New Center for Materials Research to Advance Innovation

NORTHWESTERN-LED CONSORTIUM TO HELP ANCHOR CHICAGO'S EFFORT TO BECOME HIGH-TECH HUB

A Chicago-based consortium led by Northwestern University has been awarded $25 million over five years from the National Institute of Standards and Technology (NIST), an agency of the U.S. Department of Commerce, to establish a new center of excellence for advanced materials research.

The Center for Hierarchical Materials Design (CHiMaD) will focus on developing the next generation of computational tools, databases and experimental techniques to enable the design of novel materials, one of the primary goals of the Obama administration’s Materials Genome Initiative (MGI).

Other members of the CHiMaD consortium include the University of Chicago, the Northwestern-Argonne Institute of Science and Engineering (a partnership between Northwestern and the Department of Energy’s Argonne National Laboratory) and the Computation Institute (a partnership between the University of Chicago and Argonne). Only one award was made in the national competition.

“The Center for Hierarchical Materials Design will serve as an anchor for the city of Chicago’s effort to become an international hub for high-tech innovation,” said Peter W. Voorhees, one of three co-directors of the new center. Voorhees is the Frank C. Engelhart Professor of Materials Science and Engineering in the McCormick School of Engineering and Applied Science. “Building on a long history of collaborations with NIST researchers, the center will bring together the next generation of state-of-the-art computational methods, curated materials databases and novel integrated experimental methods to design new materials,” he said.

The other co-directors are Gregory B. Olson, the Walter P. Murphy Professor of Materials Science and Engineering, and Juan de Pablo, the Liew Family Professor in Molecular Engineering at the University of Chicago.

The consortium also plans to work closely with the pioneering materials design company QuesTek Innovations, a small business spin-off of Northwestern, co-founded by Olson; ASM International, a well-known professional society of materials scientists; and Fayetteville State University. A strong cast of supporting industrial collaborators from across the nation will further enhance the mission of the CHiMaD consortium.

Designing materials employs physical theory, advanced computer models, vast materials properties databases and complex computations to accelerate the design of a new material with specific properties for a particular application — perhaps an extremely tough, light-weight composite for automobile bodies or a biocompatible cell scaffold for medicine. This approach stands in contrast to the traditional trial-and-error method of materials discovery.

The new center’s work is expected to encompass both “hard” (inorganic) and “soft” (organic) advanced materials in fields as diverse as self-assembled biomaterials, smart materials for self-assembled circuit designs, organic photovoltaic materials, advanced ceramics, and metal alloys.

CHiMaD will focus these techniques on a particularly difficult challenge, the creation of novel “hierarchical materials.” Hierarchical materials exploit distinct structural details at various scales from the atomic on up to achieve special, enhanced properties. An example in nature of a hierarchical material is bone, a composite of mineral and protein at the molecular level assembled into microscopic fibrils that in turn are assembled into hollow fibers and on up to the highly complex material that is “bone.”
Dear friends: First let me express my thanks for the generous donations from faculty, friends, and alumni to the Johannes and Julia Randall Weertman Graduate Student Fellowship Fund. Fundraising for this fellowship was announced at the October 4 Weertman Festival. Contributions now total nearly $120,000, exceeding the $100,000 phase 1 goal. This is unprecedented in McCormick history. Our goal in phase II of the campaign is to raise another $120,000 toward the $1 million needed for a full-endowed fellowship. Thank you for your support in honor of these two remarkable scholars who contributed so much to the department and to many of us individually.

I’m very pleased to share some particularly exciting news, featured as the cover story. A Northwestern-led consortium was recently named the recipient of a $25 million NIST-funded award to establish a new Center for Hierarchical Materials Design (CHiMaD). This center will provide the primary foundation for the national Materials Genome Initiative and will be co-directed by materials science faculty Peter Voorhees and Greg Olson, along with Juan de Pablo from the University of Chicago.

Spring is a time of renewal and change and that is certainly true for the department this season. It is with mixed emotions that I share the news that Katherine Faber has accepted a position on the faculty of Caltech, where her husband Thomas Rosenbaum has been named incoming president. During her tenure at Northwestern, Kathy has served in many leadership roles, including associate dean, department chair, and most recently as co-director of the Northwestern University-Art Institute of Chicago Center for Scientific Studies (NU-ACCESS). We wish them well and hope to celebrate Kathy’s contributions to MSE at this year’s annual Alumni Celebration on May 15.

Other news includes the ongoing establishment of our Energy Materials Lab on the third floor of Cook Hall. Two component laboratories of the new facility, the battery and photovoltaics laboratory, now house new equipment that will soon be available to students. We are very grateful for the alumni contributions to this new facility and are now planning a third component that will feature 3-D printing of hybrid materials in architectures used for studying phenomena such as energy conversion and storage.

Please join us on Thursday, May 15 for the annual Hilliard Symposium and the Alumni Celebration Banquet. Also, mark your calendars for Oct. 20-22, when Dan Shechtman, 2011 Nobel Laureate in Chemistry, will give the Jerome B. Cohen Lecture Series and a Dean’s Seminar.

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

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2013-14 MATERIALS SCIENCE LECTURES

Mike Bedzyk, Ian Robinson, and Morris Fine
The 2013 Morris Fine Lecture, “Nanoparticle Structure Using Coherent X-ray Diffraction,” was given by Ian Robinson, professor at the University College London, on November 19.

Mike Bedzyk, Harry Atwater, and Mark Hersam

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SUPPORT MATERIALS SCIENCE
Generous alumni support has enabled endowment of the Fine and Cohen lectures, established the Weertman Graduate Fellowship Fund, enhanced our lab and computing facilities, and created summer support for undergraduate research.

Please remember to designate the Department of Materials Science and Engineering when you give to Northwestern.

UPCOMING LECTURES

Jerome B. Cohen Lectures
APRIL 15 and 17
Steve Pennycook, Department of Materials Science and Engineering, University of Tennessee

Hilliard Symposium
MAY 15
Andrea Hodge, Department of Aerospace and Mechanical Engineering, University of Southern California

Dow Lecture
MAY 20
Jennifer A. Lewis, Hansjörg Wyss Professor of Biologically Inspired Engineering, Harvard School of Engineering and Applied Sciences
Detecting Chemicals, Measuring Strain with a Pencil and Paper

CLASSROOM PROJECT EVOLVES INTO JOURNAL PAPER ABOUT SURPRISING APPLICATIONS FOR EVERYDAY OBJECTS

Sometimes solving a problem doesn’t require a high-tech solution. Sometimes, you have to look no farther than your desktop.

Three students from the Department of Materials Science and Engineering—an undergraduate, a master’s student, and their teaching assistant—have proven that pencils and regular office paper can be used to create functional devices that can measure strain and detect hazardous chemical vapors.

A paper describing their findings, “Pencil Drawn Strain Gauges and Chemiresistors on Paper,” was published January 22 in Scientific Reports, an open-access journal from the Nature Publishing Group.

The project originated in fall 2011 in McCormick’s Introduction to Conducting Polymers course (MSE 337) during a discussion about the conductive properties of graphene, a one-atom thick layer of carbon that can be parsed from regular pencil lead. (A misnomer, pencil “lead” actually comprises graphite in a clay binder.)

“When you draw a line on a piece of paper, the graphite may shed numerous graphene sheets,” said Jiaxing Huang, associate professor of materials science and engineering.

“A student asked, ‘Can we use that graphene for something?’ That started an exploration of what pencil traces can do.’”

One team of students—including lead authors Cheng-Wei Lin (MS materials science ’13) and Zhibo Zhao (BS materials science ’13)—started by measuring the conductivity of a pencil trace on paper, then used the traces to create a rudimentary electrode. They learned that curling the paper in one direction increased the trace’s conductivity by compressing the conductive graphene particles. Curling the paper in the other direction loosened the graphene network and decreased conductivity.

The students then turned to the traces of a bendable toy pencil. (These novelty pencils are flexible because the graphite is mixed not with clay, but with a polymer binder.) Again, conductivity could be increased and decreased by manipulating the paper, but the students found it also was affected by the presence of volatile chemical vapors, such as those from toxic industrial solvents.

When the chemical is present, the polymer binder absorbs the vapors and expands, pushing the graphene network apart and decreasing conductivity. The conductivity decreased the most in the presence of vapors that are more readily absorbed by the polymer binder.

These types of chemical sensor—also called “chemiresistors”—are key elements in “electronic noses” for detecting toxic chemical vapors. In creating chemiresistors, researchers often use more expensive materials, such as networks of carbon nanotubes or metal nanoparticles, and need to disperse them in polymer matrix to form a network.

“Now our students showed that this can be done simply with a pencil and paper—and it works,” Huang said. “This is a great example showing how curiosity leads to innovative work.”

In addition to Lin, Zhao, and Huang, Jaemyung Kim (PhD materials science ’13), who served as teaching assistant for the course, co-authored the paper.
Nature builds flawless diamonds, sapphires and other gems. Now a Northwestern University research team is the first to build near-perfect single crystals out of nanoparticles and DNA, using the same structure favored by nature.

“Single crystals are the backbone of many things we rely on — diamonds for beauty as well as industrial applications, sapphires for lasers and silicon for electronics,” said nanoscientist Chad A. Mirkin. “The precise placement of atoms within a well-defined lattice defines these high-quality crystals.

“Now we can do the same with nanomaterials and DNA, the blueprint of life,” Mirkin said.

His research group developed the “recipe” for using nanomaterials as atoms, DNA as bonds and a little heat to form tiny crystals. This single-crystal recipe builds on superlattice techniques Mirkin’s lab has been developing for nearly two decades.

In this recent work, Mirkin, an experimentalist, teamed up with Monica Olvera de la Cruz, a theoretician, to evaluate the new technique and develop an understanding of it. Given a set of nanoparticles and a specific type of DNA, Olvera de la Cruz showed they can accurately predict the 3-D structure, or crystal shape, into which the disordered components will self-assemble.

Mirkin is the George B. Rathmann Professor of Chemistry in the Weinberg College of Arts and Sciences and a professor of medicine, chemical and biological engineering, biomedical engineering and materials science and engineering. Olvera de la Cruz is a Lawyer Taylor Professor and professor of materials science and engineering.

A single crystal has order: its crystal lattice is continuous and unbroken throughout. The absence of defects in the material can give these crystals unique mechanical, optical and electrical properties, making them very desirable.

In the Northwestern study, strands of complementary DNA act as bonds between disordered gold nanoparticles, transforming them into an orderly crystal. The researchers determined that the ratio of the DNA linker’s length to the size of the nanoparticle is critical. The ratio affects the energy of the faces of the crystals, which determines the final crystal shape. Ratios that don’t follow the recipe lead to large fluctuations in energy and result in a sphere, not a faceted crystal, Olvera de la Cruz explained. With the correct ratio, the energies fluctuate less and result in a crystal every time.

“If you get the right ratio it makes a perfect crystal — isn’t that fun?” Olvera de la Cruz said. “That’s the fascinating thing, that you have to have the right ratio. We are learning so many rules for calculating things that other people cannot compute in atoms, in atomic crystals.”

To achieve a self-assembling single crystal in the lab, the research team reports taking two sets of gold nanoparticles outfitted with complementary DNA linker strands. Working with approximately 1 million nanoparticles in water, they heated the solution to a temperature just above the DNA linkers’ melting point and then slowly cooled the solution to room temperature, which took two or three days. The very slow cooling process encouraged the single-stranded DNA to find its complement, resulting in a high-quality single crystal approximately three microns wide.

In addition to Mirkin and Olvera de la Cruz, authors of the paper are Evelyn Auyeung (first author), Ting I. N. G. Li, Andrew J. Senesi, Abrin L. Schmucker and Bridget C. Pals, all from Northwestern.
Atomically Thin Device Promises New Class of Electronics

The isolation over the past decade of atomically thin two-dimensional crystals — such as graphene, a single-atom-thick carbon lattice — has prompted researchers to stack two or more distinct two-dimensional materials to create high-performance, ultrathin electronic devices. While significant progress has been made in this direction, one of the most important electronic components — the p-n junction diode — has been notably absent.

Among the most widely used electronic structures, the p-n junction diode forms the basis of a number of technologies, including solar cells, light-emitting diodes, photodetectors, computers, and lasers.

In addition to its novel electronic functionality, the p-n heterojunction diode is also highly sensitive to light. This attribute has allowed the authors to fabricate and demonstrate an ultrafast photodetector with an electronically tunable wavelength response.

The research, “Gate-Tunable Carbon Nanotube-MoS2 Heterojunction p-n Diode,” was published October 21 in the Proceedings of the National Academy of Sciences.

In addition to Hersam, leading the research were Lincoln Lauhon, professor of materials science and engineering, and Tobin Marks, Vladimir N. Ipatieff Professor of Catalytic Chemistry and (by courtesy) Materials Science and Engineering.

Other authors of the paper are postdoctoral researchers Vinod Sangwan, Chung-Chiang Wu, and Pradyumna Prabhunirasha, and graduate students Deep Jarwala and Michael Geier, all of whom are affiliated with Northwestern University. This research was supported by the National Science Foundation-funded Materials Research Science and Engineering Center (MRSEC) and the Office of Naval Research.

Weertman Graduate Fellowship Fund

We thank all those whose generous donations have enabled the establishment of the Johannes and Julia Randall Weertman Graduate Fellowship Fund. If you would like to contribute, please contact Ben Porter, McCormick development director, at 847-467-5212 or at b-porter@northwestern.edu.

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- Mr. Willem Weertman

"Professor" indicates Northwestern faculty affiliation only; many others listed are professors at other institutions.
**FACULTY NEWS**

**Yip-Wah Chung** and J. Jane Wang (mechanical engineering) were co-chief editors of the new, six-volume edition of the *Springer Encyclopedia of Tribology*, published in hardcopy and online.

**Katherine Faber** co-organized a session, "Reconstructing and Deconstructing Paintings: Innovations At and Below the Surface" at the 2014 Annual Meeting of the American Association for the Advancement of Science (AAAS).

**Mark Hersam** was selected as the ACS:PMSE Arthur K. Doolittle Award for a talk at the spring 2013 ACS Meeting. He was also named director of the Northwestern Materials Research Center in September, succeeding **Monica Olvera de la Cruz**, who led the center for seven years.

**Erik Luijten** was named an American Physical Society fellow for “the development of algorithms that greatly accelerate the simulation of condensed-matter systems and for their application in elucidating the behavior of a broad range of self-assembly phenomena.”

**Chad Mirkin** was named a fellow of the National Academy of Inventors, an honorary fellow of the Chinese Chemical Society, an honorary professor at ShanghaiTech University in China, and the recipient of the Vittorio de Nora Award from the Electrochemical Society.

**David Seidman** was named a fellow of the American Association for the Advancement of Science and a 2014 AIME honorary member, nominated by TMS for “pioneering seminal research and development of field microscopy and atom-probe tomography to study basic scientific and technological problems in materials science and engineering.” He was also named the ASM Edward DeMille Campbell Memorial Lecturer for 2015.

**Sam Stupp** will receive the International Award from the Japan Polymer Society in May. The Querrey Simpson Charitable Foundation has made two gifts, totaling $25 million, to Northwestern University in support of the University’s research efforts applying nanotechnology to regenerative medicine. In recognition of the new gift, the Institute for BioNanotechnology in Medicine (IBNAM), led by **Sam Stupp**, will be renamed the Louis A. Simpson and Kimberly K. Querrey Institute for BioNanotechnology in Medicine.

**Julia Weertman** has been chosen to receive the American Association of Engineering Societies (AAES) John Fritz Medal “for her exceptional contributions to our understanding of failure in materials and for inspiring generations of young women to pursue careers in the science and engineering disciplines.” She has been named a fellow of the Materials Research Society. Professor Weertman is recognized “for pioneering contributions in materials research; and seminal and ground-breaking work on dislocations, fatigue, small-angle x-ray diffraction, and nanostructured materials.”

**Bruce Wessels** was named a fellow of the Optical Society of America “for pioneering research in epitaxial wide gap semiconductors and devices, and ferroelectric oxides for opto-electronic and electro-optic applications.”

**Christopher Wolverton** was recently named the 12th recipient of the Martin E. and Gertrude A. Walder Award for Research Excellence. Established by Joseph A. Walder, M.D. in 2002 and given annually by the provost, the award recognizes excellence in research at Northwestern.

**STUDENT NEWS**


Graduate students **Deniz Alpay** and **Lingxuan (Betty) Peng** presented materials science demos at the Career Day for Girls on February 22. More than 360 girls attended the 41st annual event for middle school and high school girls.

Junior **Edward Pang** has been awarded a Barry M. Goldwater Scholarship.

PhD student **Michael Rawlings** (Dunand) recently won the “crowd favorite” poster and second place in the research poster competition at the UT Energy Forum for his work on creep-resistant steel, which could lead to higher operating temperatures, higher efficiencies, and lower CO2 emissions from fossil fuel power plants.

Senior **Sergio Williams**, a member of the Northwestern University Microgravity Team (NUMT), took part in the NASA Reduced Gravity Flight Opportunity Program at the Johnson Space Center.

Graduate students **Karl Hujsak**, **Andrew Mannix**, **Samuel Miller**, **Christopher Serrano**, **Ashwin Shahani**, **Madeleine Wright**, and **Chyi-Huey Joshua Yeh** were awarded National Science Foundation Graduate Research Fellowships; **Sarah Clark**, **Michael Knudson**, **Garrett Lau**, **Herman Novikov** and **Lindsay Oakley** received honorable mention.
Materials Science Alumni Honored

At the 2014 Alumni Celebration on Thursday, May 15, the Department of Materials Science and Engineering 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.

ALFRED CROSBY (PhD '00)
Professor of polymer science and engineering at the University of Massachusetts Amherst; Early Career Achievement Award winner

Crosby’s research interests include mechanics of hierarchical structures, polymer adhesion, and biomimetic materials. He has received an NSF CAREER Award, the ARO Young Investigator Award, the Adhesion Society Outstanding Young Scientist Award, and the Rohm & Haas New Faculty Award.

Describe how your experience in Northwestern's MSE department shaped or affected your career.
Northwestern’s MSE department provided an incredible launching pad for my career. Of course, the classes were excellent, but the real difference was the collegiality among the faculty and students and the balance between the pursuit of fundamental materials science and materials-enabled technology. There was an obvious passion that existed within the department and it was contagious. I couldn’t stop thinking about my research and the whole field. My wife can fully attest to this!

What are some of your most memorable classes/ experiences/moments from your NU MSE years?
Julia Weertman’s class on dislocation mechanics. I loved it! I also learned so much from the evening discussions with Ken Shull in his office about research and different ways to think about adhesion. He is a fantastic teacher, mentor, and scientist. The Shull Group dinners showed me the importance of creating a strong community and how it can translate into creativity in the lab. The daily discussions with group mates, especially Cynthia Flanigan and Pete Drzal, are very memorable. I learned so much from all of the constant debate and idea generation. At my dissertation defense, I loved seeing my family and friends in the same room with my PhD committee and having the opportunity to share my thoughts and work over the previous four years.

What have been your most memorable or proudest career moments? Your most challenging?
My top three most memorable moments were: the acceptance of my first paper as assistant professor, my first Crosby group dinner, and having my research recognized by CNN Money/Fortune magazine as a breakthrough technology of 2012. One challenging moment was navigating my group’s financial situation when a company pulled committed funds. This created some tense times and creative management opportunities. It was quite a learning experience.

What advice would you give to current MSE students about to begin their careers?
Don’t underestimate the power of reflection and internal thought in the process of science and technology development. Allowing your mind to explore ridiculous dreams can stimulate fruitful discussions and new research findings if you call upon sound science and engineering principles.

Describe how your experience in Northwestern’s MSE department shaped or affected your career.
I arrived at NU in spring of 1963, straight from the Congo, which had just become independent from my home country of Belgium. The contrast of Northwestern from the Congo could not have been greater. I had no idea that a university could be so marvelous! So obviously, coming to NU affected my career, made everything possible. Indeed, since I was John Hilliard’s second student, I was one of the early Northwestern students to have graduated with a PhD degree in the field that Northwestern had invented. I was one of the first materials science PhDs ever, anywhere.

What are some of your most memorable classes/ experiences/moments from your NU MSE years?
My most memorable moment was my second day, when I met John Hilliard. I knew immediately that I wanted to work with him. It was a super choice! I chose to solve the non-linear diffusion equation of John Cahn’s spinodal theory. John Hilliard was dubious, but he let me try it out. At first I did not succeed; I was about to abandon the project, but told me, “Nonsense. If nature can do it, you can do it!” I persisted, and it worked.

What advice would you give to current MSE students about to begin their careers?
I suppose that some of my proudest career moments were associated with being given the David Turnbull and the Hume-Rothery awards; the first because I always admired David Turnbull immensely, and the second because, even as an undergraduate student in metallurgy, I had used Hume-Rothery’s textbook. I am also proud to contribute two outstanding young faculty members to NU: Mark Asta and Chris Wolverton, who had been graduate students of mine at UC Berkeley.

Describe how your experience in Northwestern’s MSE department shaped or affected your career.

DIDIER DE FONTAINE (PhD ’67)
Professor of materials science and engineering, University of California Berkeley; Distinguished Career Achievement Award winner

De Fontaine’s research interests include phase transformations in alloys, crystallography, and thermodynamics of phase changes. He has received numerous awards, including the TMS Hume Rothery Award and Exceptional Creativity Awards from the National Science Foundation.

Another memorable moment occurred when I obtained a numerical result from the computer in the form of lots of numbers. When I plotted out those numbers, point by point on graph paper, I saw a shape coming out with a profile that resembled the concentration profile of what was known as “Guinier Zones,” and for which at the time there was no theoretical explanation. I rushed into Hilliard’s office to show him the result, and he, too, was happy. Many years later when I visited John Cahn at NIST, I asked him about a new computational technique that NIST scientists were developing, the so-called phase field method. He answered, “Well, that’s what you had done for your dissertation at Northwestern.” I was shocked: without knowing it I had invented the phase field method.

What have been your most memorable or proudest career moments? Your most challenging?
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What advice would you give to current MSE students about to begin their careers?
First, pick a good adviser. Then, in the course of your studies, try to interact with specialists in your field, get them to know you, and you’ll be way ahead of the game when you start looking for a job.
Weertman Fest
A CELEBRATION OF TWO DISTINGUISHED CAREERS

On Friday, October 24 the department celebrated Weertman Fest in honor of professors Johannes and Julia Weertman. The daylong celebration featured talks by alumni and collaborators of both Weertman research groups.

Weertman Fest speakers, left to right: Sang-Hee Suh, Paul Sanders, Bill Nieman, Lyle Schwartz, Carolyn Aita, Koichi Tsuchiya, Willem Weertman, Jeffrey Eastman, Kai Zhang, Arthur Purcell