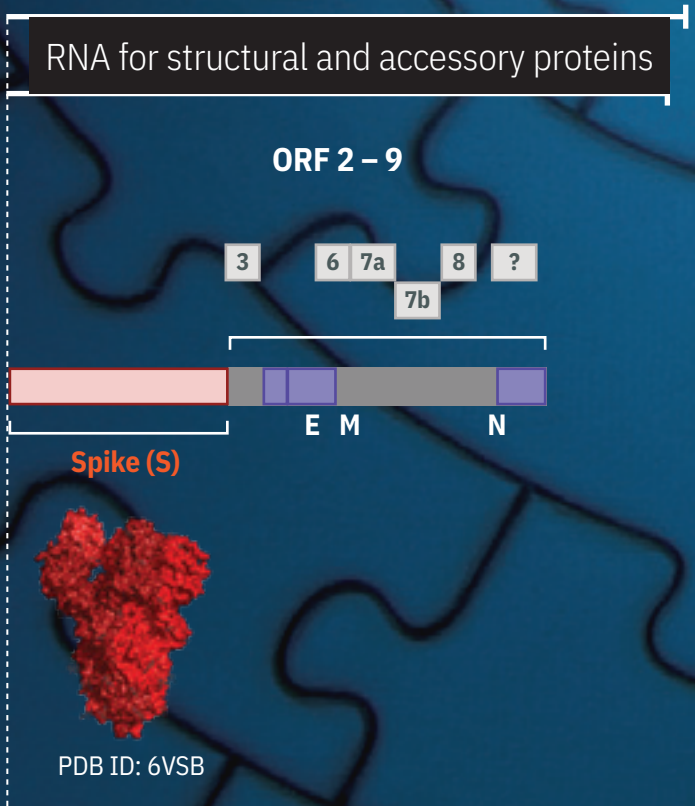


To date, there are over 1,000 structures of the parts that make up the SARS-CoV-2 virus and drugs that may interact with them. About 80% of these pictures come from X-ray crystallography and the remainder from Cryo-EM. Of the studies that look at how different drugs may bind, over 90% came from X-ray crystallography data. This includes work supported by our team in Chicago on a treatment that Pfizer is developing and work in the Crystallization Center on the main protease. Crystallography rapidly provided structural details about the smaller components of the virus, which many possible drugs could target, while Cryo-EM enabled the scientific community to look at larger pieces, notably the spike protein, and be in a position to develop the vaccines. Without the combination of X-ray crystallography and Cryo-EM, we would not have the critical information that is driving vaccine and therapeutic development today.

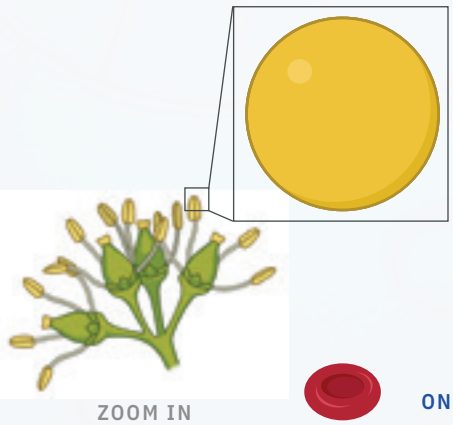
If there is ever a time to demonstrate the role of structural biology in human health, the COVID-19 pandemic is a snapshot of potential, of how when resources are available, there can be a scientific solution to disease and a solution that occurs within the lifetime of patients.

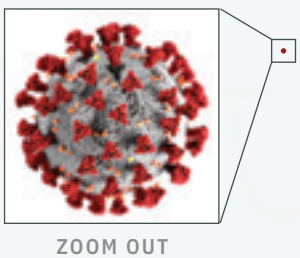
The Institute is moving into a new era with new capabilities thanks to supporters like you. The pictures you see of the virus in the media are what we do and what we will continue to do.

Vaccine Targets



VIRUSES ARE SMALL





HWI SCIENTISTS LEAD NATIONAL RESEARCH EFFORTS FIGHTING COVID-19

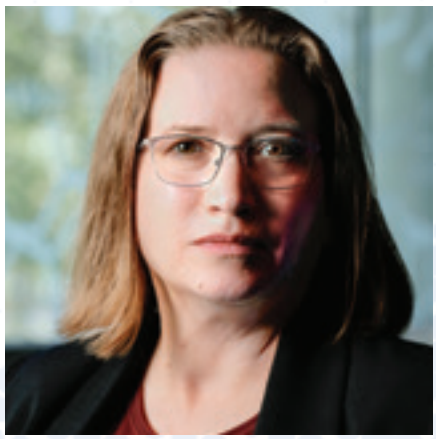
This spring, HWI received $600,000 in grants from the National Science Foundation (NSF) for research projects centered on the molecular structure of SARS-CoV-2, better known as the virus which causes COVID-19.

Dr. Sarah Bowman, Director of the National Crystallization Center, extends the Center's structural biology services for researchers working to accelerate knowledge production about coronavirus proteins and develop new experimental pipelines to accelerate response time in the face of the current and future pandemics.

$200,000 award

A collaborative effort led by Dr. Diana Monteiro from HWI and Dr. Thomas Grant from the Jacobs School of Medicine & Biomedical Sciences at the University at Buffalo uses rapid analyses to understand how proteins critical to SARS-CoV-2 viral replication function within cells of infected individuals, and how these proteins interact with potential therapeutic drug compounds.

$200,000 award



Dr. Miranda Lynch, a Staff Scientist at HWI, will develop machine learning-based computational tools for the prediction of protein-to-protein interactions involving SARS-CoV-2 and proteins in our bodies. Her team will utilize advanced computational methods to build knowledge on how the virus enters human cells and how the virus could react to potential drugs.

$199,816 award

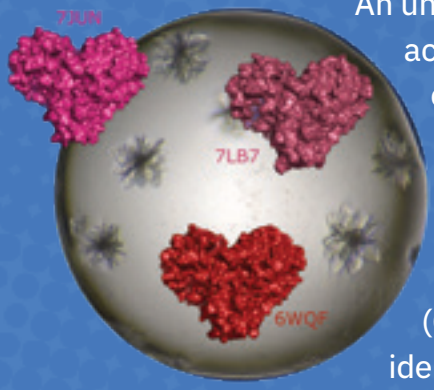
These grants were awarded by the NSF's Division of Biological Infrastructure (DBI) through its Rapid Response Research (RAPID) using funds from the Coronavirus Aid, Relief, and Economic Security (CARES) Act passed by Congress on March 27, 2020.

The funding provided to researchers at Hauptman-Woodward from the National Science Foundation will not only assist local COVID-19 research efforts, but also research of the current pandemic nationwide. "We are proud to have Western New York scientists leading the charge in studying the biology of the virus causing this global outbreak," said Congressman Brian Higgins (NY-26).

MAKING THE INVISIBLE VISIBLE

Structural biology helps scientists understand how the coronavirus enters human cells and how viral proteins interact with human proteins.

"We literally make the invisible visible," explains Dr. Edward Snell, CEO of HWI. "We try to determine what the components of the virus look like. If we can see what they look like, we can stop it from reproducing."



An unprecedented sharing of research and information across the scientific community has led to collaboration and progress as researchers seek to quickly identify treatments and vaccines for COVID-19. HWI scientists are laying the groundwork for these efforts as X-ray crystallography and cryo electron microscopy (Cryo-EM) provide the road-map for protein identification and drug development.

Dr. Sarah Bowman, the Director of the National Crystallization Center, explains how HWI's work helps scientists "see" the virus differently. By using X-ray crystallography, which acts as a map, Dr. Bowman's team is able to get a bigger picture of what molecules in the virus look like.

"The red things that are sticking out of the surface of the virus are actually a particular protein called a spike protein. The structure of the spike protein was solved really quickly, which will help us figure out what drugs might stop it from spiking into human cells and infecting people. We are also looking at how different drugs will react with the virus," says Dr. Bowman.

OUR INTERNS ARE VIRTUALLY THE BEST.

BioXFEL interns and mentors meet virtually through Zoom during the 2020 summer internship program. At the outset of the pandemic they shifted to a remote program and created new research projects and educational activities to accommodate the unique situation.


BioXFEL

SUMMER SCHOLARS

While continuing our critical research during the pandemic, we did not lose sight of our mission to educate. Last summer we worked tirelessly to shift our Duax Education Program to a virtual format, hosting students from around the country—and even from outside the USA.

Using this new virtual format, Dr. Duax continued his 10 year tradition of teaching our youngest scientists about the fundamentals of bioinformatics. This program has served as a gateway into science careers for hundreds of high school students and continues to train the next generation of scientists. To learn more about the Duax Summer Program please visit: **hwi.buffalo.edu/duax-high-school-program**.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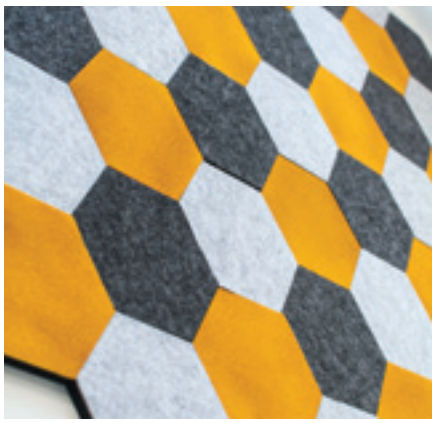


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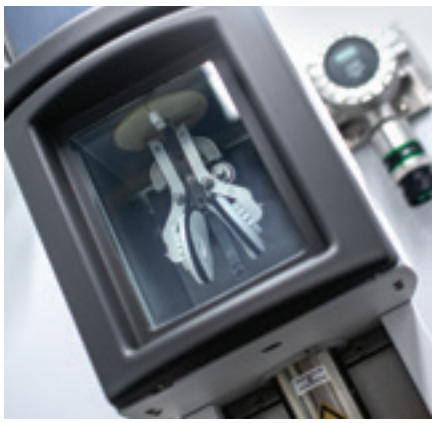
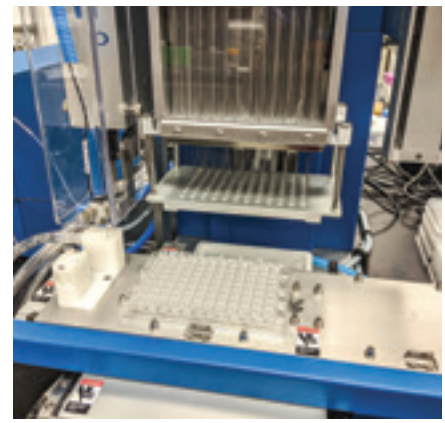
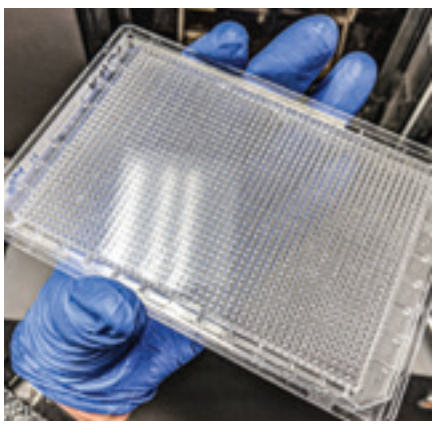
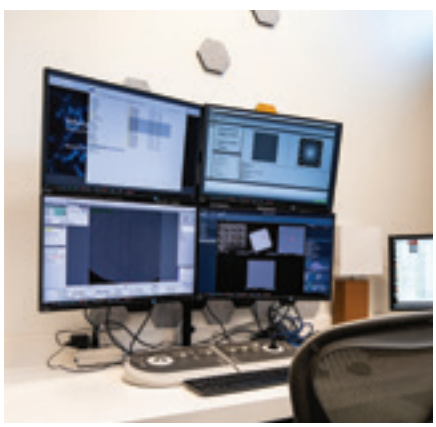







innovation starts here


HWI

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HWI

Dr. Timothy Stachowski is currently a post-doctoral researcher at St. Jude Children's Research Hospital in Memphis, Tennessee. Tim graduated in August last year earning his PhD at the Institute in the midst of the pandemic. He defended his work in front of a committee with representation from Roswell Park Comprehensive Cancer Center (RPCCC), The Jacobs School of Medicine and Biomedical Science, the Hauptman-Woodward Medical Research Institute, and in an acknowledgment of how research communities have adapted to the pandemic, a virtual member from the Hamburg Center for Ultrafast Imaging in Germany.

Tim was a graduate student in the RPCCC Molecular and Cellular Biochemistry and Biophysics program and completed his doctorate under the supervision of Dr. Edward Snell, CEO of HWI and adjunct professor at Roswell Park. Tim worked on a protein called Transforming Growth Factor Beta-1, a protein that controls the signaling in the body that turns off cell growth—something that can lead to cancer when it fails. Tim's work demonstrated that this protein could be activated by low X-ray doses, as low as those used for some treatments. This is important as radiation therapy is a common tool in some health areas. We know a lot about what happens structurally at doses that are orders of magnitude above the therapeutic dose, but very little about structural changes that can occur within this therapeutic regime. Knowledge of this may allow the development of prophylactic approaches to minimizing radiation therapy side effects that can be detrimental to treatment and recovery.

Tim demonstrated how the target protein is protected in the body and activated when needed. Using a variety of techniques, he determined what was involved with the activation and more importantly, what was not. This has direct implications for the development of therapeutics that can help impede the progression of cancer.

The work led to the development of techniques and chemical strategies to study many proteins under very low X-ray dose conditions. This is important as, while X-ray methods can reveal intricate details about how life works, many processes in the body that are critical for life can only be seen with X-rays after they have happened. It is difficult to follow how they work if the initial state is unknown. It is somewhat similar to trying to understand how a football match was won by only knowing the final score. Tim's work not only revealed a previously unknown mechanism, but it laid the groundwork to develop tools to allow others to build upon the Institute's discoveries.

Tim's work was recognized by his peers with multiple prizes from presentations at national and international meetings including a prestigious Linus Pauling award from the American Crystallographic Association for one of the best poster presentations. Tim grew from a student to a peer and we are proud to have had him train at the Institute, contribute so much to the field so early on, and see him successfully transition to an opportunity with St. Jude's.

We know he will be one of the stars of the future.

Connections Grow BioXFEL Scientific Community: Dr. Marchany Rivera

As a young girl growing up in Puerto Rico, Dr. Darya Marchany Rivera was drawn to anything having to do with science. She began participating in science fairs in 7th grade, and in 10th grade she was part of a sample preparation workshop/competition for protein crystallization in microgravity by high school students held by NASA and the University of Puerto Rico at Mayaguez. That same year she also presented a crystallization project at the International Science Fair celebrated in Cleveland, OH. Inspired in part by Ms. Marisol Colon, her wonderful high school chemistry teacher, Dr. Darya Marchany Rivera discovered that she excelled at conducting research and experiments and never looked back.

She went on to the University of Puerto Rico (UPR) to major in Chemistry. She was able to work in the lab of the professor who ran that high school competition, Dr. Juan Lopez Garriga, allowing her to focus on crystallization. She liked solving structures from crystals and making models.

A key focus of BioXFEL is to engage and build a culturally and academically diverse inclusive community of scholars. As part of its outreach efforts to students at the University of Puerto Rico, Professor Elspeth Garman from Oxford invited Dr. Marchany Rivera to the 2nd annual international BioXFEL conference. She met the BioXFEL team and scientists from Hauptman-Woodward Institute there, and was able to do a graduate internship at HWI in the summer of 2015.

"I really liked Buffalo," Dr. Marchany Rivera said. "The team at HWI was very welcoming and very supportive. They were always willing to help me when I had questions or needed advice. I ended up being there with several undergrads from the University of Puerto Rico who I didn't know beforehand. It was here for the first time I got to work with an X-ray diffractometer, which they have in-house at HWI. I worked with this on my own, which was really nice. The lab was better suited for this type of work because it was specific to crystallization."

Dr. Marchany Rivera was able to advance farther in her research than she had anticipated during her summer at HWI. It was during her time at HWI, through conversation with

Dr. William Bauer, Education and Diversity Director for BioXFEL, that she realized she wanted to become a staff scientist at a national lab.

When she returned to UPR, a few incidents caused setbacks in her lab, including the devastating effects of Hurricane Maria in 2017.

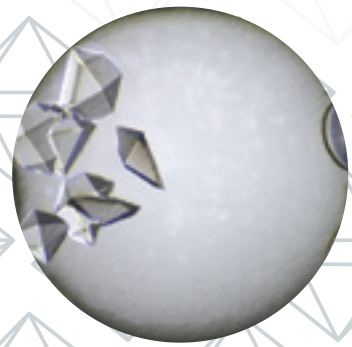
Fortunately for Dr. Marchany Rivera, due to relationships she had built through BioXFEL, she was able to go to Stanford University/SLAC National Laboratory with four other students to continue her work. She stayed there for almost a year—longer than she had expected—and continued to make connections with people who have helped her in her career.

"Dr. Marchany Rivera was instrumental in the development of BioXFEL programming for UPR researchers," according to Bill Bauer. "Not only was she one of our first UPR graduate student interns, she also assisted with creating scientific workshops, identifying the needs of the students, and is now on the BioXFEL Education and Diversity Committee. After Hurricane Maria devastated the island, we reached out to all of our UPR colleagues to offer assistance. This was very challenging because all of the island's communication systems were compromised. However, as soon as we contacted Dr. Darya Marchany Rivera, she took the lead, organized the students, and helped us deliver help to the students most in need. Her leadership, organizational skills, and scientific intuition will certainly help her become a leader in her field."

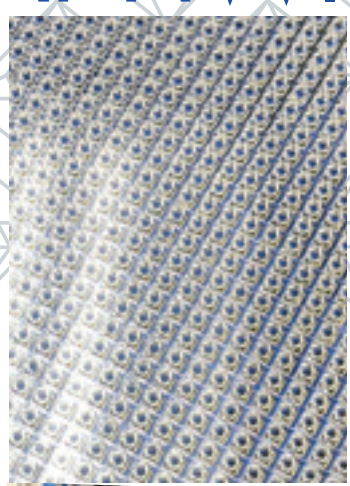
Dr. Marchany Rivera has now graduated with her PhD and is doing her post-doctoral work with another BioXFEL partner, Dr. Brenda Hogue, at Arizona State University starting this July.

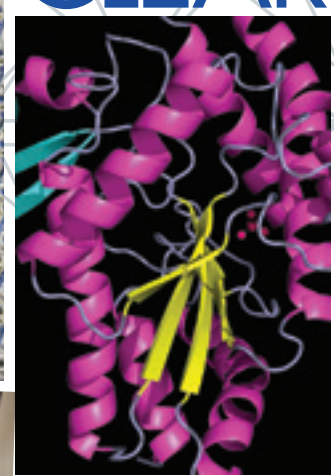
"I am so grateful that I was introduced to the BioXFEL community," Darya said. "I wouldn't be where I am in my career without their community of scientists."

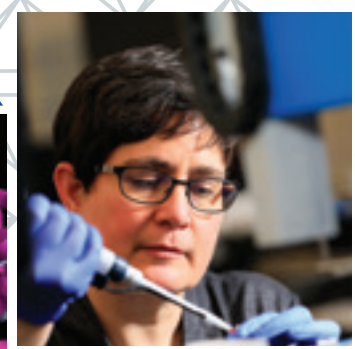
CRYSTALLIZATION CENTER RECEIVES SUPPLEMENTAL FUNDING FROM NATIONAL INSTITUTES OF HEALTH

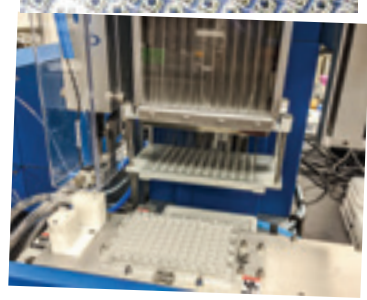


THE FUTURE AT HWI IS CRYSTAL CLEAR









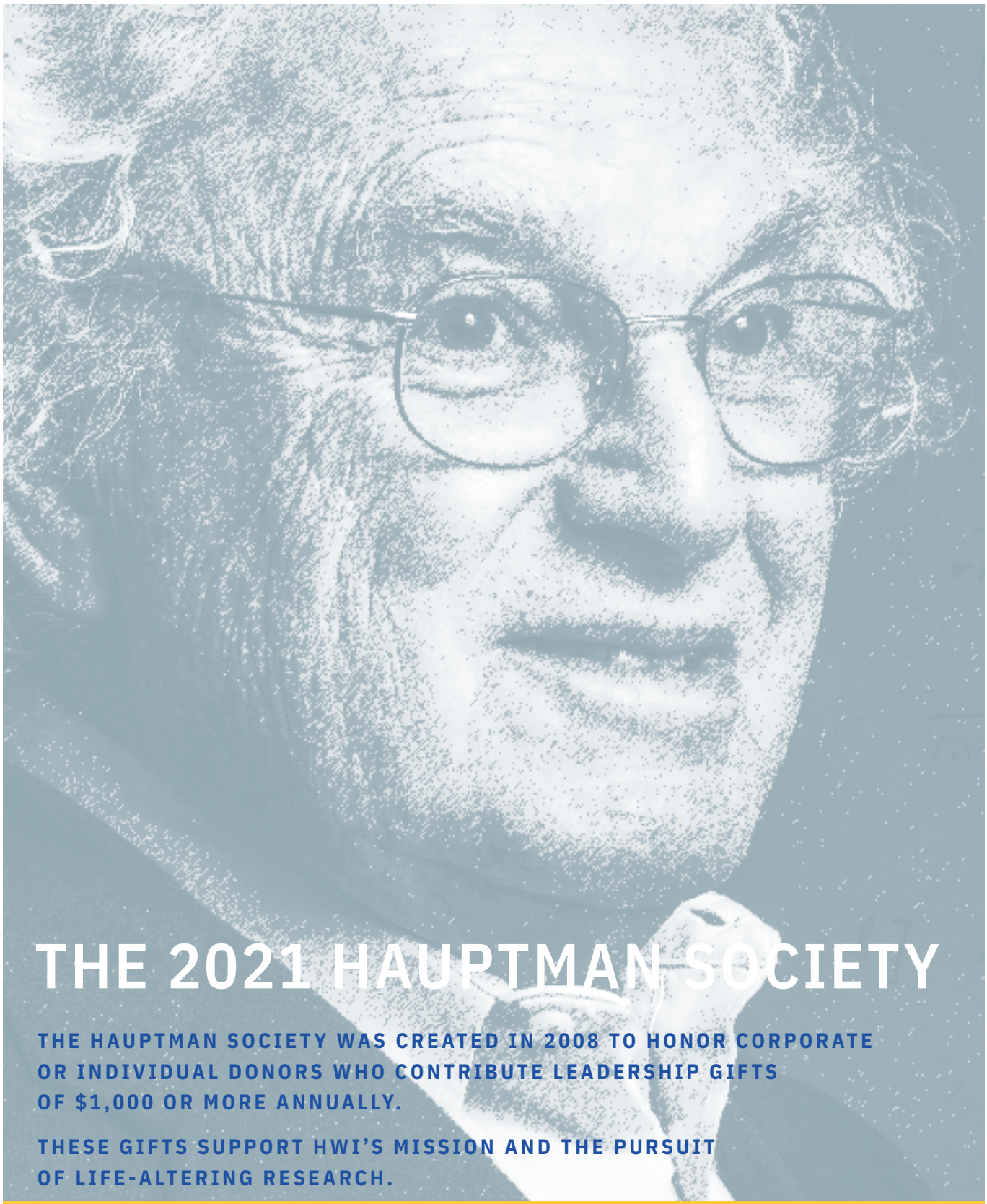
NATIONAL CRYSTALLIZATION CENTER

In an exciting footnote, the Crystallization Center has now become the National Crystallization Center, reflecting its work before and during the COVID-19 pandemic. This $4.9M grant from NIH and its impact on the Center will be described in a future edition of STRUCTURES.

Structural biology methods help us to understand fundamental principles at the base of how proteins – the molecular machines in our cells – work by enabling us to visualize molecules at an atomic level of detail. Close to 90% of all three-dimensional structures are generated using experimental methods that depend on the sample being in a crystalline form. One of the major bottlenecks is making the crystals. Searching for conditions in which a protein will crystallize can mean screening multiple different constructs against thousands of crystallization conditions, requiring large sample amounts and many person-hours in a typical laboratory set-up. The Crystallization Center at HWI specializes in resolving this crystallization problem. The Crystallization Center, in operation for over 20 years, is a high-throughput facility that provides expertise and access to state-of-the-art instrumentation to facilitate efficient and cost-effective protein crystallization. Scientists from around the world make use of the established pipelines we have developed at the Crystallization Center, in which scientists mail their samples to us here in Buffalo, NY. In the Crystallization Center, we set up the samples in our unique high-throughput 1,536 well microassay plate with our liquid handling robotics. After a crystallization experiment has been set up, we watch crystals grow using state-of-the-art imagers to monitor each of the 1,536 experimental wells.

The Crystallization Center has been operating as a National Institutes of Health (NIH) National Institute for General Medical Sciences supported Legacy resource since 2017. This NIH funding provides support for crystallization experiments to the structural biology community around the world. Since 2017, the Crystallization Center has set up samples for close to 200 different research groups from 32 US states and territories, as well as from 18 international users. These groups work on understanding the biology of many different diseases. In Buffalo, we empower each one of these studies by providing our expertise to accelerate research progress.

The COVID-19 pandemic has disrupted scientific efforts worldwide. Our Crystallization Center has remained operational as an essential research laboratory in the fight against COVID-19. We have been very successful with SARS-CoV-2 projects during the past year. However, normal operations were interrupted for the Center and for our users due to the pandemic. Many of the research laboratories that send samples to the Crystallization Center for screening were shut down for at least some period due to COVID-19. To accommodate these disruptions and enable continued support for our ongoing operations, the Center was awarded an NIH supplemental grant of $246,000, which has extended our funding at this critical time. These funds have helped keep our Crystallization Center running for both our work on SARS-CoV-2 proteins and for the other diseases under study, for which we and our users from around the world are very grateful.



THE 2021 HAUPTMAN SOCIETY

THE HAUPTMAN SOCIETY WAS CREATED IN 2008 TO HONOR CORPORATE OR INDIVIDUAL DONORS WHO CONTRIBUTE LEADERSHIP GIFTS OF $1,000 OR MORE ANNUALLY.

THESE GIFTS SUPPORT HWI'S MISSION AND THE PURSUIT OF LIFE-ALTERING RESEARCH.

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INNOVATION EDUCATION

EVENTS DISCOVERY

WAYS TO GIVE

HAUPTMAN-WOODWARD was founded because of philanthropy which then became a legacy for Helen Woodward Rivas. You too can make an impact in a multitude of ways and create your own legacy. We welcome you to contact HWI's Director of Development, Lisa LaTrovato at llatrovato@hwi.buffalo.edu or 716.898.8624 to discuss the numerous ways in which you can contribute and make a difference.

HAUPTMAN SOCIETY

The Hauptman Society was created in 2008 to honor corporate or individual donors who contribute leadership unrestricted gifts of $1,000 or more annually.

These gifts support HWI's mission and the pursuit of life-altering research. Membership advantages include our Annual member event, an invitation to exclusive speaker series, behind the scenes tour of HWI and the diffraction lab, upon request, and your name on the Hauptman Society plaque in the lobby.

MONTHLY GIVING

It is an easy, convenient, cost effective way to donate to HWI and make an impact. Your donation will be automatically charged to your credit card every month without you needing to do anything.

The same amount will be deducted on the same day of every month until you tell us you would like to increase, decrease or stop your donation.

PLANNED GIVING

A planned gift is a contribution that is arranged in the present and is allocated at a future date. These gifts historically for HWI have made significant impact at critical junctures in our history and we thank the donors who had the foresight of giving in this manner. Examples of planned gifts are listed below.

- Gifts of Appreciated Securities
- Gift of Personal Property
- Retirement Plan Gifts
- Life Insurance Gifts
- Gifts of Real Estate
- Planned Gifts
- Bequests
- Gift Annuities

IN MEMORY/HONOR OF

A donation to HWI is a thoughtful way to express your sympathy for the loss of a loved one or to honor someone special in your life or in the industry.

THE JANE F. GRIFFIN PHD EDUCATION FUND

This fund was established in 2016 to recognize HWI Emeritus Researcher Jane F. Griffin, PhD for her longstanding commitment to and establishment of HWI's education programs. The Griffin Fund supports undergraduate students with paid summer internships to work with HWI research teams and gain practical, hands-on experience in a research setting. Many students have gone on to publish results of their work from this program.

STAFFORD FELLOWSHIP

HWI has a rich history in educating the next generation of scientists. Fellowships permit new talent to be supported over the course of their studies with our world renowned research groups. The Stafford Fellowship, established by HWI Emeritus Board Chair Constance Stafford Constantine, is our longest standing fellowship and has supported numerous PhD candidates who are now prospering scholars. Donors can contribute additional funds to this fellowship that already exists.

ENDOWMENTS

Many individuals chose to contribute funds to the Institute that will ensure their gifts will continue to give for years, if not decades to come. For example, Funds contributed to an endowed chair recognize an individual or a family's legacy. Three endowed chairs exists at HWI that have varying missions, they are listed below. Contributions to these chairs which are not yet fully funded are a tremendous way to honor the spirit of both the mission of the chair and for who they are named.

Don and Vicky Hess Endowed Chair

The goal of the Donald and Victoria Hess Endowment fund is to raise permanent funds to further secure the financial strength of Hauptman-Woodward Medical Research Institute.

Herbert Hauptman Nobel Laureate Endowed Chair

This fund will support the work of an outstanding scientist whose work, echoing that of Dr. Hauptman, bridges the gap between pure science and biomedicine.

William L. Duax Endowed Chair in Crystallography

The purpose of the fund is to support the scientific work and teaching of Dr. William L. Duax, and of future generations of Hauptman-Woodward scientists.

Create your own endowment

Endowed Funds can be used to establish a chair that will enable HWI to recruit the very best scientist who will have discretionary income to support their efforts from the chair they hold.

You can read more about these opportunities on our website at hwi.buffalo.edu/giving

CURES BEGIN HERE

FOR OVER 60 YEARS, Hauptman-Woodward Medical Research Institute has worked to find cures for diseases like COVID-19, cancer, and others that impact us today. Our renowned researchers study proteins in normal and diseased states and what they learn provides a foundation for developing medicines, therapies, and cures.

Hauptman-Woodward is Buffalo's only independent research institution and has an international reputation for excellence in structural biology. We house scientists in multiple disciplines and value diversity in ideas and backgrounds to promote novel and world-leading discoveries. Our goals of innovation, discovery, and education are driven by what we describe as CURE•OSITY as we work toward the cures of tomorrow.

INNOVATION // LEADING THE WAY

Since 2004, $86 million in federal grants have been invested in HWI research.

$86 MILLION

1 NOBEL LAUREATE

Dr. Herbert Hauptman received the Nobel Prize in Chemistry in 1985 for developing a mathematical method that changed the field of chemistry. It opened a new era in research in determination of molecular structures of crystallized materials.

Since the start of the COVID-19 pandemic, the HWI Crystallization Center has received federal funding to successfully work on close over 60 projects with research groups around the nation to battle the disease.

EDUCATIONAL IMPACT

The Duax Program in Bioinformatics has hosted over **300 STUDENTS** from more than **40 LOCAL HIGH SCHOOLS** during its **11 YEAR HISTORY.** In 2020, students participated virtually instead, drawing students from states such as Oregon, Massachusetts, and California, and even a student from France.

NEARLY $3 MILLION INVESTED IN EDUCATING FUTURE SCIENTISTS

from undergraduate interns to graduate students and even postdoctoral scholars. A key value of HWI's mission is our commitment to educating the next generation, and perhaps the next Nobel Laureate.

ACCELERATING RESEARCH AND DRUG DEVELOPMENT

IMCA-CAT

Industrial Macromolecular Crystallography Association Collaborative Access Team

HWI works in partnership with IMCA-CAT, a consortium of six of the world's largest pharmaceutical companies. IMCA-CAT's mission is to accelerate drug discovery through synchrotron-based structural biology research serving the pharmaceutical industry.

→ EVERY SO OFTEN SCIENTIFIC

I sat in Buffalo with my collaborator from Oxford University and when we crunched the numbers, we both immediately realized we'd made a discovery that would—at least—result in a significant debate within our scientific community," recalled Dr. Edward Snell, "We turned the numbers into a picture and hidden within the data was an explanation of how this molecular machine worked."

"We were the first in the world to see what had been hiding there all the time. The result was stunning."

The study was about proteins that contain metal, known as metalloproteins. They play important roles in biology doing jobs in the body, regulating various pathways which often become targets for lifesaving drugs. While the amount of metal in such proteins is usually tiny, it is crucial to determining the function of these complex molecules and critical for a healthy life.

Scientists have long known that metalloproteins are vital to understanding diseases, such as cancer, and for developing new drugs since inhibitors of metalloproteins have been used to treat diseases from cancer and HIV/AIDS to bacterial infections and hypertension. But there hasn't been a reliable, analytical method for determining the identity, quantity, and position of metal atoms in metalloproteins.

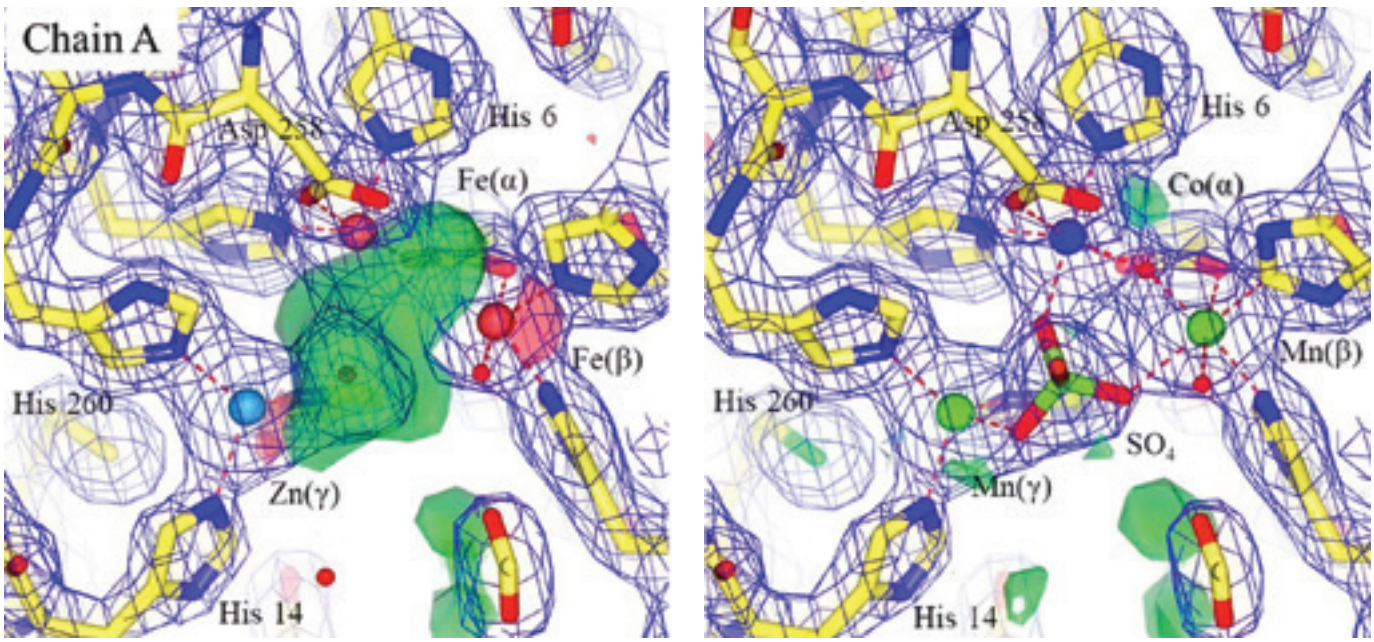
An international collaboration involving scientists from Buffalo, Rensselaer Polytechnic Institute, Columbia University, Oxford University, and the University of Surrey Ion Beam Centre (both in England) worked to couple a well-developed technique called Particle Induced Emission of X-rays, or PIXE, with the high-throughput capabilities of the HWI National Crystallization Center. The magic happened when they combined these capabilities with a touch of X-rays and applied it to a set of 30 randomly selected metalloproteins whose structure and metal content was thought to be known.

The results were dramatic—the methods previously used to determine some of these 30 random protein structures had either misidentified the metal atom or, in some cases, completely missed it. "According to our results, the current knowledge of about half of the samples we studied is incorrect," said Dr. Snell.

The Protein Data Bank is a worldwide repository for structural information and has over two million downloads of structural information per day. Of the almost 175,000 different structures that are deposited there, more than 30% contain a metal. An enormous number of researchers use these structures daily without knowledge of the potential fundamental errors that may be present. This study alerted researchers to the problem and provides a method to correct that information.

The work made use of high-technology capabilities on both sides of the Atlantic. It continues today with an analysis of more samples yielding similar results. The tools are being developed to embrace the PIXE technique and extend those tools to

DISCOVERY CAN BE STUNNING.



capabilities the Institute is developing with collaborators in Stanford, California. "Extrapolating from our results in which there was a misidentified metal in at least half of the samples studied suggests that over 300,000 models downloaded per day may not contain the correct metal," Dr. Snell said. "This has profound implications for those using the models. If these models are wrong, the understanding of the millions of people who use them becomes flawed."

Dr. Snell explained that one of the difficulties in studying metals in proteins is not only identifying them, but that they are very sensitive to X-ray radiation, so the experiment itself can change what you see. But he noted, a technique using X-ray Free Electron Lasers (XFELs), prevents this because the experiments are usually faster than any change that can occur.

Dr. Snell directs the National Science Foundation BioXFEL Science and Technology Center, (Biology with X-ray Free Electron Lasers) a consortium of the University at Buffalo, Hauptman-Woodward, and their partners. The Center is dedicated to using XFELs, which produce incredibly intense X-rays in extremely short pulses, and can help in the accurate understanding of these metals in biological systems and processes that are naturally triggered in the body but cannot be observed with other techniques.

The study has an impact beyond a single disease, it impacts the work of many on multiple diseases. It is part of the Institute's work in developing technologies and techniques that can be used by all. The paper was published in the Journal of the American Chemical Society (2020, 142, 1, 185−197) and has been read almost 2,000 times since. It involved a collaboration represented by multiple disciplines and can be summarized by a quote from Geoffrey Grime PhD from the University of Surrey, "This is an outstanding example of interdisciplinary scientific collaboration where techniques developed initially in nuclear physics labs have made a big contribution to molecular biology." Science is multidisciplinary and international.

"We were the first in the world to see what had been hiding there all the time. The result was stunning."

GAYA YADAV | SIX QUESTIONS

HOW DID YOU BECOME INTERESTED IN SCIENCE?

It was never something I was sure about. I knew I wanted to be involved in nature and thinking about how things worked and how they interconnected with each other. But it only became clear to me after I had finished my masters degree that research was the thing that would enable me to understand these things at molecular level to make discoveries. I joined a biochemistry and structural biology lab at the Central Drug Research Institute, one of the premier institutes in India for drug discovery, and began my PhD on structural and functional studies of proteins using X-ray crystallography.

WHERE DID YOUR CAREER LEAD YOU PRIOR TO HWI?

After defending my PhD in 2011, I spent about five years as a postdoctoral researcher at UT Southwestern Medical Center, Dallas, Texas followed by University of Florida, Gainesville, Florida as Senior Biological Scientist. During this time, I used different biochemical and biophysical tools to study ion channels, specially potassium ion channels and ion channels in regulated secretory pathways. We also identified a novel ion channel in secretory granules important to regulate pH in them and hence maturation of regulatory peptides or hormones such as insulin. I also had the opportunity to learn cryo-electron microscopy (Cryo-EM), which is the frequently used technology for protein structure determination nowadays and produces images of structures in native/near native state.

WHAT PROJECT HAS BEEN MOST PIVOTAL IN YOUR CAREER TO DATE?

Though all the projects I have worked on are important to my career goals at different stages, I think finding a novel ion channel in the regulated secretory pathway has been most pivotal. From the public's perspective, this discovery may have significant public impact as it opens the doors for more effective treatments for Type II Diabetes.

HOW IMPACTFUL WILL CRYO-EM BE IN WESTERN NEW YORK?

Submissions to the Electron Microscopy Data Bank (EMDB)—a popular repository for structures solved using electron microscopy—have increased exponentially in recent years, largely because of the explosive growth in the number of cryo-electron microscopes in labs worldwide. There are >14,500 entries in this database and out of that, 3,826 entries were made in 2020. These structural entries are evidence that Cryo-EM research is booming. The addition of Cryo-EM will be a resource for Western New York expediting scientific exploration in the region by providing easy access to research labs. Currently, it is difficult to find experimental time at national facilities and the resulting datasets may take months to receive. A local facility would avoid these hindrances and expedite the availability of the scope time.

WHAT DO YOU LIKE ABOUT BUFFALO SO FAR?

Contrary to people's belief, Buffalo sees its fair share of sunny days and is not so cold to make it difficult to live. City crews are plowing and salting as early as possible to keep the roads safe and drivable. There are plenty of Indian restaurants with authentic Indian taste and food prices are comparatively lower than other places I have lived so far. The city has many parks and a zoo which are nice places to visit with our kids on the weekend.

FAVORITE HOBBIES?

I do not have many hobbies, but I would like to spend time with my family as much as possible. I also enjoy watching movies. I am very fond of watching cricket, and you may know why—India has many of the best cricket players in the world.

2021 MARKS THE **TEN YEAR ANNIVERSARY**
OF DR. HERBERT HAUPTMAN'S PASSING.
WE REFLECT ON HIS RECEIPT OF THE PRESTIGIOUS
NOBLE PRIZE AND LATER IN LIFE HIS
WORK WITH GEOMETRIC SHAPES THAT
ARE STILL ON DISPLAY AT HWI TODAY.

SERVICE WITH A SMILE

Finley R. Greene, Jr. served as Vice President of Development and Communications at the Hauptman Woodward Medical Research Institute for 8 years, and most notably helped secure $24 million during the capital campaign for the Institute's state-of-the-art research facility. Finley was known for his warm smile and it was that smile that helped him connect with so many who became supporters and lifelong friends.

Finley's dedication to HWI continues to have impact today. Even recent gifts can be attributed to his education of members of our community on the impactful work of the Institute.

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HWI TAPS INTO BUFFALO'S BEST

The Hauptman-Woodward Medical Research Institute is proud to have a diverse and active board that helps guide and ensures that our activities make the biggest impact on the health of the world. In this issue, we introduce our new board members.

NENA RICH | Nena Ouellet Rich shares her passion and experience as a medical professional with the Lotus House Women and Children's Shelter in Miami, Florida, a center committed to ending child and family homelessness. The shelter also houses a community medical clinic serving the local population. Nena is a member of the board and supports several projects within the medical clinic in a volunteer capacity. Nena recently completed the Medical Writing and Editing Program at the Graham School of Continuing Liberal and Professional Studies at the University of Chicago. Her volunteer work with Lotus House includes cataloging the shelter's success and communicating it to a broader audience through journal publication.

Nena has held numerous other board trustee positions over the years including the Whyme Breast Cancer Support Network, University of Vermont Nursing School Advisory Committee, Irish Classical Theatre Company, and the Elmwood Franklin School. She has a wide range of experience across the healthcare arena, including Pediatric and Adult Home Health Care Nurse, Seattle, Washington; Quality Assurance Nurse Consultant, Seattle, Washington; Certified Case Manager – Home Care, Seattle, Washington and Buffalo, NY, and Senior Clinical System Analyst – Siemen's Corporation, Upstate NY Region. Nena was the Project Manager for the construction of the Hauptmann-Woodward Medical Research Institute's current building in 2003-2005.

Nena earned a Bachelor of Science from the University of Vermont in 1993 and has since held a professional license as a Registered Nurse.

DAN MAGNUSZEWSKI | Dan Magnuszewski is an entrepreneur, software engineer, mentor, and investor from Buffalo, NY. He began working at M&T Bank after high school and graduated with a degree in computer science from the University at Buffalo in 2005. He has been heavily involved in the WNY tech community and has been an organizer and cofounder of organizations like CoworkBuffalo and Buffalo Startup Weekend. In 2016, he received the Outstanding Young Alumnus award from UB's School of Engineering and Applied Sciences and in 2018 was included in Buffalo Business First "40 Under 40". After having worked as a software engineer at Buffalo based Synacor, he went out on his own and served as a "technical cofounder for hire" helping startups in NYC and San Francisco build their products and businesses.

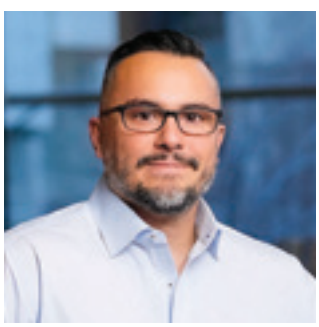
He was previously the Managing Director of Z80 Labs, a startup incubator and $5M seed fund in Buffalo, and a board member of UVANY (Upstate Venture Association of NY). In addition to this, he currently is part of UB's Computer Science Advisory Council, and has previously served as a member of the WNY Computer Science Teachers Association and Roswell Park Comprehensive Cancer Center's IT Advisory Council. In 2015, Dan cofounded ACV Auctions, a dealer to dealer marketplace for used vehicles, and is currently the CTO. In 2015, ACV Auctions won the $1 million grand prize at the 43 North business competition. In total, they raised a combined $350 million in venture capital from large venture capital firms such as Bessemer Venture Partners, Bain Capital Partners, Tribeca Venture Partners, SoftBank Capital, and Armory Square Ventures, among others. In March of 2021, ACV Auctions went public on the NASDAQ and has a current market cap of ~$4bn. ACV Auctions, which started in Buffalo, is now in markets across the entire US and expanding rapidly. ACV currently employs over 1,500 people across the country. Always dedicated to the local community, ACV Auctions was named UB SEAS Corporate Partner of the Year in 2019.

ANDREI GUDKOV | Dr. Andrei Gudkov is a pre-eminent cancer researcher and Senior Vice President, Research Technology and Innovation, Chair of the Department of Cell Stress Biology, and a member of the senior leadership team for the National Cancer Institute (NCI) Cancer Center Support Grant at Roswell Park Comprehensive Cancer Center. He is responsible for building on the basic and translational research strengths of the Cell Stress Biology program in DNA damage and repair, photodynamic therapy, thermal and hypoxic stress and immune modulation. As Senior Vice President, he assists the President & CEO in developing and implementing strategic plans for new scientific programs and enhancing collaborations in research programs with regional and national academic centers as well as with industry.

Before joining Roswell Park, Dr. Gudkov served as chair of the Department of Molecular Genetics at Lerner Research Institute, Cleveland Clinic Foundation, and professor of biochemistry at Case Western University. He earned his doctoral degree in Experimental Oncology at the Cancer Research Center, USSR and a Doctorate of Science (D.Sci) in Molecular Biology at the Moscow State University, USSR. He has authored or co-authored 135 scientific articles and holds 27 patents.

MARK BOYD | Mark Boyd is the Chief of Staff to the Hon. Crystal Peoples-Stokes. He possesses over 8 years of government and managerial experience as a confidential management employee of the municipal and state levels. He has held senior staff leadership roles being responsible for multiple office locations, with over 25 full and part time employees, and short and long-term strategic planning and more. He excels in personnel and project management; special event planning; legislative and fiscal analysis; appropriations and discretionary spending; government, community and public relations; communications; constituent services and much more. He possesses experience with fundraising and campaign finance, campaign field work and grassroots organizing.

FRANK EWING | Frank Ewing serves as Chief Executive Officer of AML RightSource. He is a licensed attorney and an anti-money laundering expert with comprehensive professional experience in global consulting, banking, and law. Mr. Ewing has extensive hands-on experience in the areas of anti-money laundering compliance, regulatory enforcement actions, regulatory affairs, internal audit, commercial litigation, corporate investigations, fraud, and risk management. Mr. Ewing earned his undergraduate degree at LeMoyne College in Syracuse, New York, and his Juris Doctor at the University of Buffalo Law School.



SAM RUSSO | Sam Russo is an investor, entrepreneur, business executive, and operator with extensive experience in a wide array of businesses and industries. As a partner at Lorraine Capital, he helps lead the private investment firm's efforts to identify, acquire, operate and grow successful businesses throughout the Northeast, with a focus on Upstate New York. A Certified Public Accountant, Russo has a strong track record as a founder and partner in several businesses, holding companies, and consulting companies. In addition to his role with HWI, Russo is an active supporter of several community organizations. In 2016, he received the 40 Under 40 award from Buffalo Business First in recognition of his professional accomplishments and dedication to the community.

ARTEM EVDOKIMOV | Artem Evdokimov leads a diverse scientific team responsible for all target discovery, validation, and implementation work. His career has included roles at Procter & Gamble Pharmaceuticals and Pfizer, where he used structural biology as a tool to assist in the development of potential new treatments for infectious diseases, CNS ailments, cardiovascular conditions and cancer. He also led the Structure and Design team at Monsanto, where his work enabled the development of novel traits to protect plants against insect predation, to elicit herbicide tolerance, or to enhance yield. Dr. Evdokimov was previously the Chief Scientific Officer and CEO at HarkerBio, a contract research company formerly located on the Buffalo Niagara Medical Campus. He holds a dual PhD in Chemistry and Structural Biology from the Weizmann Institute of Science in Israel.

LAVONNE ANSARI | Lavonne Ansari is a longtime leader in the field of community health. Since joining the Community Health Center of Buffalo, she has overseen the organization's expansion from one site to five sites across two counties. She has received numerous awards for her contributions to human rights, community involvement, and education. Dr. Ansari serves on several local and national boards, including the Mayor's Citizens' Rights and Community Relations Commission and Mosque Cares Board of Education. In addition, she is a member of the Niagara County Coalition for RACE and serves as the Coordinator of the Masjid Nu'Man Education department. Dr. Ansari earned a Bachelor's degree in Professional Studies in Recreational Therapy from Brockport State College, a Certificate in Career Development and Management in Women's Studies from Cornell University, a Master's Degree in Multidisciplinary Studies from Buffalo State College, and a PhD in Sociology of Education from the University at Buffalo.

JEFF RENZONI | In 24 years at M&T, Jeff Renzoni has served numerous roles in multiple divisions of Western New York's largest bank. In his current role, he supports talent development and employee engagement efforts for the bank's Retail Banking and Business Banking Divisions. He has also held several nonprofit board positions throughout the community, most recently at Buffalo Niagara Choirs, Inc. and Westminster Presbyterian Church. Mr. Renzoni received his bachelor's degree in Business Administration from Boston University and a Master of Business Administration from the University at Buffalo.

TRICIA BARRET | At Crowley Webb, Tricia Barrett manages the operations at one of Western New York's leading advertising agencies. In addition, she is responsible for the agency's healthcare/patient recruitment division, Praxis, where she oversees all aspects of operations for the agency's pharmaceutical and biotech clients. She is a frequent speaker on the topic of patient centricity and the role insights can play in developing effective marketing strategies for clinical research. Ms. Barrett currently serves as board chair for Leadership Buffalo, co-chair of Elmwood Franklin School's alumni council, and an advisory council member for the Tim Russert Department of Communication at John Carroll University, from which she graduated with a bachelor's degree.

BRENDA MCDUFFIE | Brenda W. McDuffie served as President and CEO of the Buffalo Urban League, Inc. from October 1998 until her retirement last year. The Buffalo Urban League is committed to ensuring that African Americans, minorities, and disadvantaged individuals have the opportunity to achieve their full potential. In her position with the Urban League, Mrs. McDuffie's energy and talent are dedicated to making real, positive changes in the lives of people in the Western New York community.

From 1994 to 1998, she was the Executive Director for the Buffalo and Erie County Private Industry Council, Inc. (PIC). In this capacity, she had the very challenging task of working with individuals and businesses to ensure that there was a high-quality workforce to allow economic bases to grow. While at the PIC, Mrs. McDuffie served as President of the New York State Association of Employment and Training Professionals (NYATEP) where she also co-chaired and was a member of the steering committee. The committee produced the recommendations for New York State's future Workforce Development System. She is currently the chair of the Erie County Industrial Development Agency.

She received her undergraduate degree from Buffalo State College and earned a Graduate Certificate in Human Resource Development from the State University of New York at Buffalo, School of Management. Mrs. McDuffie started her career as a paralegal aide for Neighborhood Legal Services. She worked for the City of Buffalo Human Resources Department as Senior Manpower Coordinator and later served as Director of Planning at the Private Industry Council where she became Executive Director in 1994.

She currently serves on several Boards of Directors. She is immediate past President of Leadership Buffalo, Secretary for Independent Health Association, member of the Board of Directors for Western New York Foundation, Buffalo State College, Buffalo Niagara Convention and Visitors Bureau, and is on the Trustee Council for Kaleida Health Systems. She has received numerous awards and recognitions including The Buffalo News Citizen of the Year; the NAACP Community Service award; Business First's Forty Under 40 award; and the United Way's Volunteer of the Year.

HWI BOARD OF DIRECTORS AND OFFICERS

Cuisine de Laboratoire

A VIRTUAL COOKING SERIES

This year we faced an unprecedented pandemic and fundraising, as we knew it, was turned on its head. In March, it was clear to us that we would not be able to execute our Brewing Science or Riedel wine tasting events. HWI had to innovate fundraising as it does with so much of the it's work and pivoted to an on-line format with a virtual cooking class we called Cuisine de Laboratoire (the Kitchen Laboratory).

Our focus, in light of the financial hardship caused by the pandemic, was to raise as much funding as we could for the crucial research, including studies fighting COVID-19, that takes place every day at HWI. We were sensitive to the challenges our local restaurants, small businesses and farmers faced. Each session highlighted a local chef, wine was provided by small local businesses and ingredients, where possible, were included in the ingredient box.

Our adventurous participants received their ingredient box, wine and recipe at their home via contactless delivery and then would tune in via Zoom for a private cooking class with the local chef featured that evening. Each session was a fun for everyone who attended and we even hosted some junior chefs! The highlight for us was the photos that were shared of the cooking process and finished dishes that showcased some of the best sous chefs in the Queen City. We even had a little fun with our plating contest and asked participants to post photos of their best presentation skills.

We are thankful to our wonderful sponsors and donors for their support of this unique event at a unique moment. Bon Appetit!

BioXFEL Conferences 2020 and 2021

The National Science Foundation BioXFEL Science and Technology Center is entering its 9th year. The Center holds an annual conference of international accord and in 2020 we returned to San Juan, Puerto Rico. BioXFEL has a strong relationship with the University of Puerto Rico and its campuses. Hosting the meeting on the island allows the Center to further enhance the meaningful programs and engage this population of students. The meeting overall drew world renowned researchers as well as up and coming students and postdocs from over the globe.

Yet, as most of us have experienced, COVID derailed our typical in-person meeting. A fully virtual meeting challenged us to find new, innovative ways to simulate the networking aspects of the conference which are critical to the formation of new collaborations and bolstering the careers of students entering the field. With special thanks to Dr. Diana Monteiro, BioXFEL was able to replicate such an atmosphere through a platform known as Gather. This 8-bit world allowed people to move around "conference rooms" and interact in small groups at live poster presentations, meet in private areas to discuss projects, or even just have playing board games. The scientific content covered various areas of XFEL science with special keynote talks from Dr. Henry Chapman (DESY) on the last ten years of serial femtosecond crystallography and Dr. Anastacia Awad (Novartis) on diversity and inclusion.

While we all relish the opportunity to travel, a virtual meeting allowed us to gather a larger and more diverse group. In this new normal, it is likely that a virtual component will always a play a role and we are pleased to have had such success in the 2021 segment. As we plan for a virtual 2022 for the safety of all our attendees, it is our aim to hybridize and include an in-person component, if possible, to maximize the positive impact of the BioXFEL International Conference.

2020 HIGHLIGHTS

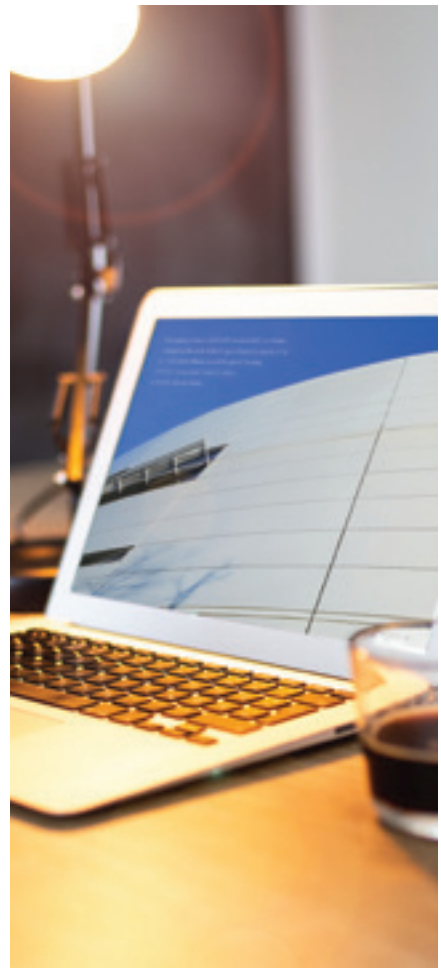
32
attended the *Write Winning Proposals* grant workshop

133
attended the conference from around the globe

2021 HIGHLIGHTS

39
attended the *Laboratory Management* Workshop

180
attended the conference from around the globe



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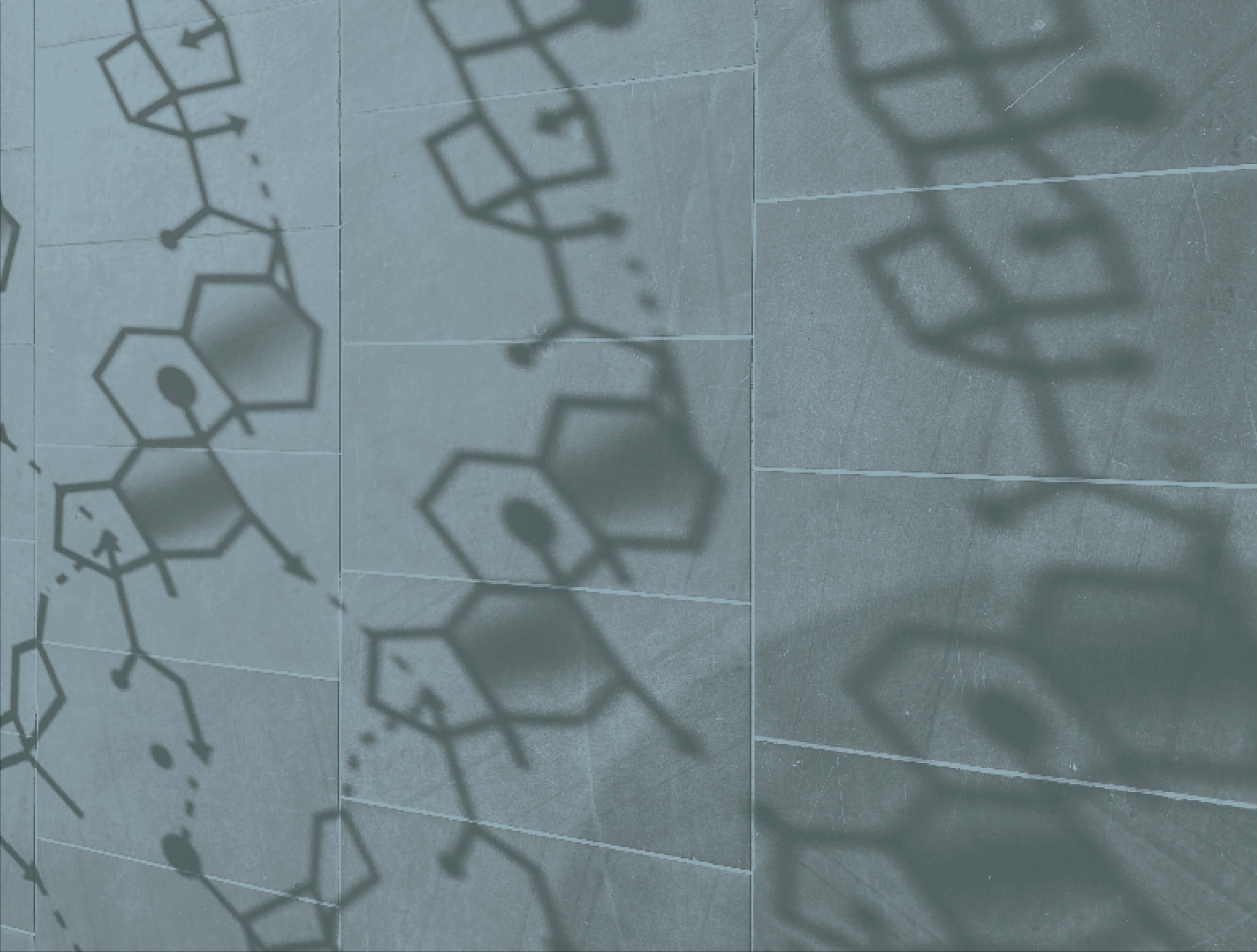
hwi.buffalo.edu/structures-magazine



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