



FALL 2014

TECHTRACKS

MATERIALS SCIENCE AND ENGINEERING

A. JAMES CLARK SCHOOL *of* ENGINEERING

mse.umd.edu

Nanobatteries

DOE renews support for Energy Frontier Research Center.

INSIDE: "ORDERED DISORDER" | \$11.4M IN ARPA-E GRANTS | TOUGHER KEVLAR

IN ADDITION TO THE RESEARCH IN THIS ISSUE, this past spring and summer members of our faculty were recognized for research resulting in a number of significant advances in the field. You can read about these in more detail on our website.

For example, Assistant Professor **Liangbing (Bing) Hu**'s paper on the transparency and conductivity of graphite was published in *Nature Communications* (ter.ps/transgraph); Professor **Eric Wachsman** received the IOM3's Pfeil Award for a paper describing the use of titanium dioxide (TiO_2) for solar water disinfection (ter.ps/tio2solarh2o); and Professor **Ichiro Takeuchi**'s thermoelastic cooling technology was reviewed in the DOE Office of Energy Efficiency & Renewable Energy's *Non-Vapor Compression HVAC Technology Report* (see ter.ps/doenvchvac). Bing and Eric also won the University of Maryland Invention of the Year Award in the physical sciences for their creation of an intrinsically safe, low cost, high-energy solid-state lithium-ion battery (see ter.ps/huwachinvent).

We've also been active in workshops. In April, Professor **Gottlieb Oehrlein** was a featured speaker at the Atomic Layer Etch and Atomic Layer Clean Technology Workshop in San Francisco. In June, Professor **Manfred Wuttig** co-hosted the Technical Meeting on Novel Nanomagnetic and Multifunctional Materials on the University of Maryland campus. In August, I co-hosted the NIST Neutron Measurements

for Materials Design & Characterization Workshop in Potomac, Md. (see www.ncnr.nist.gov/measurements).

The NIST/UMD workshop was highly successful, with more than 100 registrants gathering to develop a future roadmap for instrumentation for the NIST Center for Neutron Science (NCNR). In late September, Professor **Aris Christou** hosted the Workshop on Defects in Wide Bandgap (WBG) Semiconductors, also on campus (see nanocenter.umd.edu/events/wbg).

Don't forget—if you're an alumnus or alumna, you can share great news about your life and career by joining the "MSEUMD" group on Facebook, connecting with us on LinkedIn, or e-mailing us at mse@umd.edu. You can get the latest MSE news at any time by visiting mse.umd.edu/news.

Until next time,

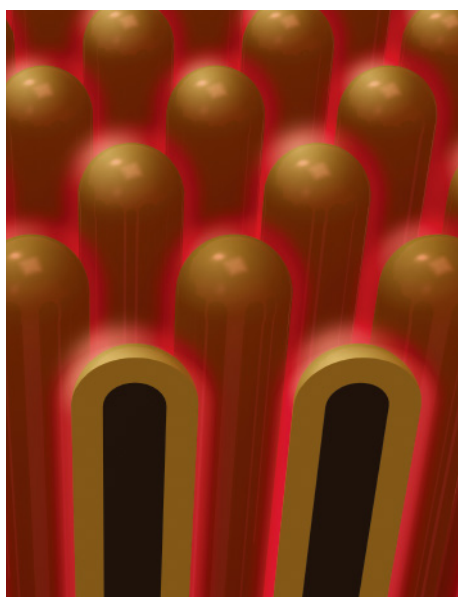


Robert M. Briber
Professor and Chair, MSE



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ON THE COVER:

This 3D model by MSE graduate student **Jiaqi Dai** depicts a battery electrode made out of a "forest" of nanowire "trees" that take up, store, and discharge lithium ions.

The central core of each nanowire (dark gray) provides a fast transport path for electrons to meet and neutralize lithium ions migrating into the outer layers (gold).

The red glow represents an electrical double layer of positive and negative ions that forms at the interface between the fluid electrolyte and the solid nanowires.

This architecture of dense nanowires is just one example of the new battery technologies being developed at the University of Maryland's Energy Frontier Research Center. For the story, see page 3.

DOE Renews Nanostructures for Electrical Energy Storage Energy Frontier Research Center

Story based on the original by Martha Heil, Maryland NanoCenter.

The U.S. Department of Energy's (DOE) office of Basic Energy Sciences has renewed its support for the University of Maryland's (UMD) Nanostructures for Electrical Energy Storage Energy Frontier Research Center (NEES EFRC) with a four-year, \$11.2 million grant. The renewal is based on both NEES EFRC's achievements to date and the quality of its proposals for future research.

NEES EFRC is a multi-institutional research center, one of 46 established by the DOE in 2009. Its goal is to develop highly ordered nanostructures that offer a unique testbed for investigating the underpinnings of electrical energy storage.

Center members study structures that are precise—each at the scale of tens to hundreds of nanometers—and ordered in massive arrays. These structures are also multifunctional, able to conduct electrons, diffuse and store lithium ions, and form a stable mechanical base. The scale and control of experimentation gives NEES EFRC researchers an exclusive gateway to probing fundamental kinetic, thermodynamic, and electrochemical processes.

In its first five years, NEES EFRC has developed a unique way of looking at the science of energy storage.

“Our agenda for the next four years is at least as creative and relevant,” says the center's director, Department of Materials Science and Engineering (MSE) professor **Gary Rubloff**. “NEES’ vision is a new generation of much better batteries that are powerful and long-lasting because they are based on carefully designed nanostructures. This requires that we understand how to precisely control the materials and shapes of the nanostructures; how to densely pack and connect them; how they behave—individually and collectively—during charging and discharging, and why; and how to make them safe

and long-lasting over thousands of charging cycles. The NEES mission is to provide the scientific insights and design principles needed to achieve this vision.”

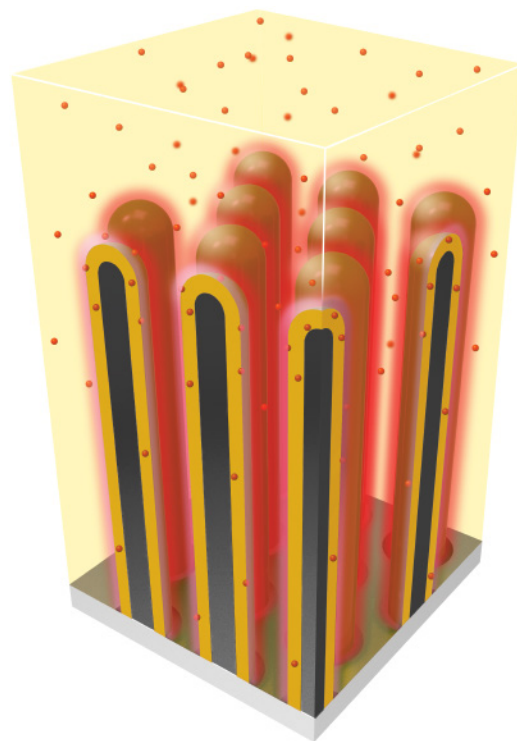
UMD is the center's lead institution and home to its largest contingent of principal investigators. The center's UMD-based research spans two colleges, the A. James Clark School of Engineering and the College of Computer, Mathematical and Natural Sciences. Rubloff notes the program has enabled the university to develop close collaborations with a diverse selection of outside universities and federal labs, with accompanying long-range benefits.

MSE professors **John Cumings** and **Liangbing Hu** say their involvement with NEES has had a positive impact on their research groups.

“It's been a valuable recruiting tool,” says **Cumings**, who works in the center's Nanostructure Interface Science research thrust. “Students are increasingly interested in solving the world's energy problems. That includes new battery technologies, and prior to NEES, that wasn't a topic within my group. Now, it provides a new motivation for my students, and it gives them a context in which they learn about energy policies and how their efforts can lead to lasting improvements in technology.”

“My students and I get a much broader understanding of electrochemical energy storage by participating in the center's workshops and meetings,” says **Hu**, who works in the Mesoscale Architectures & Ionics thrust. “We're also building strong collaborations with external members of the center, including Sandia National Laboratories. Our NEES-based work on using planar nanoscale batteries to demonstrate how electrochemical reactions can lead to the highest level of doping for a new class of optoelectronics was published in *Nature Communications*.”

Learn more at: www.efrc.umd.edu



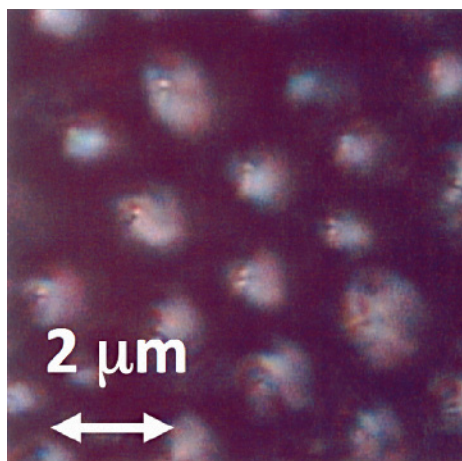
FROM THE RESEARCH GROUP OF PROFESSOR GARY RUBLOFF: ANOTHER VIEW OF OUR COVER IMAGE (SEE PAGE 2), SHOWING IONS' (RED SPHERES) INTERACTION WITH A NANOSTRUCTURED ELECTRODE (GOLD/GRAY RODS) IN AN ELECTROLYTE (PALE YELLOW).

RUBLOFF'S TEAM WANTS TO ANSWER NEW QUESTIONS THAT ARISE WHEN NANOSTRUCTURES ARE DENSELY PACKED INTO LARGER MESOSCALE ARCHITECTURES: WILL ELECTROLYTE NANOENVIRONMENTS CONTAIN AND SUPPLY IONS IN SUFFICIENT CONCENTRATION TO MAKE FULL USE OF THE ELECTRICAL ENERGY STORAGE LAYERS? WHAT DESIGN GUIDELINES ARE NEEDED TO BALANCE ELECTRON AND ION TRANSPORT TO ACHIEVE HIGH POWER? WILL SURFACE CHARGE VARY ALONG NANOSTRUCTURES, AND WHAT ROLE MIGHT THAT PLAY IN ELECTROLYTE ION TRANSPORT PHENOMENA?

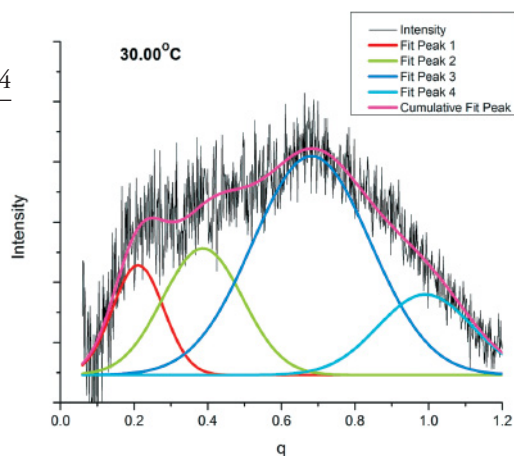
3D MODEL BY MSE GRADUATE STUDENT JIAQI DAI.

“Ordered Disorder”

MARTÍNEZ-MIRANDA DETAILS NEW TECHNIQUE FOR STUDYING NANOCOMPOSITES IN ORGANIC PHOTVOLTAICS



“SATURN RINGS” OF THE NANOCOMPOSITE CONSISTING OF THE LIQUID CRYSTAL 8CB AND FeCo FUNCTIONALIZED WITH MHDA.



THE RESULTING X-RAY SCATTERING SIGNAL FROM THE SAMPLE. BOTH FIGURES ARE FROM THE PH.D. DISSERTATION OF J. W. TAYLOR, 2013.

Understanding how electrons transfer between the light-absorbing materials used in any photovoltaic device, and how to optimize that transfer, is one of the challenges to making efficient and cost-effective products. MSE associate professor **Luz J. Martínez-Miranda** and her collaborators have combined optical microscopy and x-ray scattering techniques to uncover new information about defects in liquid crystal/nanoparticle composite materials being developed for photovoltaic applications. The work also sheds light on how electrons flow through them.

Photovoltaic materials made from organic liquid crystal nanocomposites are not as powerful or efficient as their solid-state counterparts, but they have qualities that make them good alternatives in certain situations. They can be manufactured without highly specialized equipment. They are inherently flexible, which can allow them to be worked into coatings or unusual shapes instead of being confined to a rigid solar panel. And despite their shortcomings, they cost so much less to produce that consumers still come out ahead financially.

Photovoltaic materials absorb light in different ranges of wavelengths. This energizes their electrons, creating a flow of energy. Liquid crystals are used in photovoltaics because they self-align and have an abundance of delocalized electrons that can be excited by a small voltage. The right combination of molecular order within and orientation of the liquid crystal lattice is essential to optimize electron flow, but this isn't quite as simple as it may seem.

“We are not dealing with a perfect lattice but a structure that ‘flows’ in a particular direction, and electron access to that flow is not the same from every angle,” Martínez-Miranda explains. “What we want is for as many electrons as possible to face the device’s electrodes so they can ‘go with the flow,’ which helps us create better organic photovoltaics.”

The liquid crystal photovoltaics Martínez-Miranda works with are composite materials made out of organic liquid crystals, inorganic semiconducting nanoparticles, and a functionalization compound, a type of molecule attached to the nanoparticles that acts as an intermediary to ensure they remain mixed. In her study, Martínez-Miranda found that when her nanoparticles were paired with a particular functionalization compound, they disrupted the liquid crystal order around them.

These defects, which take the form of nearly perfect circular patterns resembling blossoms or “Saturn rings,” were revealed when they scattered the light from an optical microscope. Martínez-Miranda and her team then turned to X-ray scattering to examine bulk samples at the nanometer to angstrom scale. They discovered that the disorder they observed in the local structure of the lattice was ordered across the entire sample, particularly when the concentration of nanoparticles was at 20-30%. In other words, the defects appeared in a predictable pattern.

This “ordered disorder” is not necessarily bad for a photovoltaic material, particularly if it is identified and is consistent across the entire liquid crystal lattice, because it reveals how the liquid crystal should be aligned within a device for optimal electron flow. Martínez-Miranda is currently investigating how localized disorder relates to the order of the entire liquid crystal.

“I’m looking for a sweet spot,” she explains. “If you want to build effective organic photovoltaics, you need this kind of consistency. And if there are limitations on materials, this technique will tell us where.”

For More Information:

L.J. Martínez-Miranda, *et al.*, *Applied Physics Letters* 97, 223301 (2010)

Branch, J., Thompson, R., Taylor, J.W., Salamanca-Riba, L., Martínez-Miranda, L.J., *J. Appl. Phys.* 115, 164313 (2014)

BRIBER RECEIVES INSTRUMENTATION PROGRAM AWARD

MSE professor and chair **Robert M. Briber** was one of three faculty members chosen to receive an A. James Clark School of Engineering Major Research Instrumentation Program Award. Winners were selected based on their proposals to purchase and implement a piece of equipment that would support one of the Clark School's strategic research initiatives, encourage interdisciplinary use, and be cost effective.

Briber's proposal detailed the purchase of a focused ion beam microscope to bring new nanostructure characterization capabilities to the University of Maryland. The instrument would both image and modify specimens down to the nanometer-scale using a narrow-diameter beam of charged atoms, allowing for a fully 3-D view of the internal structure of a specimen.

DISCOVER, CREATE, DEPLOY: MSE & THE MATERIALS GENOME INITIATIVE

The University of Maryland's Department of Materials Science and Engineering (MSE) is the perfect place to fulfill **President Obama's** call to accelerate the discovery, creation and commercial deployment of advanced materials, says Professor **Ichiro Takeuchi**.

Launched in 2011, the Materials Genome Initiative (MGI) supports materials research and development at U.S. institutions in an effort to solve problems at home while remaining globally competitive. The MGI is focused on materials discoveries that contribute to economic and national security, energy and human health, and stresses the use of techniques that speed up the processes and reduce costs.

Those techniques include computational design and modeling used by MSE faculty members such as Assistant Professor **Yifei Mo** and Adjunct Professor **Maija Kukla** (National Science Foundation). On the experimental side, Takeuchi uses combinatorial materials science ("combi") and other high-throughput techniques to synthesize, characterize, and catalog the functional properties of hundreds of samples at a time.

Most students, says Assistant Professor **Yifei Mo**, never have the opportunity to work with a supercomputer. That's why he designed and taught a course in which students learned to use Deepthought2, one of the nation's fastest university-owned supercomputers. Mo says the course contributes to the Materials Genome Initiative by equipping MSE students with computational skillsets they can use in future work on advanced materials design. For the full story, see: ter.ps/enma489a

Takeuchi's Combinatorial Materials Synthesis Lab houses one of the largest collections of facilities in the world dedicated to experimental materials science.

"We have a complete package at Maryland," he says. "We're 'accelerated squared.'"

The expertise extends beyond MSE, he adds, to colleagues including theorist **Peter Chung** (Mechanical Engineering) and experimentalists **J.P. Paglione** (Physics) and **Efrain Rodriguez** (Chemistry).

In May 2014, Takeuchi and his former group member, University of South Carolina (SC) professor **Jason Hattrick-Simpers** (Ph.D. '07), joined a group of experts in inorganic high-throughput materials science at a workshop co-organized by Applied Materials and SC. The event was supported by the National Science Foundation, the National Institute of Standards and Technology, and the White House Office of Science and Technology Policy (OSTP).

"So far the emphasis has been on theoretical and computational studies," says Takeuchi, "but many of the theoretically predicted materials haven't been experimentally tested. The OSTP suggested a workshop that would focus on how combinatorial materials science could contribute to the Materials Genome Initiative and validate the predicted results."

Takeuchi and Hattrick-Simpers were among the co-authors of a recently released white paper, "Fulfilling the Promise of the Materials Genome Initiative via High-Throughput Experimentation," that outlines

workshop's findings. Takeuchi also co-hosted a plenary session on the MGI and challenges in accelerated materials discovery at the Maryland NanoCenter's 2014 NanoDay.

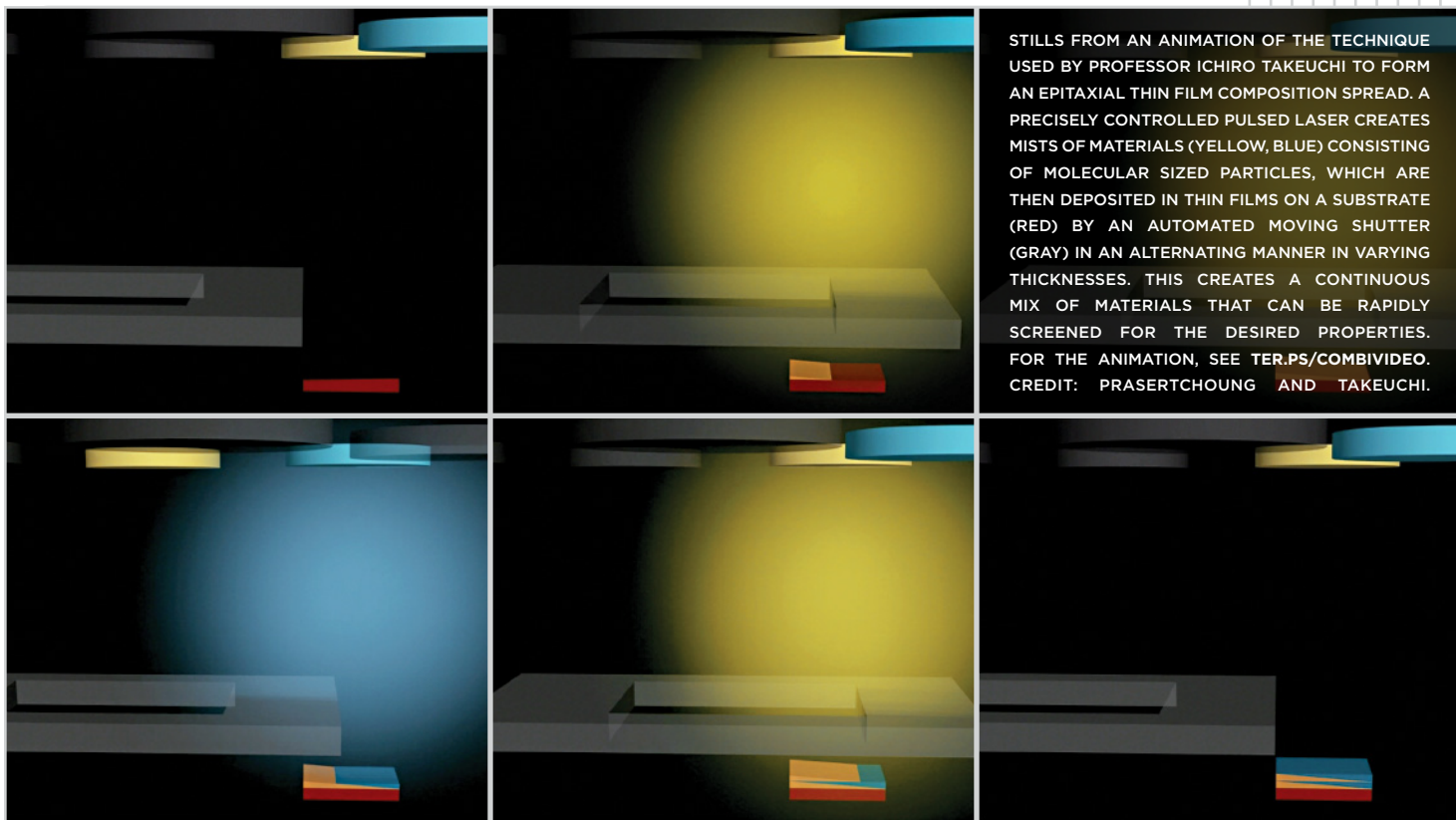
SLOAN FOUNDATION FUNDS EXEMPLARY MENTORING PROGRAM

The Alfred P. Sloan Foundation's Minority Ph.D. Program has awarded the University of Maryland's A. James Clark School of Engineering \$52,320 to establish a new Program of Exemplary Mentoring (PEM). The program, which will recruit and support highly talented, underrepresented minority Ph.D. students, is ultimately expected to serve as a model for the mentoring of all Clark School Ph.D. students.

The PEM represents a new formal collaboration among the Clark School's Center for Minorities in Science and Engineering (CMSE) and its Associate Dean for Faculty Affairs and Graduate Programs, Professor **Peter Kofinas**. It will serve students in all departments and disciplines, an expansion from the Clark School's legacy Sloan Ph.D. Network in Materials Science & Engineering and Bioengineering (MPHD).

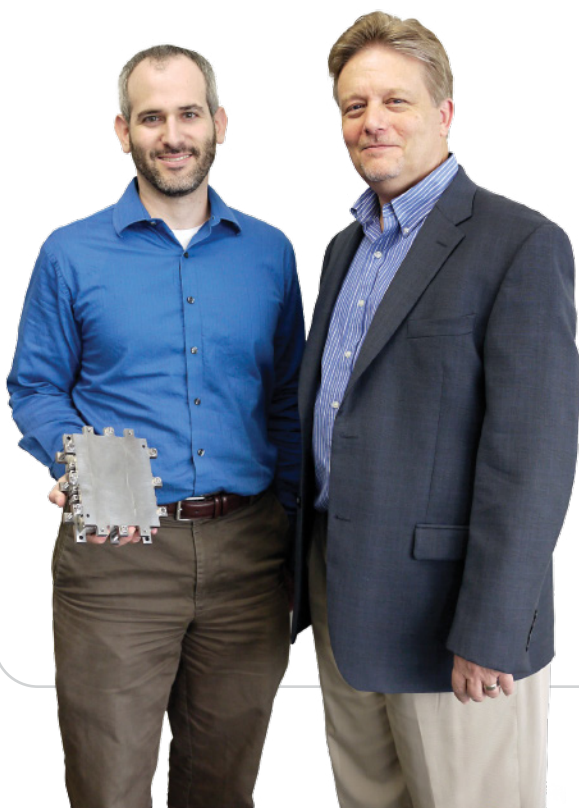
"Our objectives are to increase the number of outstanding minority Ph.D. students at the Clark School, increase the percentage of minority students who earn their doctorates, and decrease the amount of time it takes for them to do so," says MSE associate professor **Isabel Lloyd**, director of the PEM and the Legacy Sloan MPhD Network. "The program will host activities and provide professional development and mentoring that address all three of these goals."

The activities, which take place starting in the students' first semester, include networking socials at which they can meet potential peer mentors, funded trips to conferences at which they will be presenting their work, and visits to industrial and government research labs. CMSE will host a series of brown bag lunches and workshops on topics such as adjusting to graduate school culture and selecting an advisor. More formal workshops will focus on career planning, professional speaking and writing, computer modeling, and preparing for qualifying exams.



STILLS FROM AN ANIMATION OF THE TECHNIQUE USED BY PROFESSOR ICHIRO TAKEUCHI TO FORM AN EPITAXIAL THIN FILM COMPOSITION SPREAD. A PRECISELY CONTROLLED PULSED LASER CREATES MISTS OF MATERIALS (YELLOW, BLUE) CONSISTING OF MOLECULAR SIZED PARTICLES, WHICH ARE THEN DEPOSITED IN THIN FILMS ON A SUBSTRATE (RED) BY AN AUTOMATED MOVING SHUTTER (GRAY) IN AN ALTERNATING MANNER IN VARYING THICKNESSES. THIS CREATES A CONTINUOUS MIX OF MATERIALS THAT CAN BE RAPIDLY SCREENED FOR THE DESIRED PROPERTIES. FOR THE ANIMATION, SEE TER.PS/COMBIVIDEO. CREDIT: PRASERTCHOUNG AND TAKEUCHI.

Takeuchi, Wachsman Join Fuel Cell Projects Awarded Combined \$11.4 Million by ARPA-E



◀ REDOX CO-FOUNDERS BRYAN BLACKBURN (LEFT) AND PROFESSOR ERIC WACHSMAN (RIGHT) WITH A SOLID OXIDE FUEL CELL.

The U.S. Department of Energy's Advanced Research Projects Agency-Energy (ARPA-E) has awarded a combined \$11.4 million to three projects involving MSE faculty members. Individually, the three projects' grants are among the highest awarded in this round of funding.

The funding comes from ARPA-E's Reliable Electricity Based on ELeTrochemical Systems program (REBELS), which emphasizes the development of fuel cells for distributed power generation, fuel cells capable of functioning as batteries, and the use of fuel cells in the conversion of natural gas to liquid fuels. Proposed products must operate at temperatures of about 400–500 degrees Celsius, and have manufacturing costs low enough to make them commercially viable.

MICROSOFT, TRANS-TECH SUPPORT REDOX FUEL CELL DEVELOPMENT

Redox Power Systems LLC, the fuel cell company co-founded by MSE professor **Eric Wachsman**, is teaming up with Microsoft, Trans-Tech Inc., and the University of Maryland (UMD) to develop what the company describes as “transformational” fuel cell technology. The project is funded by a \$5 million REBELS grant.

Fuel cells—devices that convert the chemical energy of a fuel source into electrical energy—are optimal for distributed and on-site power generation systems, offering an alternative to the large, centralized power plants used today. Fuel cell-based systems powered by a variety of emerging and existing fuel sources could become a reality if the project is successful.

The three-year cooperative agreement has UMD partnering with Redox to improve its high-performance solid oxide fuel cells (SOFCs) and make them market-ready for a broad range of applications. The cells can provide low-cost power generation, heating and cooling for homes, and energy-efficient datacenters for companies like Microsoft. These new markets complement Redox’s existing 25 kW product, known as “The Cube,” which is designed for larger commercial structures. The team expects the technological advances resulting from the project will also open the door to applications in transportation.

Redox is focusing on lowering their SOFC operating temperatures from an already industry-leading 650°C to the 300–500°C range, reducing their start-up time to less than ten minutes, and enabling them to respond to electrical load changes from 10-90 percent power in less than one minute.

“This will be a major advancement in our fuel cell technology,” says Redox Chief Technology Officer and co-founder **Bryan Blackburn**. “It will not be incremental. We are working on every aspect of the cell—the anode, the cathode, the electrolyte. The materials will be different. Every single aspect will come together to form our highest performing, lowest-cost fuel cell.”

Trans-Tech Inc. will work with Redox and UMD to ramp up the commercial production of these new materials. The company will also work with Redox to reduce production costs. Bringing a large manufacturer like Trans-Tech into the development process early on and working with fuel cells produced using industrial processes will decrease the required time-to-market for new generations of enhanced SOFCs.

Once the fuel cell stacks meet ARPA-E cost and performance targets, they will go to Microsoft for independent live testing in the company’s server racks.

“Our vision is to bring the power plant directly into the datacenter by integrating fuel cell stacks into every server cabinet, effectively eliminating energy loss that otherwise occurs in the energy supply chain and doubling the efficiency of traditional datacenters,” says **Sean James**, Senior Research Program Manager for Microsoft Global Foundation Services. “We expect to effectively double our efficiency, from fuel to load, while cutting out many points of failure.”

“In this case the partner is also the potential customer,” explains Blackburn. “If Microsoft adopts these fuel cell systems on a large scale, they could provide just the right initial market and critical mass to drive the cost of our fuel cells down even further.”

To read Microsoft’s announcement, visit: ter.ps/redoxms

COMBINED COOLING, HEATING AND POWER SYSTEM

MSE Professor **Ichiro Takeuchi** is working with scientists at United Technologies Research Center (UTRC), Caltech, and the University of Connecticut to develop a fuel cell-based system that combines residential cooling, heating and power into one unit. The project received a \$3.2 million grant from the REBELS program.

Takeuchi is a co-PI on “Development of an Intermediate Temperature Metal Supported Proton Conducting Solid Oxide Fuel Cell Stack,” which will explore the creation of a home-scale, proton-conducting

fuel cell. He and his group will contribute their expertise in combinatorial materials science (“combi”) to rapidly create, screen and test new electrolyte and cathode materials.

“We’re looking for materials with the highest conductivity at the lowest temperature,” Takeuchi explains. “We also need long-term stability at the interfaces of the electrodes and the electrolyte. It’s not just which individual materials are the best, but what’s going to be the best combination of materials to avoid degradation where these components meet.”

Cost is another consideration, since sometimes the best materials may be too expensive to use in mass production. The team’s goal is to produce 80 percent efficient 100 Watt fuel cells, which they hope to achieve without a tradeoff between cost and performance.

Takeuchi’s colleagues include Dr. **David E. Tew** (project leader and PI, UTRC), **John Yamanis** (UTRC), Professor **Sossina M. Haile** (Materials Science and Chemical Engineering, Caltech), and Professor **Radenka Maric** (Materials Science and Engineering, University of Connecticut).

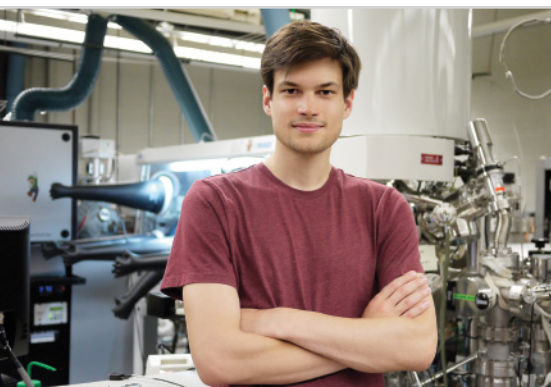
A BATTERY-LIKE FUEL CELL

Wachsman will also work with the University of South Carolina (SC) on a project titled “Bi-functional Ceramic Fuel Cell Energy System,” which received a \$3.2 million REBELS grant. MSE alumnus and SC professor **Jason Hatrick-Simpers** (Ph.D. ’07) is part of the team.

According to ARPA-E, “The University of South Carolina will develop an intermediate-temperature, ceramic-based fuel cell that will both generate and store electrical power with high efficiencies. The device will incorporate a newly discovered ceramic electrolyte and nanostructured electrodes that enable it to operate at temperatures lower than 500°C. The fuel cell’s unique design includes an iron-based layer that stores electrical charge like a battery, enabling a faster response to changes in power demand.”

Eric Schurr (Maryland Technology Enterprise Institute) contributed to this story.

Creative Catalyst Design with Graphene and ALD



ALEX PEARSE

MSE graduate student **Alex Pearse**, advised by MSE professor and Maryland NanoCenter director **Gary Rubloff**, received a 2014 Hulka Energy Research Fellowship from the University of Maryland Energy Research Center for his proposal to create new high-performance, transparent, conducting thin

films and other novel photoelectrochemical catalysts. Pearse will use atomic layer deposition (ALD) and other purpose-designed assembly methods to exploit the unique properties of graphene, which will serve as the foundation of these new materials.

The best photoelectrochemical catalysts, Pearse says, are those with highly reactive surfaces, high transparency to reduce light scattering, strong coupling to their electrodes, high surface activity, and the ability to manage intermediate reactions. Few if any catalysts, however, possess all of these qualities.

Photoelectrochemical cells, which convert sunlight into chemical energy, contain a catalyst that consists of a support layer of a material that absorbs light and generates electrons, covered by a thinner layer of catalyst particles. The electrons travel into the catalyst particles, where they can participate in electrochemical reactions with nearby reactants.

“Graphene is an ideal support for catalyst particles on because it’s highly conductive, and when it’s only a few sheets thick, it’s also transparent,” Pearse explains. “The best catalyst is a thin film of a noble metal like platinum. The problem is that metals are not transparent. The more metal you put down, the more light you block from entering your electrode. The efficiency of the system decreases despite the combination of two very good materials.”

But if you could control the placement of the catalyst particles at the atomic level, he theorizes, you could design a photoelectrochemical catalyst with the best balance of reaction sites and transparency, one atom at a time. That’s where ALD comes into play.

ALD is a procedure used to create atom-thick films for a variety of applications, often in the semiconductor and electronics industries. Material is deposited on a supporting

continues pg. 11

National Science Foundation Supports Student Research

GRADUATE RESEARCH FELLOWSHIPS: CONSERVATION, ELECTRIC VEHICLE BATTERIES

MSE graduate student **Willa Freedman** and MSE alumnus **Nicholas Weadock** (B.S. '13) were awarded Graduate Research Fellowships by the National Science Foundation (NSF).

The NSF’s Graduate Research Fellowship Program is designed to ensure the diversity and quantity of the nation’s scientists, mathematicians, and engineers by supporting outstanding graduate students attending accredited U.S. colleges or universities. NSF Graduate Research Fellowships are among the most prestigious and selective in the country.



WILLA FREEDMAN

Freedman, a member of MSE professor **Ray Phaneuf**’s research group, is exploring the use of atomic layer deposition in the conservation of monumental limestone buildings. Due to the limestone’s high porosity, these structures are particularly susceptible to the infiltration of water that promotes chemical and physical decay.

The subject of Freedman’s study is pietra di Trani limestone, found in the Apulian region of southern Italy and used in buildings such as the 13th century Castel del Monte, a UNESCO World Heritage site. She is investigating whether thin coatings of amorphous alumina, applied using atomic layer deposition, are capable of slowing the degradation of the stone by

protecting it from environmental pollutants and harsh weather. The coatings must be formulated to preserve the appearance of the stone, and must be removable without causing damage.

Weadock is currently a graduate student at Caltech, where he is a member of Professor **Brent Fultz**’s research group and developing a new electric vehicle battery.

GROW AWARD SPONSORS MICROSCOPY RESEARCH IN SWEDEN

MSE graduate student and NSF Graduate Research Fellow **Hannah Nilsson** is spending a year at Chalmers University of Technology in Gothenburg, Sweden, thanks to an NSF Graduate Research Opportunities Worldwide (GROW) award.

Nilsson, a member of Associate Professor **John Cumings**’ research

Understanding Empty Spaces to Improve a Solar Cell

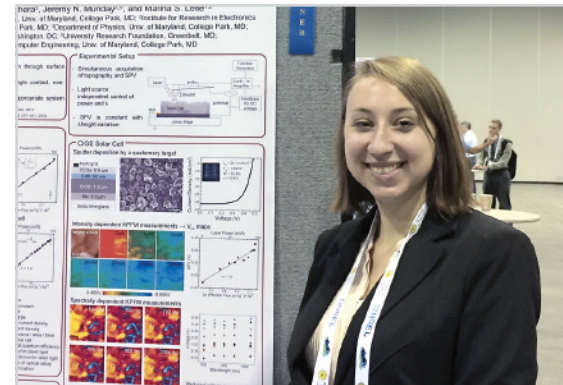
MSE graduate student **Elizabeth Tennyson** won the Best Poster Award at the 40th IEEE Photovoltaic Specialist Conference for her efforts to characterize and improve a material being considered for use in solar cells. The event gathers world leaders in solar cell research from academia, national laboratories, and industry.

Copper indium gallium selenium (CIGS) is a promising photovoltaic material that Tennyson would like to see on the market alongside devices based on semiconductors such as gallium arsenide (GaAs) and silicon. CIGS-based devices are thinner and cheaper than their commercially available counterparts, but also less efficient. Enhancement of CIGS's properties would make it a competitive material.

Under an electron microscope, CIGS resembles a few thin layers of non-uniform grains of sand (*see back cover*). It

is through the grains' interfaces—the tiny, equally uneven gaps between them—that electrons, excited by photons (particles of light), must flow to generate a voltage. This inconsistency interferes with the flow, and the interfaces may even pull electrons back into spaces vacated by others, an effect called recombination. In contrast, GaAs is a very smooth material, and more electrons travel through it at a higher speed.

If during the manufacturing of a solar cell the individual grains of CIGS could be oriented to allow for the best electron flow, its open-circuit voltage (the inherent voltage when no current is applied) would increase, improving its performance. The challenge, says Tennyson, is figuring out what that orientation is, and to accomplish that, she needed to know which kinds interfaces helped or blocked electron flow.



ELIZABETH TENNYSON

Tennyson, advised by Assistant Professor **Marina Leite** (joint, Institute for Research in Electronics and Applied Physics), used atomic force microscopy to measure the grains of CIGS in a solar cell, and a specialized form of imaging called

continues pg. 11

group, joined Chalmers Department of Applied Physics professor **Eva Olsson's** group, where she is conducting *in-situ* transmission electron microscopy experiments for the thermal characterization of graphene.

"Graphene has a theoretical thermal conductivity more than an order of magnitude higher than materials that are currently being used for heat management in electronic devices," Nilsson explains. This makes it valuable to industry. Unfortunately, she says, attempts to measure exactly how conductive it is have produced varying results that are difficult to interpret.

Nilsson believes electron thermal microscopy (ETM), a technique invented by the Cumings Group, may finally provide some concrete data on this fundamental



HANNAH NILSSON

phenomenon. ETM enables nanoscale thermometry (measuring a system's temperature or ability to transfer heat) by imaging liquid/solid transitions in small metal "islands." This allows scientists to test and observe nanoscale devices in real-time while they are inside a transmission electron microscope.

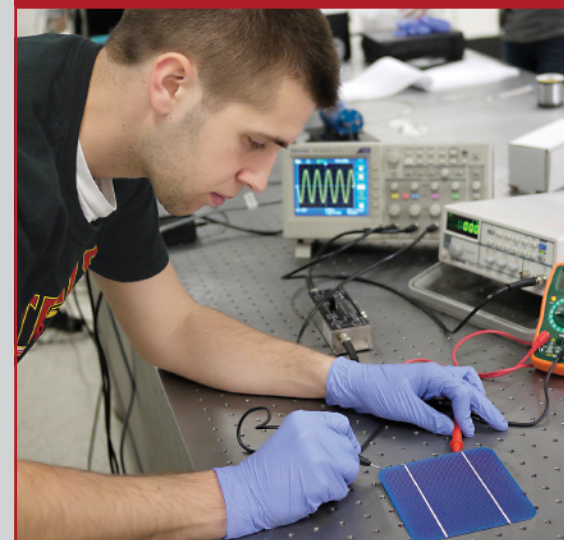
Nilsson describes ETM's application to graphene research as "a natural extension" of the Cumings Group's ongoing work in the thermal characterization of carbon nanotubes.

"I am very excited about this opportunity," she says. "The Eva Olsson Group is one of the leading electron microscopy groups in Europe. They are part of the Graphene Flagship, the EU's largest research initiative in history, so they are ideal for this collaboration."

MSE SENIOR ERIC BAILEY NAMED MERRILL PRESIDENTIAL SCHOLAR

The Merrill Presidential Scholars program honors the University of Maryland's most successful rising seniors and their most influential mentors. In addition to this award, Bailey has received scholarships and a SEEDS Undergraduate Research Fellowship. He is a Clark School Ambassador, a member of numerous honors programs, and works in Assistant Professor **Marina Leite's** research group, where he studies solar cells. For the full story, see: ter.ps/ebmerrill

To learn more about Eric Bailey's academic and research experiences in MSE, visit his profile at: ter.ps/bailey



In addition to the awards, scholarships and fellowships we've presented in this issue, we're pleased to announce the following honors:

DEPARTMENT AWARDS

The Department of Materials Science and Engineering Chairman's Outstanding Senior Award: **Kathleen Rohrbach**

The Department of Materials Science and Engineering Outstanding Materials Student Service Award:
Kari McPartland

The Department of Materials Science and Engineering Student Research Award: **Steven Lacey**

CLARK SCHOOL AWARDS

Outstanding ASPIRE Research Award: **Nathaniel Schreiber**

Dean's Doctoral Research Award: **Amy Marquardt**
Ph.D. candidate Amy Marquardt was awarded first place for her dissertation, "Application of materials science to cultural heritage: Protecting Art with Nanotechnology." Marquardt, advised by Professor **Ray Phaneuf**, is using her expertise in materials science to help museum conservators analyze, clean and preserve their art and artifacts.

To learn more about our undergraduate honorees, visit:
ter.ps/mseawards14

UNIVERSITY AWARDS

Ann G. Wylie Dissertation Fellowship: **Elliot Bartis**
(see ter.ps/bartiswylie)

NIST SURF FELLOWS

Alexander Kordell, David Marin, Rohan Mittal, Thomas Oeste, and Christopher Wong

recentGRADUATES

MAY/AUGUST 2014 B.S. GRADUATES

Christopher Andrew Berkey	Eshwari Sudarshan Murty
Luis Felipe Correa	Thomas H. Oeste
Gregory Hansten Finlayson	Glenn Robert Pastel
Samuel Justin Gillard	John Matthew Reilly
Alden De Groot Grobicki	Kathleen Marie Rohrbach
Calisa Marie Hymas	Jacob R. Steiner
Steven David Lacey	Ryan Samuel Tillman
Benjamin J. Lee (August 2014)	Mercedes Valero
Kari J. McPartland	

MAY 2014 M.S. GRADUATES

Chanyuan Liu, Nicholas Strnad, and Joshua Taillon.

MAY/AUGUST 2014 PH.D. GRADUATES AND DISSERTATIONS

Nicholas Fox-Lyon: "Plasma-surface Interactions During Reactive Plasma Processing of Hydrocarbon Films."
Advisor: Gottlieb Oehrlein

Gary Paradee: "Fatigue Properties of Graphene Interconnects on Flexible Substrates." Advisor: Aris Christou

KEVLAR, continued from back cover

being one-thousandth the width of a human hair, they are up to 100 times stronger than steel at only 1/6 the weight. The students theorized that the effective combination of the two materials would result in the product they were looking for.

After creating a prototype of its vest material, the team submitted it to the U.S. Army Research Laboratory (ARL) at the Aberdeen Proving Grounds for ballistics testing. The ARL team fired rounds of small ammunition into the samples in a controlled environment that adhered to the National Institute of Justice's standards for testing equipment used by law enforcement agencies. They recorded how many layers of fabric the bullets penetrated and the depth of the backface deformation (what happens on the inside of the vest, facing the wearer).

Over multiple tests, the modified Kevlar 29 stopped a bullet on the second or third of its 15 layers, and had a deformation of 14.23–20.2mm. Its ballistic resistance had doubled, and its tensile strength was increased by 400 percent.

Watch an in-depth video about the project at:

ter.ps/betterkevlar

alumniNEWS

ALUMNUS WINS IEEE FERROELECTRICS YOUNG INVESTIGATOR AWARD

MSE alumnus **Nagarajan "Nagy" Valanoor** (Ph.D. '01) received the Institute of Electrical and Electronics Engineers' (IEEE) 2014 Ferroelectrics Young Investigator Award.

The award, presented by the IEEE's Ultrasonics, Ferroelectrics, and Frequency Control Society, recognizes achievements in research, education, and application in the field of ferroelectric materials. Valanoor was cited for "his outstanding contributions in experiments and theory of nanoscale electromechanical phenomena in ferroelectric thin films and interfaces."

"[This] would not have been possible without UMD roots," he says.

Valanoor, currently an associate professor in the School of Materials Science and Engineering at the University of New South Wales, Australia, specializes in the synthesis and characterization of ferroelectric thin films. While at the Clark School, he was advised by MSE professors **Ramamoorthy Ramesh** (now at UC Berkeley) and **Alexander Roytburd**, and has since collaborated with MSE professor **Ichiro Takeuchi** on the development of environmentally friendly piezoelectrics.

surface called a substrate at the atomic scale and in specific locations or patterns. ALD makes it possible to manufacture devices and apply coatings with nanoscale precision.

Combining ALD and graphene, Pearse says, is a little unusual because the flat plane of a sheet of graphene is usually unreactive. Because of this the ALD process can't bind the catalyst particles to the plane. The *edges* of the sheet, however, are highly reactive, and this allows him to get creative.

"You could make a film of graphene flakes on a substrate, giving you a high density of exposed edges," he says. "The ultimate example of high surface area is if you have isolated catalyst atoms on these edges, because every side of every atom is available for reaction. Since ALD lets you precisely control how much you put down and where, you can

also control the density of your catalyst, which affects what kind of catalytic activity occurs."

Among other applications, these graphene catalyst composites could be used in lithium-air batteries or for photoelectrochemical water splitting, the direct conversion of sunlight into chemical energy using solar cells.

Perse is excited about exploring new territory. The Hulka Fellowship, he says, makes the still-speculative work possible.

"When you combine ALD's precision with graphene's unique ability to allow deposition at some places but not others, it becomes possible to create a whole new class of composite materials," he says.

To learn more about the Rubloff Group's research, visit: rubloffgroup.umd.edu

Kelvin probe force microscopy (KPFM) to map their many interface shapes, sizes and corresponding open circuit voltages.

"KPFM measures parameters related to voltage variations, enabling us to determine which interfaces are responsible for non-radiative recombination and lowering the performance of the device," she explains. "Now, in collaboration with the U.S. Naval Research Laboratory, we're using the knowledge we gained from the measurements to fabricate new CIGS solar cells with enhanced open circuit voltage and greater power conversion efficiency."

The data collecting technique she and her collaborators developed, she adds, can be used to examine any photovoltaic material.

To learn more about the Leite Group's research, visit: leitelab.umd.edu

ALUMNA WINS UMD DISTINGUISHED DISSERTATION AWARD

MSE alumna **Jane Cornett** (Ph.D. '13) received one of the Graduate School's 2014 Distinguished Dissertation Awards for her work on the behavior of thermoelectric materials. Cornett's dissertation, "Thermoelectric Transport Phenomena in Semiconducting Nanostructures," won the Mathematics, Physical Sciences, and Engineering division.

Thermoelectric materials are those that respond to changes in temperature by generating electricity, or vice versa. Thermoelectric devices have the ability to capture waste heat generated by power plants, chemical plants, computing centers, vehicles, building heating systems, or even the human body and convert it into energy that can be used to power another system. For example, a

thermoelectric device could harvest waste heat from a car's engine and use it to power its electrical system, increasing its overall fuel efficiency.

Cornett and her advisor, Associate Professor **Oded Rabin** (joint, MSE and Institute for Research in Electronics and Applied Physics), made substantial breakthroughs in understanding how thermoelectric devices function, especially at the nanoscale, and how to make them more efficient.

Cornett currently works at Analog Devices in Boston, Mass., where she is applying her expertise to the design of thermoelectric devices for small-scale energy harvesting applications.

"These energy-harvesters will convert a temperature gradient as small as 10 degrees—for example, the temperature difference between a heated floor and room temperature—into enough electrical



NAGY VALANOR



JANE CORNETT (LEFT) WITH HER ADVISOR, PROFESSOR ODED RABIN, AT THE AWARD CEREMONY.

energy to power small devices, like wireless sensors," she explains. "Harvesting 'free' thermal energy in this way is much easier than constantly replacing the tiny batteries in all of those small devices!"

To learn more about Jane Cornett's work, visit: ter.ps/thermomodel



A. JAMES CLARK SCHOOL OF ENGINEERING

Department of Materials Science and Engineering
2135 Chemical and Nuclear Engineering Bldg.
University of Maryland
College Park, MD 20742-2111

WHAT'S THIS? It looks like grains of sand, but it's actually copper indium gallium selenium, an inexpensive, promising solar cell material. The inconsistent size and spacing of its particles interferes with electron flow, reducing its efficiency. Graduate student **Elizabeth Tennyson**, advised by Assistant Professor **Marina Leite**, won an award for her work to determine how the grains can be reoriented during the manufacture of a solar cell for the best possible electron flow. For the story, see page 9.

TECHTRACKS is published for alumni and friends of the Department of Materials Science and Engineering at the A. James Clark School of Engineering. Your alumni news and comments are welcome. Please send them to:

Materials Science and Engineering
2135 Chemical & Nuclear Eng. Building
University of Maryland
College Park, MD 20742
301-405-5207 | mse@umd.edu

Department Chair: Dr. Robert M. Briber
Editor/Designer: Faye Levine

Students' Improved Kevlar Soft Body Armor Wins National Competition



LEFT, TO RIGHT: MSE ALUMNI STEVEN LACEY, CALISA HYMAS, KATHLEEN ROHRBACH, SAMM GILLARD, AND CHRIS BERKEY (ALL B.S. '14).

Specially modified ballistic grade Kevlar that could decrease the thickness and increase the strength of soft body armor took first place in the 2014 national ASM International Undergraduate Design Competition. The material, which has double the ballistic resistance of the original product, was created by a team of University of Maryland MSE students for their senior capstone design project.

Although the soft body armor used by soldiers and law enforcement officers helps protect the wearer from projectiles, it often requires so many layers of Kevlar to be effective that it loses flexibility. **Chris Berkey**, **Samm Gillard**, **Calisa Hymas**, **Steven Lacey**, and **Kathleen Rohrbach** (all B.S. '14) set out to double Kevlar's tensile strength, decreasing the number of layers required for a bulletproof vest from 30 to 15. Their goal was to make it possible to create a lighter piece of body armor that gives the user more maneuverability without sacrificing safety.

The students modified Kevlar 29 by embedding a network of crosslinked, functionalized carbon nanotubes (CNTs), using a chemical process that included etching, soaking and curing the fabric. CNTs have many unusual properties, including their strength: despite

continues pg. 10