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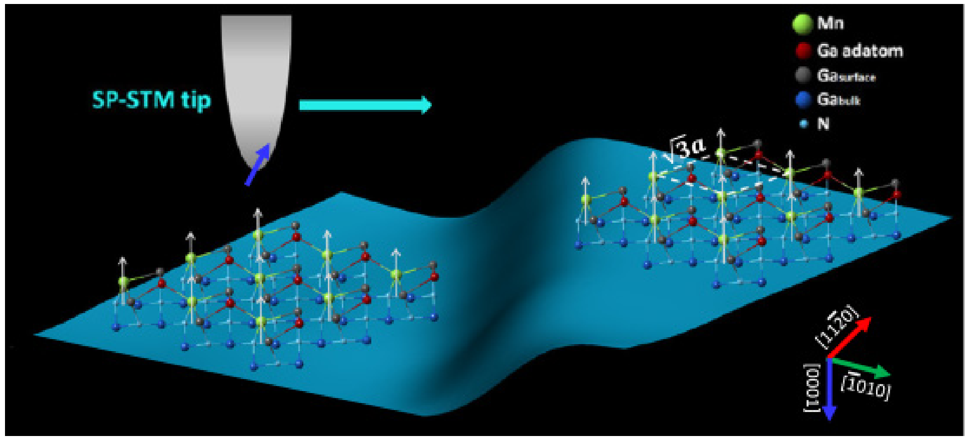
Uncovering 2D Ferromagnetism at Room Temperature

Seen on almost all household refrigerator doors, magnets are commonplace items. Yet scientists are still working to fully understand how magnetic structures form, especially at the atomic level. Magnetism, or the phenomenon that creates attraction or repulsion between particles based on their spin orientations, can be produced in a variety of materials. Yet typical household magnets display only one version of this intriguing natural wonder, ferromagnetism, which represents a perfect magnetic collective alignment of all spins. Ferromagnetism is well characterized in three-dimensional objects (imagine a cube, for example) but is often difficult to produce at reduced dimensions. In a paper published in *Nano Lett*. 2018, 18, 158–166, Physics professor & NQPI member Arthur R. Smith and co-workers reported the discovery of ferromagnetism in a two-dimensional material (akin to an isolated cube face) at room temperature.



A visual representation of SP-STM measurements to characterize ferromagnetism in 2D-MnGaN (Image courtesy of Arthur R. Smith)

"We're really looking at the ultimate limit of thin-film ferromagnetism," Smith said. "This isn't the first time people have seen ferromagnetism in atomically thin structures, but in the past they've seen it only at very low

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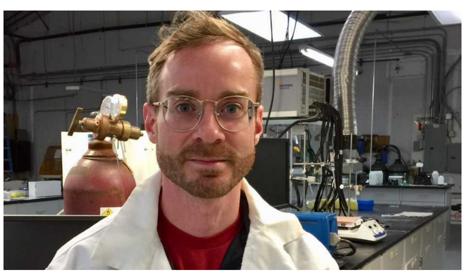
Using Carbon Quantum Dots for Bladder Cancer Detection



John Staser in his laboratory in Stocker Center

Materials expert and NQPI member John Staser is extending his expertise in carbon quantum dots to use these remarkable nanostructures for medical treatment.

Carbon quantum dots, about five nanometers in diameter, display unique optical and electronic properties due to their small size. In particular, they are photoactive, or "fluorescent," over the ultraviolet range. Staser, an associate professor of Chemical and Biomolecular Engineering in the Russ College of Engineering and Technology, said the fact that these dots are fluorescent and that they are carbon-based—and therefore biologically benign—has inspired researchers like himself to explore their applications in the medical sector, especially for cancer detection.

"The idea is simple," Staser said. "We attach carbon quantum dots to a cancer antibody and inject them into a person. If the person has cancer cells, the antibody will go to those cells, and we will be able to see that happen by shining (a) UV light onto his body."

Staser and his colleague Dr. Ramiro Malgor, an associate professor and medical doctor from the Ohio University Heritage College of Osteopathic Medicine, have conducted preliminary experiments to assess the idea's feasibility. Staser provided Malgor with carbon quantum dots, who injected them into a cell culture to test two things: whether these dots are safe for the cells, and whether they can be detected in the culture.

After two days of cultivation, Staser and Malgor were excited to find out that 95 percent of the cells were alive after being exposed to the quantum dots. And as they shed UV light on the culture, the dots appeared clearly either on the surface of or inside the cells. They concluded these carbon quantum dots can be used for medical imaging.

"Using carbon quantum dots for medical imaging is not a completely new idea. But for the first time, we are applying it to the detection of bladder cancer," Staser said. Bladder cancer affects millions of people around the globe every year and is treatable if diagnosed early. The current detection involves inserting a probe through the urethra, a painful procedure, especially for male patients. In contrast, quantum dots would be both less invasive and more tolerable.

The potential for this technology is far reaching, as it can be applied not only to cancer detection but cancer treatment. However, work along these lines has just begun, Staser cautioned. A new drug product needs to go through years of testing before it can be used on humans. Staser and Malgor are taking the long road from laboratory experiments to cancer treatment, to find more efficient and effective ways to alleviate cancer.

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Director's Corner

Dear Colleagues:

Warmest greetings from the Athens campus of Ohio University; we hope you enjoy reading the 21st edition of the NQPI newsletter. As another semester winds down, it is a pleasure to go over the many accomplishments of our members and students and share them with you.

I wish farewell and a happy retirement to Donna Welch! Donna has served as the Administrative Specialist for CMSS/NQPI since 2011. From assisting visitors and helping students to putting together our large student research poster events, Donna was essential to the operation of the Institute. She said she is looking forward to being her own boss and spending time with her husband. We will certainly miss her. Best wishes, Donna!

Springtime this year includes the sounds of construction outside of Clippinger Labs as progress continues on OHIO's investment in a new Chemistry Building. The new facility will provide our fellow Chemistry faculty, students, and NQPI members with modern research and teaching space. This is an exciting time and we look forward to working with our members and colleagues to take this opportunity to enhance and modernize our research infrastructure, essential to the continued success of our faculty and students.

This newsletter highlights several faculty and student achievements, including the growth of the first 2D ferromagnetic material, an extraordinary success by Arthur R. Smith. Exciting progress has been made on the development of cancer-detecting methods as described in the articles about Doug Goetz and his work on esophagus cancer, as well as on John Staser's production of biologically compatible carbon quantum dots.

I'm delighted to announce that Larousse Khosravi Khorashad is the winner of the 2018 NQPI Outstanding Dissertation Award. Read about Khosravi Khorashad and his research on the back page.

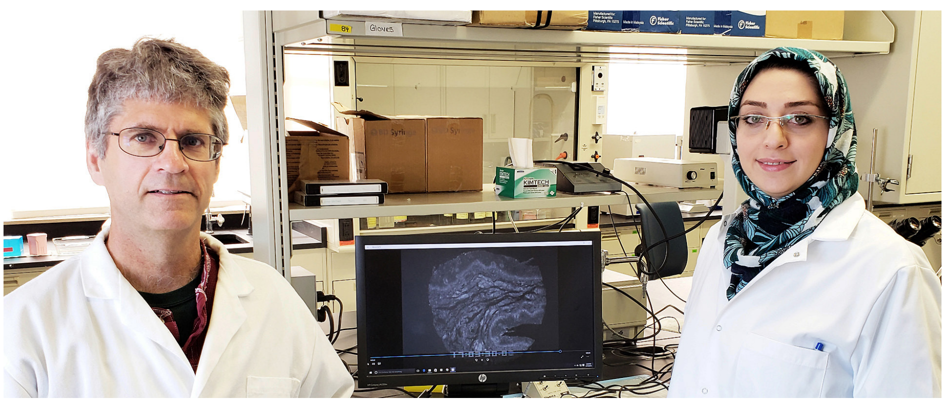
As always, I invite you to visit our website **ohio.edu/cas/nqpi** to learn more about all NQPI research, seminars, special events and other activities.

Sincerely,
Eric Stinaff, NQPI Director

NanoBytes

- In 2018, a total of eight patents were granted for inventions developed at Ohio University, including two by NQPI member Khairul Alam and one by NQPI member Doug Goetz.
- Mechanical Engineering professor in the Russ College of Engineering and Technology and NQPI member Khairul Alam was recently elected to the National Academy of Inventors (NAI) as a senior member.
- The American Physical Society (APS) held its annual March Meeting this year in Boston, MA. A group of nine NQPI members and graduate students presented contributed talks and posters during the week of March 4-8.
- Distinguished Professor of Physics and NQPI member Alexander Govorov has surpassed 25,000 reads and reached over 11,000 citations on ResearchGate.

Detecting Esophageal Cancer with Adhesive Molecules



Doug Goetz and Mahboubeh Noori stand in front of an endoscopic image of esophageal tissue.

Cancer of the esophagus typically carries a grim prognosis. According to the American Cancer Society, only about 20 percent of patients survive five years after diagnosis. Unfortunately, esophageal cancer goes mostly undetected until more severe stages of the disease are reached. If earlier detection were possible, patients' survival rates could increase dramatically. A team of Ohio University researchers are working to help make earlier detection a reality.

Currently, detecting esophageal cancer requires an invasive endoscopy, meaning most individuals are not screened regularly. Although endoscopic methods may allow physicians to identify structural surface changes, these procedures do not reveal molecular details about the biochemistry of the cells.

NQPI member Doug Goetz, a professor of Chemical and Biomolecular Engineering in the Russ College of Engineering and Technology, and doctoral chemical engineering student Mahboubeh Noori, recently reported in *Integrative Biology* that by using particles engineered with specific ligands (molecules that bind to other molecules), they can detect molecular changes that are unique to cancerous esophageal cells. Goetz and Noori's work on this project was done in collaboration with Monica Burdick, an associate professor of Chemical and Biomolecular Engineering, David Drozek, associate professor of Specialty Medicine in the Heritage College of Osteopathic Medicine, former chemical engineering doctoral student Grady Carlson and undergraduate chemical engineering major Evan Streator.

The team developed an adhesion assay (test) to detect cancer cells in vitro with the ligand-conjugated particles. The researchers infused the bioengineered particles over the surface of cancer and normal cells in a Petri dish via an endoscope. Next, they allowed the particles to incubate with the cells, applied a rinse to remove unbound particles, and examined the state of both types of cells. They observed that the engineered particles remained bound to the cancer cells but not to normal cells.

"They (the bioengineered particles) stick to the cancer cell surface, through the ligand-receptor interaction," Goetz said. He stated that the molecular mechanism by which the particles stick is similar to Velcro hooks binding to a looped fabric.

In a clinical application, endoscopes would douse the interior of a patient's esophagus with the bioengineered particles. Ideally, the particles would then bind exclusively to cancerous tissue. If cancer were present, an alarming number of ligand-bound particles would remain on the tissue revealing the cancerous tissue to a clinician.

Goetz said he hopes that one day this research will lead to highly sophisticated future applications. For example, he foresees the possibility of a patient swallowing a pill carrying ligand-conjugated particles that can be detected via an app on the patient's smartphone. In this future scenario, patients could detect esophageal cancer on their smartphones. Currently, the group's research is providing a path for the development of such technology.

Tackling Water Pollution in Ohio and El Salvador

Dina López in her office in Clippinger Labs

When hydrogeochemist Dina López first came to Ohio University 24 years ago, she was already an expert in a widespread environmental problem in the Athens area: acid mine drainage. The brownish streams are a remnant of the state's legacy of coal exploitation, and the chemicals they contain—such as pyrite—have been contaminating drinking water and killing fish inhabiting local rivers.

With her expertise in chemistry, physics, and geology, López led a multidisciplinary research team to address this issue. They established "beautiful correlations between the velocity of the flow, the chemistry of the water, and the bacteria in the stream," López said. The correlations can be used to evaluate remediation measures, such as adding alkaline substances to reduce acidity.

Similar to abandoned mines, active mines also pose pollution risks. Last year, López's team developed a model to predict how an underground mine is likely to form a pool, overflow, and discharge acidic waters into the environment.

Outside Ohio, López has been concerned about environmental problems and public health in her home country, El Salvador. An important research topic she is interested in is how volcanic activity releases arsenic, a toxic chemical that is associated with various cancers, into the water, soil, and air, impacting humans.

Arsenic and heavy metals can arise from low quality agrochemicals such as pesticides and fertilizers, which is a probable cause for the exponential growth of chronic kidney diseases in El Salvador and neighboring countries, López explained. She and her colleagues are using a statistical measure known as geographical weighted regression to assess the relationship between the environmental variables in those countries and the prevalence of kidney disease.

"Human health is not my specialty. However, as I started to work in the environmental issues related to this disease and was able to know the patients and see young faces dying, that's really heartbreaking," López said. "When law enforcement is not in place, what we can do is to educate people of the consequences and the ways to protect themselves."

This year, López is working with Sebastian Barket, a new master's degree student with a biology background who is returning to the multidisciplinary study of acid mine drainage. "Ohio has contributed a lot to the wealth of this country with coal mining, but the environmental costs are high, too," López said. While the acidic streams can exist for hundreds of years, all remediations we have today are temporary—there is still a lot of work to do for scientists like López.

NQPI Undergraduate Researcher Models Ammonia Synthesis

Environmental & Plant Biology Professor Morgan Vis presents a blue ribbon to Esther Grossman at the Ohio University 2018 Student Research and Creative Activity Expo. (Photo: Jean Andrews)

Modeling a chemical process with computational software is no easy task, but Ohio University Honors Tutorial College Engineering Physics student Esther Grossman isn't afraid to take on the challenge.

Grossman is currently completing her honors thesis under the supervision of Distinguished Professor of Chemical and Biomolecular Engineering and NQPI member Gerardine Botte, and Assistant Director and Lecturer Damilola Daramola of the Center for Electrochemical Engineering Research. The team is working to characterize the process of ammonia synthesis.

"I love the synergy between experimental work and theoretical work, especially in electrochemical engineering where processes (occur) in the lab; there's just so many things involved," Grossman said. "So it's interesting (to see) how we can get computational accuracy … but there's still so much that leaves you wondering when you simplify a system so much that you can do it on the computer."

Ammonia is one of the most widely-used industrial compounds and is synthesized through a complex, multi-step procedure that is highly sensitive to external conditions. Many researchers are interested in finding alternative synthetic pathways to save energy costs.

Grossman uses a program called Gaussian to visualize clusters of atoms involved in ammonia synthesis. She is modeling the adsorption energies, bonding sites and site preferences that are involved in the synthesis process. For her thesis, Grossman compared different computational functions to account for the effect of mutual atomic interactions (represented by Van der Waals forces) within the molecular system.

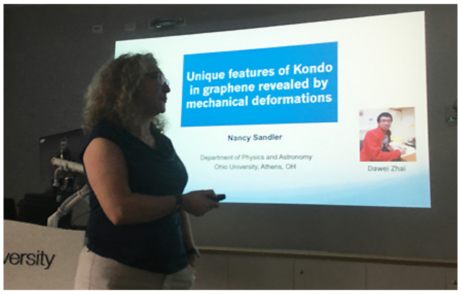
"With these computational schemes, under the umbrella of density functional theory (a numerical technique used to model many-component systems), there's no direct way to put a Van der Waals force into a numerical formula. It's a very hard thing to model," Grossman said. "So what we have is these functionals (approximations for the actual interactions among charged particles) that tack on a dispersive term to the whole function."

Grossman applied three different density functionals to her system. Two of these functionals applied a dispersion effect, which helps mimic the effect of Van der Waals forces. She found that, when applied under the dispersive functionals, the bonding energies reflected more accurately those observed under experimental conditions.

Ultimately, Grossman said she hopes her work will be useful to other researchers who are studying ammonia synthesis. Next year, she plans to pursue her graduate degree in electrical engineering, where she hopes to apply her background in physics and computation to model electrical systems.

"Working with Dr. Botte was an awesome experience because she's so knowledgeable," Grossman said. "It was such a cool experience."

Sandler Brings Her Research to Australia



Nancy Sandler presents at Monash University.

At one atom thick, graphene is the thinnest, flattest material known to date. It is also the most impermeable, and strongest material in the world. It is electrically conductive, flexible, and incredibly lightweight. These attributes make it one of today's most researched materials, evoking interest from physicists all over the world.

This past December, NQPI member Nancy Sandler, a professor of Physics & Astronomy, was invited to Melbourne, Australia by her colleague, Monash University professor Michael Fuhrer. As chair of the fourth International Conference on Two-Dimensional Materials and Technologies, or ICON-2DMAT 2018, Fuhrer invited Sandler to talk on: "Deformed Graphene Membranes: from Electronic Waveguides to Valley Filters," i.e. how graphene can be a canal for electrons to travel through.

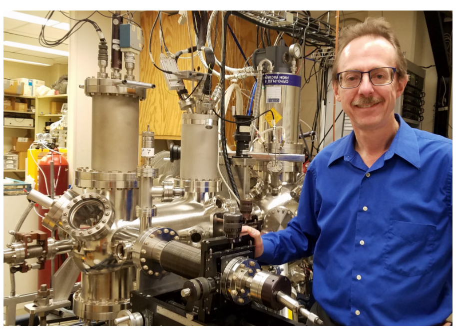
While in Melbourne, Sandler had the opportunity to visit the FLEET center at Monash University, funded by The Australian Research Council as a Centre of Excellence in Future Low Energy Electronics Technologies. At FLEET, a leading institution for the advancement of electronics, she toured the facilities and presented a seminar on the persistence of magnetic properties for atoms placed on top of graphene.

"I wanted to know if the magnetic nature of the atom was maintained after deposition on graphene and if it depended on the specific position where the atom attached," Sandler said.

Melbourne, a city crossed by the Yarra River, impressed Sandler with its considerable diversity. She said that people from all over the world mix there with amazing architecture, local art and fantastic food. "It was an honor to be invited to speak at the conference about my research. The hospitality of my hosts and lively culture of Melbourne was the icing on the cake."

Uncovering 2D Ferromagnetism

Continued from page 1



Arthur R. Smith poses in front of his group's spin-polarized scanning tunneling microscope.

temperatures … and in terms of any possible future applications, this is much more applicable."

Smith, along with former doctoral physics students Yingqiao Ma and Abhijit Chinchore, synthesized 2-dimensional (2D) manganese gallium nitride on top of a layer of semiconductive gallium nitride. They characterized the 2D-MnGaN's electronic and magnetic properties using spin-polarized scanning tunneling microscopy (SP-STM).

Previously, the group had demonstrated that manganese, gallium, and nitrogen atoms (on the surface of gallium nitride) order in a unique configuration.

"In essence, it forms a quasi-hexagonal structure," Smith said. "Imagine a 2D layer of atoms in a distorted hexagonal network. Each nitrogen-bonded, magnetic manganese atom is indirectly coupled to six manganese neighbors through an intervening network of gallium atoms."

Using this system, the groups characterized the topographical structure of the material. In addition, they generated images of magnetic arrangements. Their results demonstrated a uniform orientation of spin direction across the sample at room temperature, evidence of ferromagnetism. These findings were supported with theoretical calculations by their collaborators, University of Buenos Aires professor María Andrea Barral and Valeria Ferrari, a professor at the National University of San Martín, co-authors on the paper.

Currently, Smith's group is completing follow-up research on this system. Collaborating with Ohio State University Physics professor Fengyuan Yang, they are employing a technique called superconducting quantum interference device (SQUID) magnetometry to generate quantitative measurements of ferromagnetism in their samples. In addition, the group is pursuing other experiments in which the manganese gallium nitride structure is manipulated to produce different magnetic effects.

Dissertation Award

Larousse Khosravi Khorashad (Photo: Robert Hardin)

NQPI is proud to announce Larousse Khosravi Khorashad as the recipient of the 2018 Outstanding Dissertation Award.

Khosravi Khorashad received his Ph.D. from Ohio University in 2017. His research area is a combination of computational physics and plasmonics with applications to nanotechnology. His dissertation is titled, "Theoretical and Computational Study of Optical Properties of Complex Plasmonic Structures."

Khosravi Khorashad's work involved theoretical and computational studies of optical properties of different nanostructures. He used a variety of software programs to simulate light scattering from nanostructures with different nature-inspired symmetric shapes.

After graduating from OHIO, Khosravi Khorashad worked as a post-doctoral scholar at the University of California, San Diego. This year, he returned to OHIO as a post-doctoral researcher to work with his Ph.D. advisor, NQPI member Alexander Govorov. Govorov said, "Larousse is very good at computational nanoscience."

Khosravi Khorashad said he felt honored and appreciative of the support that helped him earn this award. "I would like to thank my Ph.D. adviser, Professor Govorov and my family, without whose support and help I would not be able to receive this honor," Khosravi Khorashad said.

Writing, design, editing, interviewing and photos by Amanda Biederman, Ryan Flynn and Ling Xin. Editing by Dr. Nancy Sandler and Jean Andrews. Please email nqpi@ohio.edu with comments.