A PUBLICATION OF THE UNIVERSITY OF VERMONT DEPARTMENT OF PHYSICS SUMMER 2011

Physics@UVM

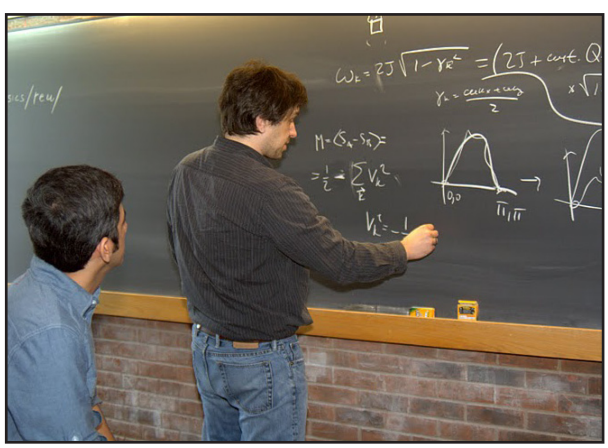
Faculty Notes

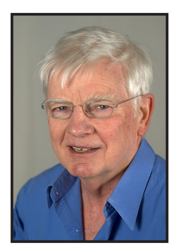
Dr. Madalina Furis, Assistant Professor of Physics, received a prestigious Faculty Early Career Development (CAREER) award of $600,000 from the National Science Foundation on the basis of her research proposal entitled "Imaging Excitons, Spin Coupling and Magnetism in Discotic Crystalline Organic Semiconductors." The CAREER award supports outstanding junior faculty members in science and engineering with the potential to become leading teacher-scholars in their respective disciplines.

Dr. Adrian Del Maestro is joining the UVM physics faculty starting in Fall 2011. Dr. Del Maestro, currently a postdoctoral fellow at the Institute for Quantum Matter at Johns Hopkins University, is a theoretical condensed matter physicist whose current work focuses on properties of interacting bosons in low dimensional systems.

Professor Jun-ru Wu was a featured speaker at the International Symposium on Therapeutic Ultrasound in New York in April 2011. His lecture was titled "Feasibility study of cell surgery using high intensity focused ultrasound."

Dr. Valeri Kotov was reappointed to the faculty as Assistant Professor of Physics. His reappointment becomes effective in Fall 2011. Dr. Kotov is an invited lecturer this summer at a workshop titled "Synergies between field theory and exact computational methods in strongly correlated quantum matter" held at the International Centre for Theoretical Physics in Trieste, Italy. His lecture is titled "The spinon gas model and its numerical tests."





Dr. John F.W. Perry was promoted to Lecturer III. His new appointment becomes effective in Fall 2011.

Megan Force named GTF of the Year

Megan Force, a physics M.S. student, was named Graduate Teaching Fellow of the Year in the Department of Physics. Megan received a certificate of achievement and a membership to the American Physical Society at the physics department awards reception on May 4, 2011. Megan will be attending Dartmouth College in the fall to pursue a Ph.D. in astronomy.

Awards and Honors

From left to right: Jacob Wahlen-Strothman, Isaac Backus, Professor Clougherty and Isabel Kloumann at CAS Honors Day.

Two departmental awards were presented to physics undergraduates at the College of Arts and Sciences' Honors ceremony held in Ira Allen Chapel on May 20, 2011. Junior physics major Jacob Wahlen-Strothman received the Albert D. Crowell Award for his research performed under the supervision of Professors Kelvin Chu and Madalina Furis on the magneto-optic and optical properties of solution and self-assembled thin films of biologically-relevant small molecules, including metal ion derivatives of meso-tetraphenylporphyrin. He presented his research results at the 2011 March meeting of the American Physical Society in Dallas, Texas.

The David W. Juenker Prize for outstanding scholarship in physics was awarded to two senior physics majors: Isaac J. Backus and Isabel M. Kloumann. Isaac, from Burlington, Vermont, majored in Philosophy and Physics and developed a strong interest in astronomy during his junior year. Under the faculty supervision of Professor Joanna Rankin, his research has centered on comparing two radio pulsars with similar mode-switching effects. His work took him first to the Arecibo Observatory in Puerto Rico and then to the Giant Metrewave Radio Telescope in India. One publication reporting his research has been published and a second is in final preparation. Isaac will be attending the University of Washington in Fall 2011 to pursue a Ph. D. in physics.

Isabel, also a Burlington native, was a double major in Physics and Mathematics. Under the supervision of Professor Rankin, Isabel carried out a large study of a pulsar that nulls two-thirds of the time. As a junior, she became involved with NanoGRAV, the international effort to detect gravitational waves using pulsar timing. On the basis of her outstanding undergraduate research, Isabel completed an Honors thesis titled "Characterizing the behavior and stability of pulsar radio frequency emission." Isabel will pursue a Ph.D. in Applied Mathematics at Cornell University this fall.

2011 Sigma Pi Sigma Inductees

Three undergraduates were inducted in the UVM chapter of Sigma Pi Sigma in May 2011: Brad Michael Diamond of Westford, Vermont; Darcy Elizabeth Glenn of Hopewell, New Jersey; and Cody James Lamarche of Newport, Vermont. Founded in 1921, Sigma Pi Sigma is the national physics honor society. Sigma Pi Sigma honors outstanding scholarship and service in physics, encouraging and stimulating members in their scientific pursuits.

Isaac Backus inducted into Phi Beta Kappa

Isaac Backus, a 2011 UVM physics graduate, was inducted as a new member into Phi Beta Kappa honor society. Phi Beta Kappa is the oldest honor society in the country, and among the most prestigious. From the society's website: "The ideal Phi Beta Kappan has demonstrated intellectual integrity, tolerance for other views, and a broad range of academic interests. Each year, about one college senior in a hundred, nationwide, is invited to join Phi Beta Kappa." The Alpha Chapter of Vermont was chartered in 1848. In 1875, it became the first chapter in the nation to admit women to its membership.

Nota Bene

We would enjoy hearing from all UVM physics alums and friends. Send your email to physics@uvm.edu.

Summer Internships and Awards

Ian C. Goyette, a graduate student in physics, was awarded a paid summer internship in the Surface, Materials Science and Chemistry Laboratory at the IBM facility in Essex Junction, Vermont. Ian's summer project is titled "Ellipsometry of Films Critical to State of the Art Device Fabrication." Under the supervision of researchers at IBM, Ian will determine optical characteristics that will be used in IBM labs for manufacturing films for microelectronic applications.

Stephanie Young, a junior physics major, was awarded 2011 APLE Summer grant. APLE Summer awards provide a stipend of $3,000 for undergraduate students. Typically only two awards are given each year in the College of Arts and Sciences. Stephanie's research project is titled *Searching for Core Emission in Classical Double Conal Pulsars*. She will spend her summer examining pulsars that are extremely dense, rapidly rotating neutron stars with strong magnetic fields that emit beams of radiation. In her previous research, Stephanie successfully identified a weak core emission component in certain pulsars, where only conal emission had previously been known. This summer she will be developing new techniques and computer methods to reliably identify weak emissions. This software development will be key to further research since no one has looked at pulsars this way before. Stephanie will be submitting her results for publication in *Monthly Notices of the Royal Astronomical Society* by the end of the summer.

Recent Faculty Grants and Awards

Professor Madalina Furis was awarded $600,000 by the National Science Foundation to study magneto-optical properties of discotic organic semiconductors.

Professors Dennis Clougherty and ***Madalina Furis*** were awarded $286,000 by the National Science Foundation for the establishment of an REU (research experiences for undergraduates) site on complex materials.

Professor Randall Headrick was awarded $550,000 by the US Department of Energy to continue his studies of the mechanisms of roughening and smoothing during thin film deposition.

Professor Valeri Kotov was awarded $200,000 by the US Department of Energy for theoretical studies of graphene.

Professor Joanna Rankin was awarded $283,000 by the National Science Foundation to study how pulsar timing can be used to detect gravitational waves.

Slicing Proteins with Occam's Razor

By Joshua Brown

A cheetah lies still in the grass. Finally, a gazelle comes into view. The cheetah plunges forward, reaches sixty-five miles per hour in three seconds, and has the hapless gazelle by the jugular in less than a minute. Then it must catch its breath, resting before eating.

A blue whale surfaces, blasting water high from its blowhole. It breathes in great gasps, filling its thousand-gallon lungs with air. Then it descends again to look for krill, staying below for 10, 20, even 30 minutes before taking another breath.

Both animals need oxygen, of course. And both depend on the protein myoglobin to store and then release that oxygen within their working muscles. But how they need oxygen differs. The whale must have enough to last a whole dive. Its muscles have a high concentration of myoglobin that delivers oxygen steadily. In contrast, the cheetah's myoglobin must perform like a fast-shooting cannon. The cheetah needs to suddenly take up and release large doses of oxygen to stoke its explosive speed.

How does myoglobin do all that? For decades, biologists have wondered how – and with what atomic motions, exactly – the folded structure of myoglobin allows it to hold and release oxygen.

Now, two physicists at the University of Vermont have an answer. They've developed a new way to peer into the inner workings of proteins and detect which specific atoms are at work. Their work was published in the Aug. 27 issue of the journal Physical Review Letters.

Atomic bondage

Using myoglobin as a test, the scientists were able to home in on the critical functional piece of the protein, separating it from the vast number of other "jigglings and wigglings of atoms" says William DeWitt, a UVM graduate student and the lead author on the paper that describes the finding.

"We've been able to identify the motion of one particular amino acid – this group of atoms called the distal histidine – that controls the binding process," he says.

Shaped a bit like a tennis racket over a basket, this tiny arm of the protein moves, through thermal fluctuations, to open or close the binding site near the myoglobin's iron-filled center. "As the atoms move in one direction it becomes easier to bind oxygen," says DeWitt, "and as they move in the reverse direction it becomes less easy."

And how this distal histidine moves should vary between the whale and the cheetah. "I would imagine," says Kelvin Chu, associate professor of physics and DeWitt's co-author, "that there has been evolutionary pressure on every species to adapt this motion in the myoglobin for their particular oxygen-binding needs."

"That's a testable hypothesis," Chu says. "What we would expect to see across species is that the tennis rackets are in different places or move different amounts."

DeWitt and Chu's work extends far beyond myoglobin. The two physicists see broad application of their new method in creating custom-crafted proteins.

"Once you know what these motions are and what the important atoms are," says Chu, "you can make mutants of proteins that have different binding attributes." And these different attributes have promise in developing new biotechnologies "ranging from blood substitutes to organic solar cells," he says.

Grad student William DeWitt and Professor Kelvin Chu, Department of Physics, have invented a new way to peer into proteins. Their paper in Physical Review Letters pinpoints which atoms within the protein myoglobin hold and release oxygen to meet the unique needs of different animals. (Photo: Joshua Brown)

Slicing Proteins with Occam's Razor, *continued*

Function follows form

Proteins are a cell's heavy laborers: hauling water, taking out the trash, carrying in the groceries – and trillions of other tasks that make life. But how the shape of a protein determines its function remains one of the most vexing and important questions in the physics of biology.

Proteins are not the static, Lego-like objects you might see in an x-ray photograph in a biochemistry textbook. Instead, made from long chains of amino acids scrunched into various blobs and globs, a protein is always jumping between slightly different structural arrangements due to thermal motion of its atoms. Even a modest-sized protein like myoglobin has more possible arrangements of its atoms than there are stars in the universe. And each of these arrangements slightly changes a protein's function.

"But what are the important motions that control its function?" asks Chu.

"Relating the structure of a protein to what it is doing is the holy grail," he says. For myoglobin at least, the two UVM scientists seem to have brought the prize a lot closer to hand.

The power of parsimony

Their method – called temperature derivative spectroscopy or TDS – involves cooling myoglobin to as low as -450 degrees Fahrenheit, about 18 degrees above absolute zero, and then measuring its oxygen-binding process. At these chilly temperatures, each protein basically gets stuck in just one arrangement. These individual atomic arrangements can't be observed directly, but, using infrared light, a pack of myoglobin molecules does yield a kind of group portrait – a summing, called a TDS surface – of the position of all the proteins as they bind to the oxygen in carbon monoxide.

The Vermont scientists' innovation comes largely from what they have been able to do with this group portrait.

"This scenario is called an inverse problem," DeWitt notes, "we have measured the effect but want to determine the cause." Unfortunately, a bit like asking what two numbers add up to ten, there are many solutions.

But, usually, nature does not build wasteful structures – and though the universe is undoubtedly complex, it does not seem given to capricious complexity. In other words, the scientific principle of parsimony – what philosophy students encounter as Occam's Razor – suggests that the least complex explanation is the most likely.

Applying a mathematical version of this idea from Bayesian statistics, called the principle of maximum entropy, DeWitt and Chu went looking for the simplest solution to the TDS surface created by their group of myoglobin molecules. And the answer: the motion of the distal histidine most simply explains how myoglobin regulates oxygen binding.

They followed this prediction by performing a computer simulation of the molecular dynamics of the distal histidine, which confirmed their interpretation.

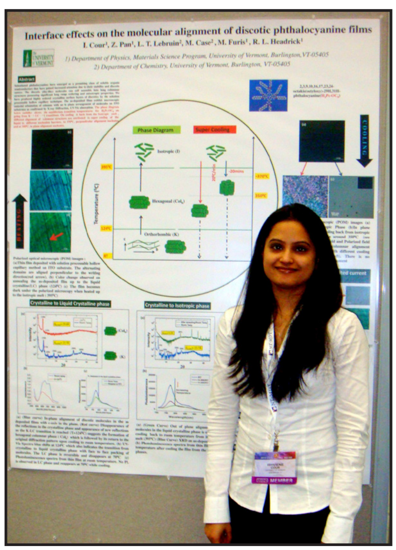
"Will did a lot of this on his own," says Chu, "He took the data, and the analysis was done on a MacPro," plus some time on the National Science Foundation's high-performance computer network, the TeraGrid.

"He's a clever guy," says Chu.

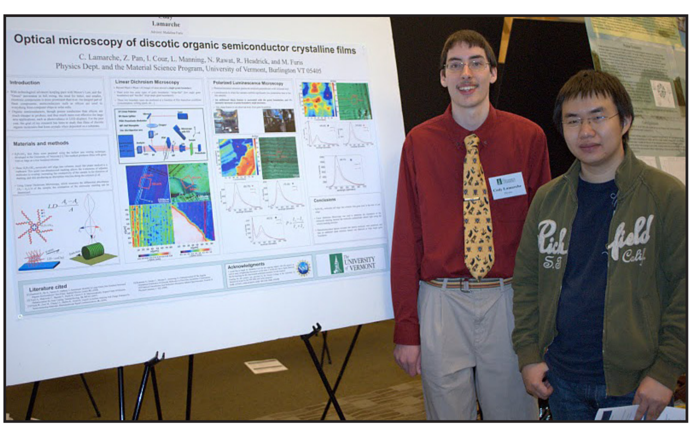
Student Research

From left to right: Isabel Kloumann, Professor Rankin, Stephanie Young and Megan Force at the 2011 UVM Student Research Conference. Isabel's poster is titled "Characterizing the Radio Frequency Timing Stability of Fast and Millisecond Pulsars."

Cody Lamarche, a junior physics major, was a recipient of an NSF Research Experience for Undergraduates (REU) award from the National High Magnetic Field Laboratory (NHMFL) at Florida State in Tallahassee Florida. His project involved conducting a magnetic circular dichroism experiment to measure magnetic properties of organic semiconductors in very high magnetic fields. He was part of a UVM/NHMFL collaborative team led by Dr. Stephen McGill (NHMFL/FSU) and Prof. Madalina Furis (UVM) that developed the first optical spectroscopy experiments for the new record 25T split–coil HELIX magnet commissioned in June by NHMFL.



Ishviene Cour, a Ph.D. candidate in the Materials Science Program, presented research at the 2010 Fall meeting of the Materials Research Society in Boston, Massachusetts. Her poster is titled "Interface Effects on Molecular Alignment of Discotic Phthalocynanine Films."



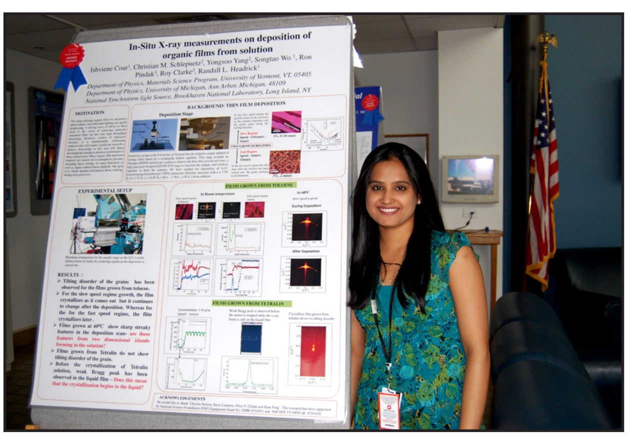
Undergraduate physics major Cody Lamarche with graduate student Zhenwen Pan at the 2011 UVM Student Research Conference. The project performed under the supervision of Professor Furis is titled "Optical Microscopy of Discotic Organic Semiconductor Crystalline Films."

Student Research, continued

Yanting Zhang, a Ph.D. candidate in the Materials Science Program, gave an oral presentation at the 2011 March meeting of the American Physical Society in Dallas, Texas. The title of her talk was "Dissipative Effects in Quantum Sticking."

Dr. Songtao Wo, a recent graduate of the Materials Science Program, gave an oral presentation titled "Grain Nucleation and Growth Effects on Charge Transport in Solution-processed Organic Semiconductor Thin Films" at the 2010 Fall meeting of the Materials Research Society in Boston.

Jacob Wahlen-Strothman received a UVM Undergraduate Research Award to work with Professor Kelvin Chu on magnetic circular dichroism of metal-substituted tetraphenylporphyrins. This $5000 summer internship is based upon the work that he presented at the American Physical Society meeting in Dallas TX and forms the basis of his honors thesis. In his previous research, Jacob performed measurements on solution and self-assembled organic molecules. He is extending his experimental and analytical techniques to biologically-relevant compounds and is using density functional theory to determine the electronic structure of his samples.



Ishviene Cour, a Ph.D. candidate in the Materials Science Program, presented research at the May 2011 annual users meeting of the National Synchrotron Light Source in Upton, New York. Her poster, titled "In-situ X-ray Measurements on Deposition of Organic Films from Solution," won a best poster award at the meeting. It reported on a collaboration between Headrick's group at UVM and groups from Brookhaven National Laboratory and from the University of Michigan

Trouble with Sputter? Blame Giant Nanoparticles

By Joshua Brown

When you tear open a bag of potato chips or pop in a DVD, you're probably putting your hand on sputter deposition. No, don't run for the soap.

Sputter deposition is an industrial process used since the 1970s to spray – sputter, that is – thin films onto various backings, like the metallic coating on potato chip bags, the reflective surface on DVDs, or the electronics on computer chips.

Mostly, the process works very well. In a vacuum chamber filled with an inert gas, like argon, high voltage is applied to a magnet. This energizes the argon, which, in turn, bumps particles of, say, tungsten metal from a source near the magnet out into the cloud of gas. Some of these extremely hot, charged tungsten particles zip at high speed through the argon and deposit onto the target, forming a thin film.

But sometimes the coatings peel off or the product bends in on itself and cracks, as if the film was stretched tight before it was applied to the surface. Other times, the films are just too rough. For decades, scientists have been baffled – and manufacturers frustrated – about why these problems happen.

Particle pile-up

Now researchers at the University of Vermont and the Argonne National Laboratory near Chicago have an explanation: "it's nanoparticles," says Randy Headrick, professor of physics at UVM, "sticking and pulling together."

The discovery, led by Headrick's graduate student, Lan Zhou, was published August 10 in the journal *Physical Review B*.

Using high-powered x-rays, the team measured the size of tungsten particles depositing on a target and were amazed. Above a critical pressure in the argon gas (eight one-millionths of an atmosphere), the size suddenly jumped. Instead of single atoms or several-atom molecules – as would be expected in the high-heat, high-velocity environment of a sputter chamber – they detected relatively gigantic blobs of hundreds of atoms: what the researchers call a "nanoparticle aggregation."

"It's a condensation, like clouds, like mist," says Headrick, "this is something we really didn't expect."

These nanoparticles pull together and fuse, drawing the film tight as tiny "nano-voids" between particles are eliminated. This can create stress in thin films strong enough to pull electronic wafers into a cup shape or roughness that distorts the delicate coatings of optical lenses.

One nanometer, please

"No one realized that in the gas phase you could produce a particle so large," says Al Macrander, a physicist at Argonne National Laboratory and a co-author on the article. "They're highly energized, so it's counter-intuitive that they would stick – because of their velocity," he says. But stick they do.

In the sputter deposition chamber, "particles start off with temperatures of around ten thousand degrees," UVM's Randy Headrick explains. But even as they are moving in the gas, they cool slightly and "once they cool," he says, "they want to go back to being a solid."

"This has large implications," Macrander says, "for many industries, not only optics." For his part, the new findings are likely to help accelerate the creation of advanced x-ray lenses that he has been helping to develop.

So far, the efforts to make these lenses have not succeeded since the sputter deposition process has produced coatings that are still too rough with too much tension – despite using state-of-the-art techniques.

Trouble With Sputter?.... *continued*

"These lenses are intended to focus x-ray beams on smaller dimensions than have ever been achieved," he said, "down to one nanometer." To make these lenses requires more than a thousand layers of thin film. "Stress builds up and becomes a problem," he says.

The team's new insight into the basic physics of sputter deposition points the way toward a solution, but the equation is complex. "If you want to get real smooth surfaces, you have to deposit at lower argon pressures," says UVM's Lan Zhou. But at this very low pressure, the particles hit with such velocity that the thin films want to expand, creating the opposite problem by pulling films apart.

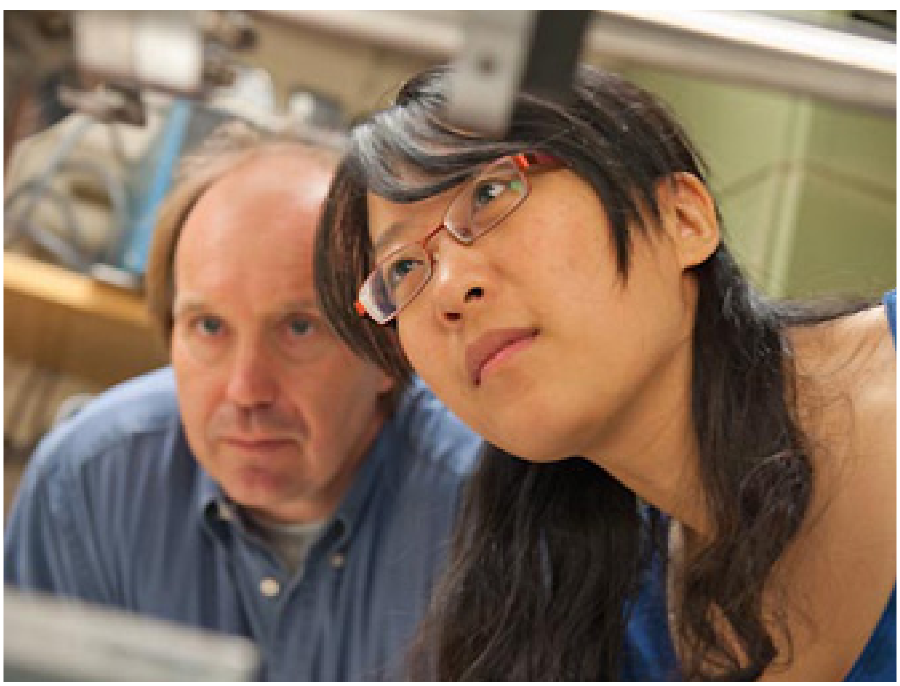
"Its still an open question: what do you do to make a film with zero stress and as smooth as possible?" says Headrick.

"At least now we understand what is happening," says Zhou, "so people can try to optimize the film deposition conditions, for structure and roughness."

Hard thought

Still, what are problems in one application might be a benefit in others. "There is a lot more to this finding than lens coatings," says Headrick, "there are many kinds of materials where you want to make nanoparticles, like some kinds of catalytic converters or solar cells. This could be a good way to make nanoparticles cheaply."

But the cost of figuring it out was steep. "This took years for us to understand," says Zhou, with the slightly worn smile that PhD students wear best, "it was hard to think of aggregate particles forming in the middle of a flux."



Graduate student Lan Zhou and her advisor Randy Headrick made a fundamental discovery in physics that may improve computer chips, solar panels, x-ray lenses, and even your next pair of mirrored sunglasses. (Photo: Sally McCay)

NanoDays 2011

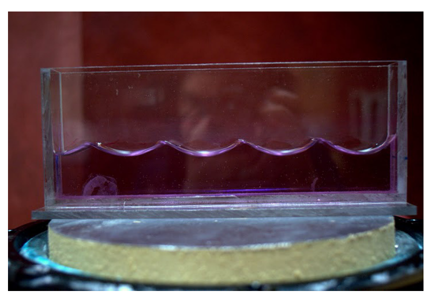
The UVM chapters of the Society of Physics Students and Sigma Pi Sigma organized a series of events for NanoDays 2011, an annual national celebration of nanoscale science, technology and engineering that includes hands-on activities, demonstrations and lectures for the general public. The ECHO Science Center was the site for all events.

The 2011 NanoDays team with the UVM SPS banner. From left to right: Cody Lamarche, Brad Diamond, Darcy Glenn, Jessica Titterton. Eli Kinigstein, Cody Duquette, Isabel Kloumann, Dan Khalaf, Stephanie Young, Mateus Teixeira, Dave Hammond, Jacob Wahlen-Strothman and Professor Clougherty.

Physics Fun @ ECHO

David Hammond with assistance from UVM chapter of the Society of Physics Students designed and organized "Physics Fun@ECHO," a program of lake-related physics at the ECHO Science Center on January 29, 2011. Over 400 people learned about topics such as buoyancy, waves, solitons and seiches. UVM physics students performed demonstrations and engaged the public in discussion of the science. Many of these demonstrations were designed and built by Dave Hammond.

Back row, left to right: Jacob Wahlen-Strothman, Lane Manning, Anand Sharma, Colin Riggs. Middle row: Professor Clougherty, Owen Myers, Mateus Teixeira, Dan Khalaf, Ian Goyette. Front row: David Hammond, Lisa Carpenter, Isabel Kloumann, Megan Force, Stephanie Young, and Naveen Rawat.



A wave demonstration from the Physics Fun @ ECHO program in January 2011.

Lane Manning, a Ph.D. candidate in the Materials Science Program, makes waves for attendees of the Physics Fun @ ECHO program.

2011 Graduates

Bachelor of Science degree recipients

Isaac Backus
Daniel Khalaf
Eli Kinigstein
Isabel Kloumann
Colin Riggs

Master of Science degree recipients

William DeWitt
Megan Force
Minghao Li

Ph.D. Materials Science recipients

Dr. Di Chen
Dr. Songtao Wo
Dr. Lan Zhou

Congratulations graduates!

From left to right: Professor Clougherty, Dan Khalaf, Colin Riggs, Isabel Kloumann, Isaac Backus, and Eli Kinigstein. From UVM's 207th Commencement ceremony held in the Athletic Complex Multipurpose Facility on May 22, 2011.

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Giving Opportunities

Your gift to the Department of Physics is invaluable and deeply appreciated. We offer naming opportunities for capital gifts in support of our departmental priorities, and we accept gifts in all amounts to any one of our departmental funds listed on the right. We also welcome deferred gifts and other gift-planning vehicles, which we understand can often make more substantial gifts possible. Contributions can be made online at **https://alumni.uvm.edu/giving/**

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- Albert D. Crowell Research Fund
- Physics Colloquium Fund

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