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NQPI
OHIO UNIVERSITY

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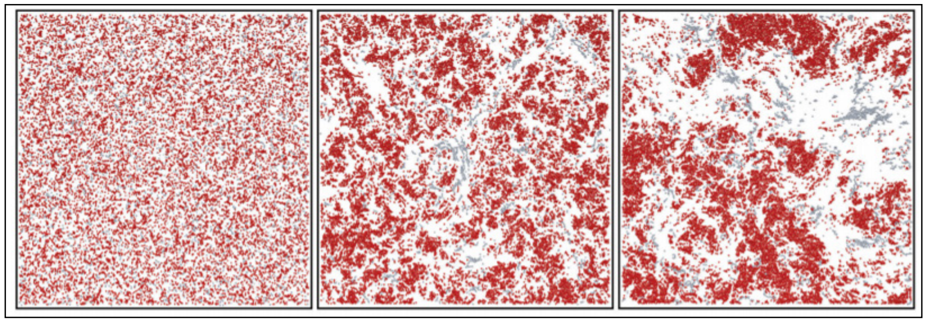
Castillo Models Granular Systems on the Move


Simulated packing densities with regions of fast (gray) and slow (red) moving particles.

Fluidized granular systems show some puzzling behaviors, especially when they are about to get stuck.

Ohio University Physics & Astronomy professor and NQPI member Horacio Castillo is working to understand phenomena happening in dense granular matter. To Castillo, dense granular matter are like crowded subway cars.

"If the car is crowded and people do not get out of the way, you cannot move," Castillo said. "This is sort of reinforcing because the person who would actually like to move for you cannot move because there is someone else blocking their motion."

Granular materials are the second largest group of materials manipulated by humans, after water. Practical applications include asphalt, concrete and various powders in the chemical, pharmaceutical and manufacturing industries.

Castillo and his colleagues ran numerical simulations of two-dimensional granular systems. They modeled elastic and inelastic collisions between particles in a fluid state.

As the density of the system in Castillo's simulation increases, particle collision results in a gradual slowing of system dynamics. At high enough density, the system can reach a

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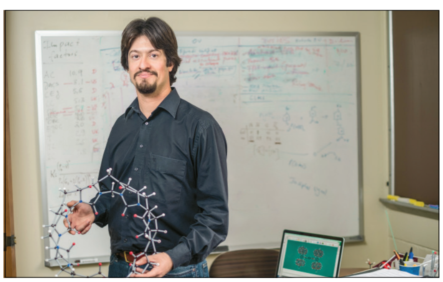
Engineering Pumpkin-Shaped Molecular Transporters


Eric Masson studies pumpkin-shaped Cucurbituril molecules.

Named after the gourd family Cucurbitaceae, a unique group of molecules are known for binding things in tight complexes. While pumpkins are said to whisk fairy tale characters off to royal balls, the Cucurbiturils transport molecules to specific targets.

Ohio University Chemistry & Biochemistry professor and NQPI member Eric Masson studies cucurbiturils, macrocyclic molecules that form a hollow, cylinder-like structure and contain oxygen atoms along their outer rims.

The cavities of Cucurbiturils are largely hydrophobic, and it is known that they bind hydrophobic "guests" readily in water. In a paper published in *Organic Letters* last August, Masson and Ph.D. student Ramin Rabbani showed that eight-unit cucurbiturils (i.e., CB[*8*]) can bind two guests at once, one being a hydrocarbon.

"(CB[*8*] is) basically a supramolecular handcuff that can connect two things together," Masson said. "You have CB[*8*], and you have the (first) substituent … Then you have this cavity that is still available for another guest. In that remaining cavity ... we captured hydrocarbons."

In the paper, the team described the binding of 20 hydrocarbon guests, which they visualized using nuclear magnetic resonance spectroscopy. Now they are characterizing the binding of terpenoids, small molecules found in natural oils such as lavender and basil. The technique can be used to identify oils extracted from different geographic regions. The project, supported by the American Chemical Society Petroleum Research Fund, may be used in quality control and detection of counterfeit products.

Additionally, Masson is working on a project funded by the National Science Foundation on the development of CB[*8*] dynamic polymers that regulate biological systems. The team is synthesizing molecules that link to cucurbiturils on either side, forming a long chain with properties reminiscent of alpha helical structures of proteins. While the central chain is rigid, the substituents can bind biological targets, such as enzymes and other proteins involved in pathological pathways.

Masson said this research may play a major role in drug delivery, allowing for precise, effective treatments that minimize off-target side effects for patients. His group is currently writing two papers on the project.

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Director's Corner

Dear Colleagues:

Warmest greetings from the Athens, Ohio campus of Ohio University. We hope you enjoy reading the 18th edition of the NQPI newsletter and learning about the latest research activities being conducted by our members. With grants and funding becoming harder to obtain each year and university budget cuts becoming more commonplace, we all have to find ways to work "smarter." Good communication between groups and effective collaborations are just some of those ways.

One such exciting example is work being performed by Dr. Horacio Castillo and his collaborators on moving particles within granular systems. Dr. Castillo compares particle movement to the movement of people from a crowded subway car; the first have to move before anyone else can move. We are certain you will enjoy reading about this work.

We also spoke with Dr. Amir Farnoud about his new piece of equipment called the Zetasizer, which measures particle and molecule size. Additionally, we hope you enjoy our last "installment" of the first Nanocar Race in which the OHIO team achieved a very respectable second place finish.

We invite you to learn about NQPI's newest member, Dr. Anthony Stender, a Chemistry & Biochemistry professor who brings his expertise on new spectroscopic techniques as they pertain to the study of forensics. We are excited to welcome Dr. Stender to NQPI!

We also take serious pride in our students' work. We hope you enjoy the article on current biological sciences graduate student and NQPI writing intern Amanda Biederman, who has recently completed her second trip to Antarctica where she studied the physiology of icefishes.

As always, we keep more current information and other news on our website, *www.ounqpi.org*. Thank you for reading our newsletter and I wish you a productive winter season.

Sincerely,
Eric Stinaff, NQPI Director

NanoBytes

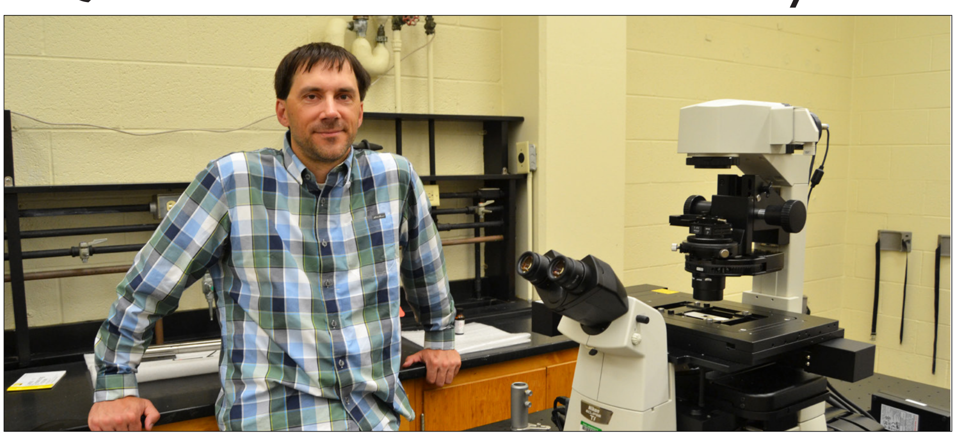
■ Physics & Astronomy professor Nancy Sandler was recently an invited speaker for the conference of Transport at the NanoScale at the Centro Internacional de Ciencias in Cuernavaca, Mexico.

■ An article entitled "Anomalous Kondo resonance mediated by semiconducting graphene nanoribbons in a molecular heterostructure" by Physics & Astronomy professor Sergio Ulloa was published in *Nature Communications* in October 2017.

■ NQPI will be sending a delegation to the 2017 Fall Meeting of the Matierials Research Society in Boston in late November. NQPI members attending include Electrical Engineering and Computer Science professor Wojciech Jadwisienczak, Physics & Astronomy professor Alexander Govorov and two graduate students.

■ Visit *www.ounqpi.org* to read about Physics & Astronomy professor Arthur Smith's accomplishments during his recent sabbatical.

NQPI Welcomes Forensics Faculty Member Anthony Stender



Anthony Stender in his microscopy lab at Clippinger. He joined NQPI in March 2017.

The tenure track venture in academia is a windy road.

"It never crossed my mind that I would eventually be a chemist," said Anthony Stender, NQPI's newest member and Chemistry & Biochemistry professor.

Before he was encouraged to try forensic science, Stender completed a bachelor's in Math at the University of Wisconsin at River Falls and a master's in Meteorology from the South Dakota School of Mines and Technology. Set on attaining a Ph.D. level position, he would find himself studying rod-like plasmons at Iowa State University.

"The joke we shared in our research group was: 'on paper, I'm an analytical chemist', but none of us were doing traditional analytical chemistry research," Stender said.

Jokes aside, Stender has developed a hefty set of scientific proficiencies; multiple forms of optical microscopy, nanoengineering and a fellowship at Rice University help craft a unique approach toward nano-forensic research.

"One thing that appealed to me (at OHIO) was the opportunity that I could do some nano-related research," Stender said. "I could do some microscopy, but I could also do some forensic-related research."

Specifically, Stender hopes to use a "single particle at a time" approach to investigate the gap between the macro- and nanoscale levels of measurement. Forensic microscopy rarely ventures below the microscale, but there is a growing interest to go there. In the end, Stender's goal is to understand how properties change as you take a particle from one end of this scale to the other.

"Once you start growing beyond 100 nanometers … you start to blur the lines of 'is it nanoscale behavior, or is it like a bulk material?'" Stender said. " It seems like there is an opportunity there to do some interesting research with students."

Staff Writer Amanda Biederman Explores Antarctica

NQPI editorial intern Amanda Biederman explores in the region of the Western Antarctic Peninsula.

Heading south for the summer might sound counterintuitive to some, but go far enough and you will hit colder temperatures. Ph.D. student and NQPI's editorial intern Amanda Biederman spent the past summer at Palmer Station, Antarctica studying the fish and their warming climate – though this is not her first time.

"Since this is my second season at Palmer Station, I went in with a much clearer idea of what to expect," Biederman said. "I spent the year before deployment designing a set of experiments to complete at Palmer for my dissertation."

Inspired by her advisor Lisa Crockett, OHIO Biological Sciences professor, Biederman studies how Antarctic fish are impacted by climate change. Before actually going to Antarctica, her pursuits led her into graduate research on membrane biology.

"I found (my advisor's) work with Antarctic fishes particularly exciting because it's so relevant to climate change, which is such an important topic for discussion among our society today," Biederman said.

Antarctica is a temporary home for Biederman and other researchers, but the cold does not stop experimentation. Additionally, the climate does not even stop the team from taking time off to relax.

"We all had a big celebration for the winter solstice (in June)," Biederman said. "We all come up with creative ways to have fun despite the cold and isolation. A lot of people go out boating or hiking on our day off."

For Biederman personally, the research highlights pinnacle moments for her academic career.

"It feels very satisfying to have completed two major milestones (comprehensive exam and proposal defense) as a graduate student," Biederman said. "The preparation that I went through in order to accomplish this has definitely helped me to build a research plan and to succeed the best I can in the field."

Creating Memories in Hawai'i, a Proposal for Data Storage

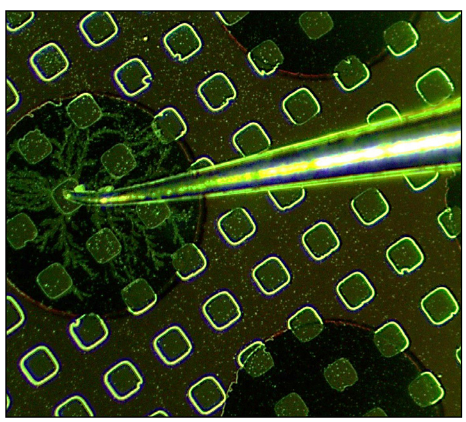
For NQPI members and Physics & Astronomy professors Gang Chen and David Drabold, there might one day be a "memory to rule them all."

In a proposal sent to the Semiconductor Research Corporation, Chen and Drabold together with a team at Arizona State University aim to further investigate the scalability of new memory chip material in flash devices such as USB sticks, solid-state drives and picture memory cards. The material of interest is what is known as a solid electrolyte glass or a so-called Conductive Bridging Random Access Memory material that is much faster at writing and storing information and consumes less power than today's devices.

"If you want to go to some limit of miniaturization … some kind of a memory cell that has 100 atoms … that would be a kind of 'Holy Grail'," Drabold said.

Scaling memory devices down means not only making them physically smaller but rearranging the atomic structure of the flash memory material so that a higher storage density can be achieved.

The solid electrolyte glass under study



Silver deposits with an electron probe and branching dendrites.

was comprised of a nonstoichiometric material and ionized silver. When electrodes were placed on both ends of the glass, a silver nanowire was constructed, forming a high-resistance, low-conductivity state that stores information.

During his sabbatical, Chen led to an additional discovery that there were a strong and intermediate conducting state before the formation of the silver wire – a state that resembled semiconductors, never totally insulating or conducting. He presented his findings and led discussions at various institutions in Southeast Asia, such as the National Sun Yat-Sen University in Kaohsiung, Taiwan and South China University of Technology in Guangzhou, China.

"Our research was based on the hypothesis of the existence of the semiconducting phase, and we proved it to be true," Chen said.

Another challenge involves figuring out the conduction pathway generated by this interaction.

"I realized I know how to compute the conductivity, but I don't know how to compute the path," Drabold said.

Drabold is currently working on a potential working theory to help explain this phenomenon. In the end, it's all a part of the scientific process.

"It happens, this sort of serendipitous, random good luck that we had that interaction," Drabold said. "It led us to more in the usual spirit of science: we started out looking this way and we deviated a bit to another interesting topic."

Nano Wagon Team Makes The Podium

The Ohio University BobCat Nano Wagon took home the silver medal from the first ever Nanocar Race hosted at CEMES (Centre d'Élaboration de Matériaux et d'Etudes Structurales) in Toulouse, France.

NQPI members Saw Hla (Physics & Astronomy) and Eric Masson (Chemistry & Biochemistry) led their respective students in a joint effort to guide the Nano Wagon to the 100nm finish line. Hla, stationed in Athens, Ohio at the time of the race, drove the nanocar along a gold surface while Masson, in Toulouse, monitored the race.

Although short of the 100nm goal, finishing 2nd at 43nm is still a remarkable accomplishment. Relaying information in real-time between the teams is a challenge itself. Each competitor attending the meeting in France remotely controlled their vehicles' trajectories by communicating with their pit crews at home. For the OHIO team, graduate student Kyaw Zin Latt stayed in Athens to oversee the racing conditions.

Moving the nanocar involved subliming the vehicle's molecules onto the gold track and probing it with an electron from a STM tip. The pit crew had to be careful not to upset the Nano Wagon's molecular configuration; probing nanocars with STMs gradually heats the gold surface. At higher gold surface temperatures, the Nano Wagon risked destruction while at lower ones, propulsion was unlikely.

The OHIO team secured a victory in constructing the largest supramolecular nanovehicle for the event. Constructed with 644 atoms, the Nano Wagon was awarded "The Texan" for its sheer size. Graduate student pit crew member Kondalarao Kotturi said that synthesis of this "monster truck" has opened avenues for his nano-car research proposal.

"We have to build different versions of the car ... to understand whether the wheels are rolling or sliding by designing other models," Kotturi said.

According to his recent findings, Masson said that the Wagon wheels are likely to be rolling.

"The primary data and our personal experience with that molecule (is) there is almost no friction," Masson said. "When the axel is inside the wheel, the wheel can rotate with virtually no friction."

While the BobCat Nano Wagon might have seen its last race, the same cannot be said for future models. Another Nanocar Race is currently in the works at CEMES.

"We don't know what the rules are going to be," Masson said. "I'm sure there's going to be another exciting challenge, but there will be a race."

Pit crew members (left to right) Karthi Permual, Kondalarao Kotturi, Mersad Raeisi and Ramin Rabban.

Granular Systems

Continued from page 1

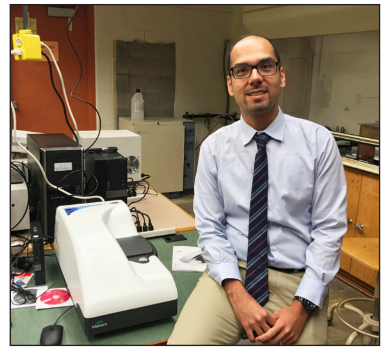
state known as dynamical arrest, in which the dynamics are almost completely stopped. A phenomenon called dynamic heterogeneity accompanies this slowdown, generating regions of fast- and slow-moving particles.

In the initial research published in *Physical Review Letters*, Castillo and his colleagues reported that as the system became denser, the size of slow and fast regions in this two-dimensional system grew dramatically.

In a further study published in *Soft Matter,* they examined the distributions of region sizes in more detail. They found that the distribution of fast region sizes was unremarkable, but the distribution of slow region sizes showed a power law behavior characteristic of percolation transitions. These transitions appear, for example, in the study of forest fires, rock porosity and fluid diffusion in random media.

Castillo said researchers have conducted follow-up studies to understand the differences between two- and three-dimensional systems. This work has established clearer connections between how dynamical arrest and dynamical heterogeneity occur in fluidized granular systems and how they occur in other soft matter systems.

A Zetasizer for OHIO



Amir Farnoud with the Zetasizer ZS.

NQPI member and Chemical and Biomolecular Engineering professor Amir Farnoud was awarded a grant from the 1804 Fund titled "Acquisition of a Zetasizer ZS to enhance nanotechnology research and education at Ohio University."

The Zetasizer ZS is an instrument that uses dynamic light scattering to measure particle size and two oppositely charged electrodes to determine particle charge.

The former process involves shooting a beam of light off particles inside a glass vial. As this light scatters, its intensity fades over time, and this information is stored as data to determine particle size. The faster the scattered light diffuses, the smaller the particle is likely to be.

Two electrodes are positioned on opposing sides of the sample; thus, particle charge is approximated by how quickly each particle moves to either electrode. In order to calculate this velocity, one must measure the time difference between two moving particles.

The acquisition of a Zetasizer ZS is a strong step forward for researchers like Farnoud, who are interested in developing a multi-user facility at the Athens campus at OHIO.

To read longer version of this article describing Farnoud's recent work, visit *www.ounqpi.org*.

Writing, design and editing by Amanda Biederman and Ray Humienny. Editing by Dr. Nancy Sandler and Kay Kemerer. Please e-mail nqpi@ohio.edu with comments.