McCormick

Northwestern Engineering

Materials Science and Engineering

Robert R. McCormick School of Engineering and Applied Science
Northwestern University

SPRING 2013

Northwestern-Art Institute Partnership Expands With Mellon Grant

CENTER WILL BE A NEW NATIONAL MODEL OF COLLABORATIVE SCIENTIFIC RESEARCH IN THE ARTS

Northwestern has received a $2.5 million grant from the Andrew W. Mellon Foundation to establish the Center for Scientific Studies in the Arts (NU-ACCESS), expanding an innovative partnership between the University and the Art Institute of Chicago that has led to unlocking secrets about many of the museum's masterpieces and developing new methods and technologies to investigate art.

Breaking new ground, the conservation science partnership, funded over six years, will offer its scientific tools and expertise to users from across the country.

In the United States, scientific research on cultural heritage objects typically is conducted within the boundaries of a specific museum or cultural institution, with only a few dozen such institutions equipped with the necessary tools and expertise nationally.

"I am thrilled that what we have accomplished over the past eight years has been recognized as valuable," said Katherine T. Faber, a Walter P. Murphy Professor in materials science and engineering. "Now, we are ready to build upon this solid foundation to offer our expertise to others beyond our institutions."

Faber and Francesca Casadio, the Andrew W. Mellon Senior Conservation Scientist at the Art Institute, launched the museum-academic partnership in 2004 with Mellon support.

Many of the partnership's remarkable discoveries over the years have been woven into major exhibitions at the Art Institute, including "Matisse: Radical Invention, 1913-1917" in 2010 and "Watercolors by Winslow Homer: The Color of Light" in 2008.

The current show "Picasso and Chicago" (Feb. 20 to May 12) includes findings from a study of Modern bronze sculptures in which Northwestern and Art Institute researchers traced some of Picasso's unmarked sculptures to the Valsuani foundry in Paris, based on material evidence.

The new center will serve as a collaborative hub, facilitating interdisciplinary research partnerships in art studies and conservation on a national scale. Academic researchers and scholars in training will meet and engage in mutual learning with scientists, conservators, and curators.

Kathy Faber (right) of the Department of Materials Science and Francesca Casadio of the Art Institute of Chicago will co-direct the Center for Scientific Studies in the Arts. One piece of artwork already studied through the NU-AIC collaboration was "Head of a Woman (Fernande)" by Pablo Picasso (at left).

Conservation scientists in and outside Chicago have learned about the partnership's work through the Art Institute's exhibitions as well as academic papers and seminars. They have been eager to have the opportunity to study their own treasures, using the latest science and engineering tools offered by Northwestern and the Art Institute.

"Art and technology are prime material evidence of humanity's accomplishment," Casadio said. "By bringing the two together in this center, we will have a chance to enhance our understanding of the world's shared cultural objects and preserve them for future generations.

"This landmark initiative represents a tectonic shift from the isolated museum scientist to a dynamic hub that will serve as incubator of new ideas and significantly accelerate the rate of discoveries by providing the latest technological innovations brewing in the academic environment," she said.

Casadio and Faber will be co-directors of the Center for Scientific Studies in the Arts, which will be

continued on page 5

SAVE THE DATES

Annual Hilliard Symposium and Alumni Celebration
Thursday, May 16

Weertman Festival to Honor Hans and Julia Weertman
Friday, October 4

See page 2 for more information.

Letter from the Chair

Spring quarter finds the materials science department as busy as ever. Looking through the pages of this newsletter you will find that 2012-13 has been an exciting year. And there is more to come.

In September, President Morton Shapiro announced that the University and the National Institute for Materials Science in Japan would launch a joint research center to address global materials-related challenges in energy, environment, health, and security. Co-directed by Robert Chang, the center will enable our department to tackle new and exciting challenges in these important areas.

Shortly after New Years, Northwestern announced another exciting collaboration, this time with the Art Institute of Chicago. For several years, our institutions have partnered in a groundbreaking program that applies materials science characterization to the field of conservation science. Now, thanks to a sizeable grant from the Andrew W. Mellon Foundation, the new Center for Scientific Studies in the Arts will offer research opportunities to museums around the country. Katherine Faber will co-direct the center.

Meanwhile, our enrollments have increased at both the graduate and undergraduate levels. Research activity also remains high and we continue to publish exciting work. In addition, we are developing new opportunities for students to be involved in materials innovation through our soon-to-be available Battery Lab ("BatLab"), the first component of a planned Energy Materials Lab.

I hope you will join us for our second annual Alumni Celebration on Thursday, May 16. The day will begin with the Hilliard Symposium, which will feature graduate student posters and presentations, as well as a keynote address by alum Todd Steyer, manager of extreme environment materials at The Boeing Company. In the evening, we will celebrate alumni, student, and faculty accomplishments at the second Alumni Celebration Banquet. You can read more about the alumni honorees on page 7.

In the meantime, please save another date: Friday, October 4, 2013 — Homecoming Weekend — when the Weertman Festival will honor Hans and Julia Weertman.

Please join us for lively discussions, an update on research by our students, and a great opportunity to connect with old friends and new acquaintances. I hope to see you in May!

Michael J. Bedzyk
Chair, Department of Materials Science and Engineering

Michael J. Bedzyk

"We are developing new opportunities for students to be involved in materials innovation through our soon-to-be available Battery Lab ('BatLab'), the first component of a planned Energy Materials Lab."
Michael J. Bedzyk

Department Announcements

"BATLAB" COMES TO MSE

Materials science students and faculty will soon have access to a new, state-of-the-art Battery Lab ("BatLab"). Located on the third floor of Cook Hall in a space that previously housed the ceramics lab, the lab will include a suite of desktop-sized equipment for the synthesis, processing, device fabrication, and device testing for batteries and related devices.

The new facility will streamline the hands-on experience of students exploring high-performance battery and capacitor materials. The BatLab will be the first component of a planned Energy Materials lab, which will serve as a platform for student (graduate and undergraduate)-driven innovation in the broad arena of materials related to energy.

The BatLab is being funded by the generous contributions of alumni and supporters. The department is seeking funding for the Energy Materials lab at-large. If you or your company is interested in donating or becoming a corporate sponsor, please contact Ben Porter, McCormick's director of development, at (847) 467-5212 or b-porter@northwestern.edu.

2013 UPCOMING EVENTS: HILLIARD SYMPOSIUM, ALUMNI CELEBRATION, WEERTMAN FESTIVAL

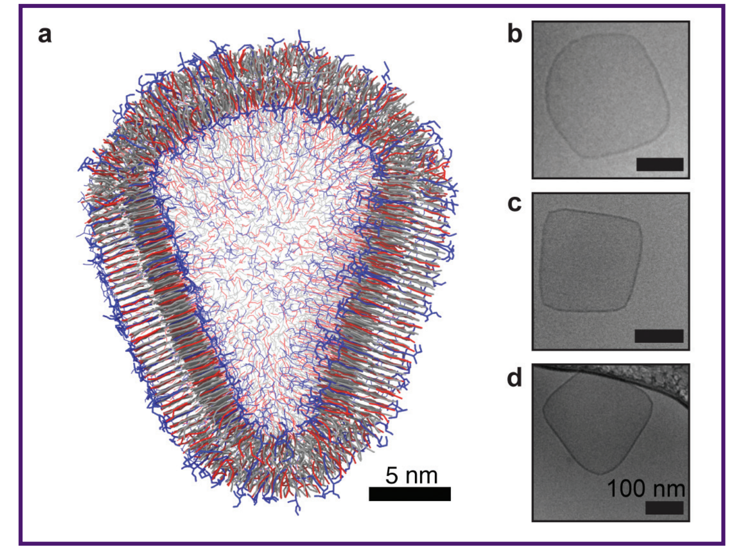
Join the Department of Materials Science and Engineering for the Annual Hilliard Symposium of graduate research on Thursday, May 16. The keynote speaker will be Dr. Todd Steyer, manager of extreme environmental materials at The Boeing Company. The symposium will be followed by the 2nd Alumni Celebration Banquet at the Hilton Orrington Hotel in downtown Evanston.

And on Friday, October 4 — during Homecoming Weekend — the department will host the Weertman Festival in honor of Hans and Julia Weertman, faculty emerita of materials science and engineering at McCormick.

Please join us! Program and registration details will be sent via e-mail as they become available. Information will also be available on the departmental website: www.matsci.northwestern.edu.

New Geometries: Researchers Create New Shapes of Artificial Microcompartments

AS IN NATURE, VARIOUS SHAPES COULD BE MORE EFFICIENT FOR SPECIFIC FUNCTIONS



A simulation shows the edges of a polyhedra-shaped micro compartment are fluid-like bilayers. Electron microscopy and x-ray scattering were used to image the multi-length scale structure.

In nature, biological functions are often carried out in tiny protective shells known as microcompartments, structures that provide homes to enzymes that convert carbon dioxide into energy in plant cells and to viruses that replicate once they enter the cell.

Most of these shells buckle into an icosahedron shape, forming 20 sides that allow for high interface with their surroundings. But some shells — such as those found in the single-celled Archaea or simple, salt-loving organisms called halophiles —break into triangles, squares, or non-symmetrical geometries. While these alternate geometries may seem simple, they can be incredibly useful in biology, where low symmetry can translate to higher functionality.

Researchers in the Department of Materials Science and Engineering have recently developed a method to recreate these shapes in artificial microcompartments created in the lab: by altering the acidity of their surroundings. The findings could lead to designed microreactors that mimic the functions of these cell containers or deliver therapeutic materials to cells at specific targeted locations.

"If you want to design a very clever capsule, you don't make a sphere. But perhaps you shouldn't make an icosahedron, either," said Monica Olvera de la Cruz, Lawyer Taylor Professor of Materials Science and Engineering, Chemistry, and (by courtesy) Chemical and Biological Engineering at McCormick and one of the paper's authors. "What we are beginning to realize is maybe these lower symmetries are smarter."

To create the new shell geometries, the researchers co-assembled oppositely charged lipids with variable degrees of ionization and externally modified the surrounding electrolyte. The resulting geometries include fully faceted regular and irregular polyhedral, such as square and triangular shapes, and mixed Janus-like vesicles with faceted and curved domains that resembled cellular shapes and shapes of halophilic organisms.

The research was conducted by three McCormick faculty members: Olvera de la Cruz; Michael J. Bedzyk, professor of materials science and engineering and (by courtesy) physics and astronomy; and Samuel I. Stupp, Board of Trustees Professor of Materials Science and Engineering, Chemistry, and Medicine.

A paper about the research, "Molecular Crystallization Controlled by pH Regulates Mesoscopic Membrane Morphology," was published November 27 in the journal *ACS Nano*.

Other authors of the paper include lead co-authors Cheuk-Yui Leung, Liam C. Palmer, and Bao Fu Qiao; Sumit Kewalramani, Rastko Sknepnek, Christina J. Newcomb, and Megan A. Greenfield, all of Northwestern; and Graziano Vernizzi of Siena College.

Tresa M. Pollock, Alcoa Professor of Materials at the University of California at Santa Barbara, with Michael J. Bedzyk (left) and Peter Voorhees at the John E. Dorn Memorial Lecture on February 12.

2013 MATERIALS SCIENCE LECTURES

This year's **Morris E. Fine Lecture**, "Watching Microstructure Evolve in Three Dimensions," was presented by Peter W. Voorhees, Frank C. Engelhart Professor of Materials Science and Engineering, on January 8.

The 2013 **Eshbach Lecture**, "Electrocrystallization of Coatings for Orthopedic and Dental Implants," was presented by Professor Noam Eliaz of Tel-Aviv University, Israel, on January 15. Eliaz, who is from the School of Mechanical Engineering and the Materials and Nanotechnologies Program at Tel-Aviv, is visiting the department and teaching a course in corrosion.

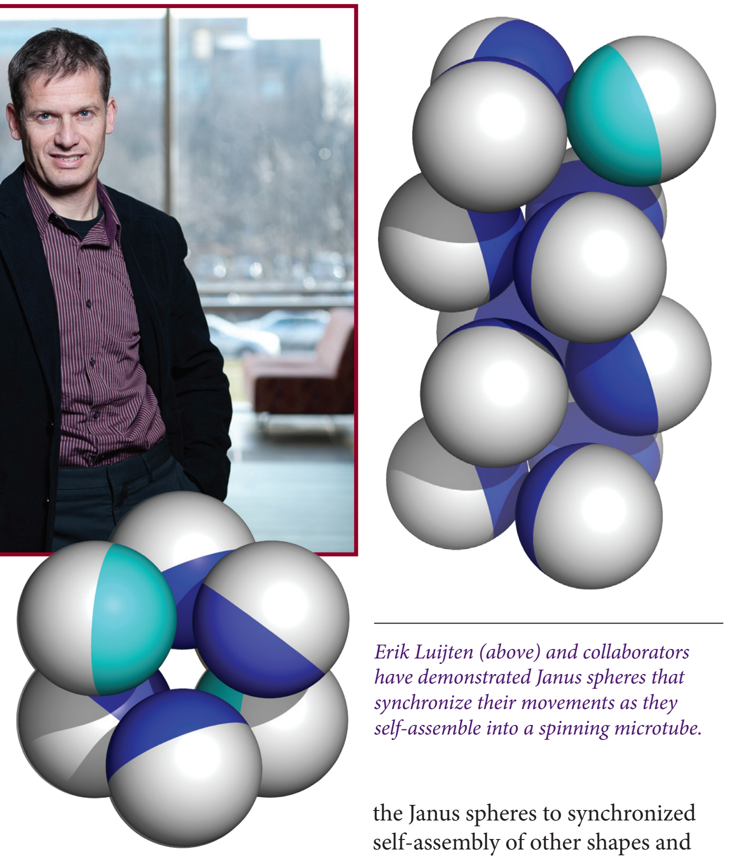
The 2013 **John E. Dorn Memorial Lecture**, "A New Tri-Beam Tomography System: How Much Information is Enough?" was presented by Tresa Pollack, Alcoa Professor of Materials at the University of California, Santa Barbara, on February 12.

The 2013 **Dow Lecture**, "Electrical Properties in Polymer Nanocomposites," was presented on February 26 by Karen I. Winey, professor of materials science and engineering at the University of Pennsylvania.

New Structures Self-Assemble in Synchronized Dance

APPLICATION OF FUTURE TECHNOLOGIES COULD BE IN MEDICINE, CHEMISTRY, AND ENGINEERING

With self-assembly guiding the steps and synchronization providing the rhythm, a new class of materials forms dynamic, moving structures in an intricate dance.



Erik Luijten (above) and collaborators have demonstrated Janus spheres that synchronize their movements as they self-assemble into a spinning microtube.

Researchers from McCormick's materials science department and the University of Illinois have demonstrated tiny spheres that synchronize their movements as they self-assemble into a spinning microtube. Such in-motion structures, a blending of mathematics and materials science, could open a new class of technologies with applications in medicine, chemistry, and engineering.

The results were published November 22 in *Nature*.

"The world's concept of self-assembly has been to think of static structures — something you would see in a still image," said Steve Granick, Founder Professor of Engineering at the U. of I. and a co-leader of the study. "We want shape-shifting structures. Structures where a photograph doesn't tell you what matters. It's like the difference between a photograph and a movie."

The researchers used tiny particles called Janus spheres, named after the Roman god with two faces, which Granick's group developed and previously demonstrated for self-assembly of static structures. In this study, one half of each sphere is coated with a magnetic metal. When dispersed in solution and exposed to a rotating magnetic field, each sphere spins in a gyroscopic motion. They spin at the same frequency but all face a different direction, like a group of dancers in a ballroom dancing to the same beat but performing their own steps.

As two particles approach one another, they synchronize their motions and begin spinning around a shared center, facing opposite directions, similar to the way a couple dancing together falls in step looking at one another.

"They are both magnetized, which causes them to attract each other, but because they're moving, they have to move in sync," said Erik Luijten, professor of materials science and engineering and of applied mathematics at McCormick. He co-led the research with Granick.

Soon, the pairs and clusters of dancing spheres assemble themselves into a microtube — a long, hollow structure. The entire tube spins, even as each individual sphere continues its motion as well, like dancers in a line dance completing their individual steps as the line moves.

"It's spontaneous. We don't force it to form," said U. of I. graduate student Jing Yan, the first author of the paper. "We saw that during the self-assembly process, the synchronization also happens. If you look at the spheres, every one is doing a different thing. Only when they come in close contact will they do something cooperatively. The two concepts are intricately related in this system."

Now that the researchers have detailed the delicate choreography of synchronization and self-assembly, they hope to explore applications for this new class of moving structures. One potential application of a dynamic, self-assembled microtube is to transport and release cargo. A particle or collection of molecules could be encapsulated in the tube and transported to a different location. Then, the tube can be disintegrated, releasing the cargo at a target point.

"We're looking for the new applications that people haven't dreamt up yet because they didn't have the capability," said Granick, a professor of materials science and engineering.

"Traditionally in self-assembly, you make a specific building block that will organize into a specific structure. If you want a different structure you have to make a different building block. Here, with one building block, we can control the structure by exploiting the synchronization effect." *Erik Luijten*

Next, the researchers are working to further understand the properties governing synchronized self-assembly and ways to guide it for functionality, such as manipulating the structures with an electrical or magnetic field. They also plan to explore directing the Janus spheres to synchronized self-assembly of other shapes and structures, allowing even more applications.

"Traditionally in self-assembly, you make a specific building block that will organize into a specific structure," Luijten said. "If you want a different structure you have to make a different building block. Here, with one building block, we can control the structure by exploiting the synchronization effect."

The U.S. Army Research Office, the Department of Energy and the National Science Foundation supported this work.

U. of I. research scientist Sung Chul Bae and Northwestern graduate student Moses Bloom are co-authors of the paper.

"For to be a Farmer's Boy" by Winslow Homer

based physically at Northwestern. The center will be staffed by a senior scientist and two postdoctoral fellows and will act as an umbrella for all research and educational activities related to the conservation science partnership.

"I am thrilled that what we have accomplished over the past eight years has been recognized as valuable. Now we are ready to build upon this solid foundation to offer our expertise to others beyond our institutions." *Katherine T. Faber*

Interested parties from museums and cultural institutions will be required to submit proposals for merit review to study objects in their own collections or perform object-inspired research. Faber and Casadio expect three to five major projects and up to 10 minor projects to be carried out each year by researchers from inside and outside Northwestern and the Art Institute.

"Bathers by a River" by Henri Matisse

"The new center will be built on the solid foundation of collaborations between the Art Institute of Chicago and Northwestern University that have long been nurtured by the enlightened support of the Mellon Foundation," said Douglas Druick, president and Eloise W. Martin Director of the Art Institute of Chicago.

"As the first such initiative in the United States, the center will inspire a new model for research partnerships between museums and academia, and we are especially excited by the promise of bringing museum professionals, researchers, and students together to contribute original and groundbreaking research to their respective fields," he said. "We remain exceedingly grateful to the Mellon Foundation for the important scholarship made possible by their support of these key partnerships and look forward to sharing our findings with the broadest audiences possible in the coming years."

"The new center promises to enhance research and education on works of cultural heritage with new partners at museums and cultural institutions who would benefit from the scientific tools and expertise we collectively offer," Northwestern Provost Daniel Linzer said.

"I have appreciated the many discoveries this highly productive partnership in conservation science has made possible and look forward to future findings as the collaboration expands its scope," he said.

Linzer noted the partnership and its center address all four core areas of the University's strategic plan: to discover creative solutions, integrate learning and experience, connect our community, and engage with the world.

For more information on the Center for Scientific Studies in the Arts, go to http://www.nuaccess.northwestern.edu.

"A Sunday on La Grande Jatte - 1884" by Georges Seurat

Brief summaries of some of the groundbreaking discoveries resulting from the Northwestern-Art Institute partnership follow:

"Head of a Woman (Fernande)" by Pablo Picasso. Findings from a study analyzing the metal alloys of Modern sculptures are part of the Art Institute's current major exhibition "Picasso and Chicago" (Feb. 20 to May 12). A research team determined that many of the museum's Picasso sculptures are made of high-zinc brass alloys, a fact that enabled them to trace the works to the Valsuani foundry in Paris.

"Fernande," on the other hand, has a low-zinc bronze composition that is more typical of sand-cast sculptures, but the piece is unlike those cast at the Rudier foundry. The search for its unknown casting foundry is one of the open questions the new Center for Scientific Studies in the Arts hopefully will be able to address by extending the alloy study to a wider range of collections.

"Bathers by a River" by Henri Matisse. Researchers from Northwestern's Department of Electrical Engineering and Computer Science developed imaging technology to colorize archival black-and-white photographs of early versions of this painting. This provided insights into Matisse's working methods and the coloristic development of this masterpiece over time and was part of the Art Institute's 2010 show "Matisse: Radical Invention, 1913-1917."

"For to be a Farmer's Boy" by Winslow Homer. Conservators discovered the painting's white skies were originally painted in unstable red and orange dyes that have almost completely faded. A team including Northwestern chemists has been working to determine exactly what the original colors were. The findings were featured in the museum's 2008 exhibition "Watercolors by Winslow Homer: The Color of Light."

"A Sunday on La Grande Jatte - 1884" by Georges Seurat. The luminous yellow in this painting began to change within years of Seurat's completing the masterpiece, but no one knew why. Scientists determined that exposure to a humid climate and burning coal caused the darkening of the zinc yellow pigment used by Seurat.

"Sketch of Margaret Sloane, Looking Right" by Mary Cassatt. A research team removed tiny colored flecks from this pastel study and examined them using a highly sensitive technique called surface-enhanced Raman spectroscopy. The researchers were able to detect and identify organic pigments that could be matched to pastel sticks in Mary Cassatt's paint box.

Department News

FACULTY NEWS

Mike Bedzyk *and* ***John Torkelson*** were named fellows of the American Association for the Advancement of Science (AAAS).

Morris Fine was profiled in a recent *TMS Materials Technology* article. He was honored in March at a special symposium at the TMS 2013 Annual Meeting in San Antonio, Texas.

Mark Hersam received the Bette and Neison Harris Chair in Teaching Excellence beginning on September 1, 2012. He was also named a 2012 Fellow of the American Physical Society.

Jiaxing Huang has received the 2013 Outstanding Young Manufacturing Engineer Award from the Society of Manufacturing Engineers. In addition, Huang's inspiration for crumpled graphene — crumpled paper in a trashcan — was cited by *Chemistry and Industry* magazine as an example of scientific creativity.

An article by ***Derk Joester***'s group describing the role of growth factors in calcite crystal growth was highlighted as an editor's choice in the November issue of *Science*. Post-doctoral fellow ***Regina Knapp*** was first author of the original article, which was published in the *Journal of the American Chemical Society*.

Erik Luijten, graduate student ***Wei Qu***, and collaborators at Johns Hopkins University have discovered how to control the shape of nanoparticles that move DNA through the body and have shown that the shape of these carriers is key to how they work. The study was published in *Advanced Materials* and featured on a podcast by the National Academy of Engineering.

Tobin Marks has been selected to receive the Gabor A. Somorjai Award for Creative Research in Catalysis from the American Chemical Society (ACS). He will receive the award at the ACS meeting in April.

Chad Mirkin has been selected to receive the 2013 Walston Chubb Award for Innovation from Sigma Xi.

Monica Olvera de la Cruz has been elected to the Basic Energy Advisory Committee of the U.S. Department of Energy.

In October, ***David Seidman*** visited Tel Aviv University as Mortimer and Raymond Sackler Lecturer.

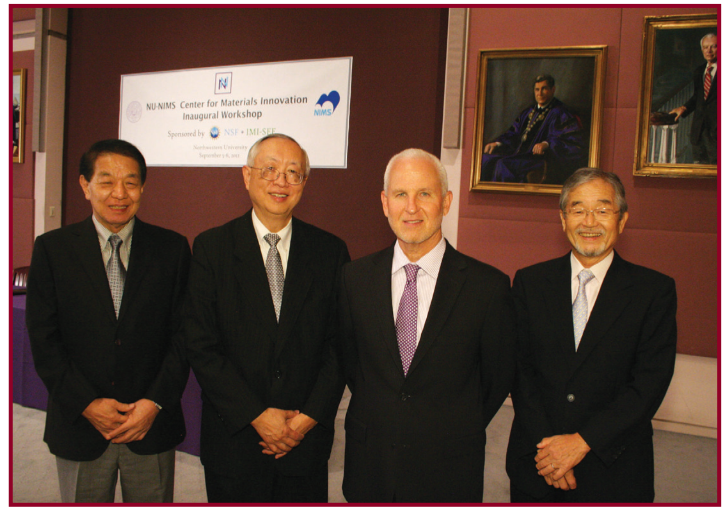
Kenneth Shull will present a weeklong series of lectures June 17-21 as the 2013 Turner J. Alfrey Visiting Professor at the Michigan Molecular Institute and will make daylong site visits to Dow and Dow Corning the following week.

Peter Voorhees has been chosen as a fellow of the Minerals, Metals and Materials Society (TMS) class of 2013 for "seminal studies on the thermodynamics and kinetics of phase transformations." He was also named 2012 Teacher of the Year by the materials science department.

STUDENT NEWS

A group of materials science undergraduates won first prize in the ASM Materials Education Foundation's 2012 Undergraduate Design Competition for their project, "TRIP-150 Blast Protection Alloy," in which they created a computational design for an improved blast-resistant steel. Team members ***Ruilong Ma***, ***Wisaruth Maethasith***, ***Ben Richardson***, ***Eric Schwenker***, and ***Zhibo Zhao*** completed the project as part of their MatSci 390 coursework under the guidance of Zack Feinberg (PhD '12, Olson) and Greg Olson. The team received an award at the ASM Leadership Awards Luncheon at the MS&T 12 conference in Pittsburgh, Penn.

Global Materials Research Center Established



Northwestern and the National Institute for Materials Science (NIMS) in Japan have established a joint research center to address global materials-related challenges in energy, environment, health, and security. The center will be based at Northwestern and co-directed by R.P.H. Chang of the materials science department and alum Yoshio Aoki, director of NIMS' External Collaboration Division. Pictured at the September 6 ceremony, from left to right, are Aoki, Chang, Northwestern President Morton Schapiro, and NIMS President Sukekatsu Ushioda.

Jiayan Luo (Huang) received a Graduate Student Gold Award and ***Jeff Doak*** (Wolverton) won a student presentation award at the Fall 2012 MRS meeting.

Post-doctoral researcher ***James Saal*** (Wolverton) has received a Young Leader Award from TMS and will attend the March meeting in San Antonio.

Postdoctoral fellow ***Ivan Blum*** (Seidman) won the $200 first-place prize in a poster competition organized in December by the student group Tomographers Anonymous; the competition was sponsored by Dow. Graduate student ***Anthony Johnson*** (Voorhees) won the $100 second-place prize.

ALUMNI NEWS

Jennifer Andrew (BS '02), assistant professor of materials science and engineering at the University of Florida, received a 2012 NSF CAREER award to study "Structure-property relationships arising from interfacial coupling in bi-phasic ceramic nanocomposites."

Ampika Bansiddhi (PhD '09) and thesis adviser ***David Dunand*** were awarded an excellent thesis award — within the top 10 of 150 theses submitted — by the National Research Council of Thailand.

Mariana Bertoni (PhD '07, Mason) has accepted a position as assistant professor of electrical, computer, and energy engineering at Arizona State University.

Yongwoo Kwon (PhD '08, Voorhees) began a new position at Hongik University on March 1.

Justin Scott (PhD '11, Dunand) has joined TMS as technical project leader, leading the development of an integrated approach to key TMS strategic technology projects, including integrated computational materials engineering, advanced manufacturing, and energy materials.

Boris Vuchic (PhD '95, Marks) has generously provided funding toward support of the new Battery Lab (BatLab), the first component of the Energy Materials Lab.

Materials Science Alumni Awards

ALUMNI CELEBRATION: THURSDAY, MAY 16

At the 2013 Alumni Celebration on Thursday, May 16, the Department of Materials Science will honor two outstanding alumni with the Distinguished Career Achievement Award for Alumni of Materials Science and Engineering and the Early Career Achievement Award for Alumni of Materials Science and Engineering. This year's honorees spoke to us about their McCormick experience and how it has helped shape their careers.

Pulckel M. Ajayan (PhD '89)
Benjamin M. and Mary Greenwood Anderson Professor of Engineering, Rice University
Distinguished Career Achievement Award winner

Ajayan's research interests include synthesis and structure-property relations of nanostructures and materials science and applications of nanomaterials. He is one of the pioneers in nanotechnology and specifically the field of carbon nanotubes. He has published one book and 450 journal papers, many in high impact journals.

1) Describe how your experience in McCormick's MSE department shaped or affected your career.
Coming to the MSE department at Northwestern was a major milestone in my life. I was going abroad from India for the first time and I was very anxious for various reasons. MSE was very welcoming and I learned quickly that I could excel if I worked hard. I had a great time in the MSE department from several points of view — learning, research, relationships, and friendships. The four years I spent there was perhaps the most significant time in my life in terms of formulating my thoughts and goals for my professional and personal life. I developed my confidence and basic love for science there. My professional life clearly took shape at Northwestern.

2) What are some of your most memorable classes/experiences/moments from your McCormick MSE years?
A couple classes still remain in memory. The stereology class I took from the late Professor John Hilliard and the elasticity course I took from Professor John Dundurs (in civil engineering) remain clearly in memory. Professor Laurie Marks (my adviser — I was his second student officially, but the first to graduate) was a great mentor, and I am obliged to him in many ways. His style, approach to science, and even some mannerisms (strangely enough) have remained with me to date.

One thing I remember vividly is my first year in Chicago. It was so biting cold (and remember, I had just come from India directly) that I thought I would die for sure by the end of winter. On the other hand, I developed some deep friendships with fellow graduate students, which remain strong to this day.

3) What have been your most memorable or proudest career moments? Your most challenging?
I think I have been lucky to be at the right places (at the right times) throughout my career. After my graduate study I decided to go to Japan to pursue a post-doctoral fellowship at NEC Corporation in Tsukuba. This happened to be an amazing choice, since within a few months of my arrival, our group (headed by Sumio Iijima) initiated the pioneering works on carbon nanotubes, and I was fortunate enough to be part of some of those early breakthroughs. Several of the early works on nanotubes, published in journals such as *Nature*, had a defining impact on my career and were some of the proudest moments.

The most challenging thing, I would say, was finding a permanent academic job back in the U.S. after a long postdoctoral stay in Japan and Europe — although I should say I had the greatest time during these early days of my career. The experience and outlook in life I gained during my stays in these international locations were simply irreplaceable. I think these international stays gave me a much broader perspective and more liberal approach to doing science as well as living my life.

4) What advice would you give to current MSE students about to begin their careers?
Motivation and passion for doing things are most important. Identify what is important for you early on and pursue that. Don't follow trends or what may appear to be rewarding for the time being. Make rational decisions. Be honest to yourself. Think outside of the box. And from my experience, I suggest traveling the world and working abroad (at least for a brief period) to develop a broader perspective both in your career development and personal life. And of course, don't forget to enjoy life during your graduate life — this is the best time of your life.

Beth Dickey (PhD '97)
Professor and director of graduate programs, Department of Materials Science and Engineering; associate director, Analytical Instrumentation Facility
North Carolina State University
Early Career Achievement Award winner

Dickey joined NCSU's Department of Materials Science and Engineering in 2011. Prior to NCSU, she was a professor of materials science and engineering and an associate director of the Materials Research Institute at Penn State University. A primary focus of Dickey's research is on developing processing-structure-property relationships for material systems in which the macroscopic physical properties (mechanical, electrical, thermal, etc.) are governed by grain boundaries or internal interfaces.

1) Describe how your experience in McCormick's MSE department shaped or affected your career.
I consider my experiences in McCormick's MSE department to be the cornerstone of my professional career. The department maintained a high standard for and appreciation of scientific rigor and elegance. Moreover, there was a high degree of mutual respect for the scientific contributions of everyone in the department. These attributes are hallmarks of a truly outstanding organization.

2) What are some of your most memorable classes/experiences/moments from your McCormick MSE years?
One of my most memorable experiences was pulling an "all-nighter" doing research and grading lab reports for Professor Buckley Crist's X-ray diffraction course, and walking out to a stunningly vibrant coral-colored sunrise over Lake Michigan.

My favorite classes were Professor Peter Voorhees' thermodynamics and phase transformation classes, and I still have an elusive dream of understanding thermodynamics as well as he does!

3) What have been your most memorable or proudest career moments?
My proudest moments are when I hood my own PhD advisees during their graduation ceremonies.

4) What advice would you give to current MSE students about to begin their careers?
Persevere!

Best of Both Worlds: Hybrid Approach Sheds Light on Crystal Structure Solution

Understanding the arrangement of atoms in a solid — one of solids' fundamental properties — is vital to advanced materials research. For decades, two camps of researchers have been working to develop methods to understand these so-called crystal structures. "Solution" methods, championed by experimental researchers, draw on data from diffraction experiments, while "prediction" methods of computational materials scientists bypass experimental data altogether.

While progress has been made, computational scientists still cannot make crystal structure predictions routinely. Now, drawing on both prediction and solution methods, McCormick researchers have developed a new code to solve crystal structures automatically and in cases where traditional experimental methods struggle.

Key to the research was integrating evidence about solids' symmetry — the symmetrical arrangement of atoms within the crystal structure — into a promising computational model.

"We took the best of both worlds," said Chris Wolverton, professor of materials science and engineering and an expert in computational materials science. "Computational materials scientists had developed a great optimization algorithm, but it failed to take into account some important facts gathered by experimentalists. By simply integrating that information into the algorithm, we can have a much fuller understanding of crystal structures."

The resulting algorithm could allow researchers to understand the structures of new compounds for applications ranging from hydrogen storage to lithium-ion batteries.

Chris Wolverton

A paper describing the research, "A Hybrid Computational-Experimental Approach for Automated Crystal Structure Solution," was published November 25 in *Nature Materials*.

While both computational and experimental researchers have made strides in determining the crystal structure of materials, their efforts have some limitations. Diffraction experiments are labor-intensive and have high potential for human error, while most existing computational approaches neglect potentially valuable experimental input.

When computational and experimental research is combined, however, those limitations can be overcome, the researchers found.

In their research, the authors seized onto an important fact: that while the precise atomic arrangements for a given solid may be unknown, experiments have revealed the symmetries present in tens of thousands of known compounds. This database of information is useful in solving the structures of new compounds.

The researchers were able to revise a useful model — known as the genetic algorithm, which mimics the process of biological evolution — to take those data into account.

Bryce Meredig (PhD '12) was the paper's lead author.

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