HYDROGEN PRODUCTION VIA OXIDE SEMICONDUCTORS

LEARN MORE ON PAGE 3
Greetings to our MSE alumni! In the last issue of *MSE News*, you might recall that I highlighted the Materials Genome Initiative, a national science policy initiative whose goal is to discover and deploy materials twice as fast and at half the cost. It is envisioned that these ambitious goals will be reached through a combination of high-throughput experimentation and computational simulations. The Materials Science and Engineering Department is already responding to this challenge through changes in our research and education programs.

On the research front, we have recently hired Dr. Elizabeth Holm, whose specialty is computational materials science and engineering. Holm is currently a distinguished member of the technical staff at Sandia National Laboratory, and she has more than 20 years of experience in modeling materials. As a member of the National Materials Advisory Board, she has been part of the working group for Integrated Computational Materials Engineering; the report from this group is widely viewed as the forerunner of the Materials Genome Initiative announced by President Obama last year. Holm will officially join the MSE faculty this Fall, and she is expected to lead our research efforts related to the Materials Genome Initiative.

In parallel, our current MSE faculty members—led by Professor Chris Pistorius—are actively re-examining our curriculum to assess our current use of computation. Our goal is to integrate the use of computation and simulation into the existing core of Materials Science and Engineering courses, rather than create separate courses focusing on these topics. This reflects our opinion that these tools are integral to the field, rather than a separate subject. The goal is that our students will be better able to use computation and simulation in problem solving when they move on to graduate schools and/or careers in materials engineering.

In this issue, we profile a MSE alum who is also leading our field into the future: Dr. Warren Hunt, who was recently named Materials Innovation Director at The Minerals, Metals, and Materials Society (TMS), after serving as its Executive Director. See page 7 to learn more about this high-profile graduate of our Department.

This edition of *MSE News* also highlights exciting changes happening to MSE’s facilities, specifically the recently completed renovation of the C-level laboratories in Doherty Hall (see page 9). We are currently updating the A-level space in this building to add leading-edge labs and equipment that will help take MSE into the next generation in materials education and research.

This Fall, the Department of Materials Science and Engineering will host its annual Saltminers Dinner right here on campus on Monday, October 8, in conjunction with the 2012 MS&T meeting that is being held in Pittsburgh. I hope you will be able to join us for this event, which provides a way for you to reconnect with other MSE alumni—as well as see firsthand the many exciting changes in the Department. I look forward to seeing you there!

Gregory S. Rohrer,
W.W. Mullins Professor
The image on the cover of this edition of *MSE News* is a Piezo Force Microscopy (PFM) generated image of the surface of BiFeO₃. The main contrast in the image arises from the ferroelectric domains within the material’s structure. This image was recorded by Yiling Zhang, an MSE doctoral student who is studying the relationship between domain polarization and photochemical reactivity.

Zhang’s project is motivated by the possibility of using oxide semiconductors as relatively inexpensive catalysts to photochemically split water to produce hydrogen. The current limitation in photochemical hydrogen synthesis is the low efficiency of known catalysts. One factor that reduces efficiency is the small size of the catalyst particles, which are typically less than 100 nm in diameter. The confinement of both the excitation and the reaction to such a small volume leads to enhanced recombination of photo-generated electron-hole pairs within the particle, as well as the back reaction of intermediate species on the surface of the particle.

While one might think a simple solution is to use larger particles, the surface-area reduction associated with larger particles quickly offsets any gains that arise from reduced recombination. Considering this situation, it was hypothesized that if particles could be electrically polarized, then the oppositely charged photo-generated charge carriers would be transported in opposite directions. Because of this charge-carrier separation, recombination would be less likely. Furthermore, if the oxidation and reduction half reactions occur at different spatial locations, then the rate of the back reaction would be reduced.

BiFeO₃ was selected for this study because it is a semiconductor with a relatively narrow band gap of about 2.5 eV that is photocatalytically active in visible light. More important for this work, it is also ferroelectric — with spontaneous polarization along the pseudo-cubic <111> directions of 6.1 mC/cm². Zhang and his co-workers have shown that spontaneous polarization in the ferroelectric domains leads to band bending that transports photo-generated electrons and holes in opposite directions. As a result, the oxidation and recombination reactions are spatially selective.

This study of BiFeO₃ is part of a larger project in which Zhang is working with fellow doctoral students Li Li and Andy Schultz to explore the photochemical reactivity of composite oxide catalysts in which interfacial charge is used to separate photo-generated charge carriers.

The team’s work has shown that photochemical reduction and oxidation reactions on ferroelectric surfaces, and even on the surfaces of titania films supported by ferroelectrics, are spatially selective and correlated to the domain structure. The mechanism appears to be that when electron-hole pairs are created in the space charge regions, they move in opposite directions — so that some surfaces have excess electrons and promote reduction, while others have excess holes and promote oxidation. This also suppresses the recombination reaction and leads to enhanced composite reactivity. The details of these research findings can be found in the following recently published papers:

Assistant Professor Christopher Bettinger has won the prestigious National Academy of Sciences (NAS) Award for Initiatives in Research for his innovative work on advanced materials for next-generation implanted medical devices.

The NAS Award for Initiatives in Research was established by AT&T Bell Laboratories in honor of William O. Baker, a former President of Bell Labs who advised five U.S. Presidents on scientific matters. The award, which includes a prize of $15,000, is supported by Lucent Technologies. Its purpose is “to recognize innovative young scientists and to encourage research likely to lead toward new capabilities for human benefit.” Bettinger received the award on April 30 at the 149th annual meeting of the NAS in Washington, D.C.

“This is a wonderful honor as I continue to work to improve materials that will degrade benignly in the body, and ultimately, to develop materials that will sense their surroundings and respond deftly to help cure disease,” says Bettinger.

The diverse list of past NAS Initiatives in Research Award winners includes experts in multidimensional spectroscopies, mathematical algorithms, carbon nanoelectronics, and photonic crystal devices. Bettinger is the first materials scientist to win this highly competitive award since 2006.

AWARD-WINNING RESEARCH CROSSES DISCIPLINES

Bettinger, who joined MSE in 2010, has worked at the interface of materials science and biomedical engineering for more than 10 years. At Carnegie Mellon, he holds a joint appointment in the Department of Biomedical Engineering.

Bettinger has conceived and produced a number of innovations that aim to better integrate medical devices with the human body. These technologies include new synthetic materials that mimic the natural properties of soft tissue, as well as biodegradable electronics that could usher in a new era of electronically active implants. Bettinger’s work is designed to lead to broader advances in the field of medical devices to reduce the burden of human disease and improve quality of life.

In his Laboratory for Therapeutic Biodegradable Microsystems, Bettinger’s research team works to develop biomaterials-based MEMS for use in a wide range of biomedical applications including regenerative medicine, neural interfaces, and drug delivery. They use interdisciplinary strategies to develop next-generation medical implants that combine extraordinary properties of biodegradability and biocompatibility with unique mechanical properties and electronic functionality.

RECENT ACCOLADES BRING ATTENTION TO MSE

The NAS award is just one of many recent accolades for Bettinger that bring a global spotlight to the Department of Materials Science and Engineering. Earlier this year, his group earned a grant from the National Institute of Biomedical Imaging and Bioengineering, part of the National Institutes of Health (NIH). In 2011, Bettinger was selected to Technology Review magazine’s TR35 list, which honors top innovators under the age of 35. He was also invited to attend the prestigious National Academy of Engineering’s 17th annual U.S. Frontiers of Engineering Symposium, which brings together exceptional researchers in industry, academia, and government.

“Everyone in the Department is pleased by the many awards and accolades won by this energetic young faculty member,” says MSE Department Head Gregory S. Rohrer. “With his groundbreaking interdisciplinary research and his many international honors, Christopher Bettinger is bringing a lot of attention to the innovative work being done here at MSE.”

Bettinger received an S.B. in Chemical Engineering in 2003, an M.Eng. in Biomedical Engineering in 2004, and a Ph.D. in Materials Science and Engineering in 2008 as a Charles Stark Draper Fellow, all from the Massachusetts Institute of Technology. He completed his post-doctoral fellowship at Stanford University in the Department of Chemical Engineering as an NIH Ruth Kirschstein Fellow in 2010.
Professor Gregory S. Rohrer has won a second-prize award in the prestigious Sapphire Prize competition, given to the best papers published in the Journal of Materials Science during 2011, the publication’s Sapphire (45th) Anniversary Year. Rohrer’s paper, entitled “Grain Boundary Energy Anisotropy: A Review,” was chosen from more than 5,000 manuscripts the journal received last year — of which 971 were published. Sapphire Prize winners were honored at the 2011 Fall Materials Research Society meeting, held in Boston in November. Journal publisher Springer will sponsor Open Access to Rohrer’s paper, and he also received an award of $1000.

In May, Professor Jay Whitacre announced that his start-up company, Aquion Energy, will manufacture sodium ion batteries and energy storage systems at the site of a shuttered Sony television factory in Westmoreland County. The build-out of the base facility and factory infrastructure will begin immediately and continue throughout 2012. Initial product manufacturing is scheduled to commence in 2013. As part of a first-phase manufacturing commitment at this site, Aquion expects to create over 400 high-tech manufacturing jobs by the end of 2015. Based on Whitacre’s research, Aquion has developed a novel, sodium-ion, aqueous electrolyte battery that will enhance the electrical grid by providing flexible, emissions-free capacity.

Assistant Professor Mohammad Islam was a featured speaker at the Gotham-Metro Condensed Matter Meeting, sponsored by the New York Academy of Sciences and held in New York City on April 20. This biannual conference brings together leading experts in condensed matter physics to share their research and ideas. Islam’s research focuses on experimentally investigating the microscopic structure and dynamics of synthetic and biological soft matter, in order to better understand traditional concepts such as phase transitions, self-assembly, and the relationship between microscopic structure and macroscopic properties. Islam’s presentation described his research team’s fabrication of single wall carbon nanotube based foams, which they call SWCNT aerogels, as well as aerogel based composites.

Professor Robert Davis has been chosen as a Science & Engineering Ambassador by the National Academy of Sciences and the National Academy of Engineering. Leaders of these two groups visited Pittsburgh in May to announce that the city was chosen as a pilot for a new program created to increase public awareness of scientific issues. Pittsburgh was chosen as a pilot site for the new Science & Engineering Ambassador Program because of its rich energy heritage, its eminent universities, its engineering and science leaders, its cultural assets, and the participatory spirit of its citizens. While the program will initially focus on energy issues, the plan is to expand to additional topics in the future. To learn more about the program, visit www.scienceambassadors.org.

Professor Sridhar Seetharaman — along with members of his research group and collaborators at NETL — has been selected to receive the American Ceramic Society’s Spriggs Phase Equilibria Award for their paper, “Phase Equilibria in Synthetic Coal-Petcoke Slags (Al2O3-CaO-FeO-SiO2-V2O3) Under Simulated Gasification Conditions.” The paper was published in Energy & Fuels in 2011. The complete list of authors includes MSE alum Piyamanee Komolwit (Ph.D. 2009), as well as Jinichiro Nakano, Kyei-Sing Kwong, James Bennett, Thomas Lam, and Laura Fernandez. The award will be presented at the American Ceramic Society Banquet, held at the MS&T meeting here in Pittsburgh later this year.

Professor Katayun Barmak has joined Columbia University as its Philips Electronics Professor in the Department of Applied Physics and Applied Mathematics. She had been a faculty member at MSE since 1999. The Department wishes her the best in all her future endeavors!
Jennifer Wai-Man Shih (B.S. 2009) has accepted an offer from the Division of Enforcement B, Office of Compliance, Center of Devices and Radiological Health at the U.S. Food and Drug Administration (FDA). Shih will be working within the division that manages cardiology, vascular, circulatory, orthopedic, radiology, anesthesiology, and neurology devices.

Scott Pisula (B.S. 2001) has been working for U.S. Steel since graduating from MSE. He started at the Edgar Thomson Works in Braddock and was transferred about three years ago to the Clairton Works in Clairton. Pisula writes that he has been extremely lucky to be able to utilize his MSE degree the entire time he has been with U.S. Steel. Since receiving his MSE degree from Carnegie Mellon, Pisula has also earned a masters degree in Materials Science and Engineering from the University of Pittsburgh. He is the proud father of a beautiful son, Mikey.

Jennifer Singelyn (B.S. 2005) completed her Ph.D. at the University of California at San Diego in August 2010. Since then, she has been working at Becton, Dickinson & Company (BD)—a medical device company with headquarters in New Jersey. Since she is a native of New Jersey, Singelyn writes that it has been great to be near her family, after being on the West Coast for five years. Singelyn is in BD’s Technology Leadership Development Program, a rotational program meant to develop the company’s future R&D leadership. Her first rotation has focused on BD’s injection systems business, where she has been Team Lead and R&D Lead on projects to move BD products into global markets. She has traveled to India, Switzerland, and China in the last year. Singelyn is quick to credit her MSE education for helping her achieve her current position.

Franco Fabiilli (M.S. 2010) is a Coating Production Engineer at Perrigo Company in Allegan, Michigan. Perrigo develops and manufactures generic pharmaceuticals and store brand over-the-counter medicines. As a Coatings Production Engineer, Fabiilli’s role is to develop and improve manufacturing processes with regard to safety, efficiency, and technology. He also troubleshoots any issues related to tablet defects. He reports that the position is a really great experience, and his materials science/chemistry background has been very useful.

Elise Selinger (B.S. 2000) is working for Conley Rose, a boutique intellectual property law firm, as an Associate in their Dallas office. She manages patent prosecution in the telecommunications industry, as well as the oil and gas industry. The firm handles high-tech work for patents as well as trademarks, copyrights, and trade secrets. Selinger is excited and enjoying this new professional opportunity.

Married MSE alums Pranay Choudhary (M.S. 2006, Ph.D. 2010) and Abhilasha Bhardwaj (M.S. 2006, Ph.D. 2009) write with exciting news! In April, they welcomed a new daughter named Aashi. Congratulations to the happy family from everyone at MSE.

Tom Matta (B.S. in MSE and M.B.A., Tepper School of Business 2007) is the Chief Operating Officer and Co-Founder of StatEasy, a software firm created to give coaches and athletes access to the most accurate form of feedback imaginable: statistics synchronized with video. “Coaches commonly record live statistics and video during any sporting event,” explains Matta. “To make the most of this data, the information needs to be married together and, with StatEasy, coaches are able synchronize video and stats via a simple one-click process.” Matta is working to adapt the unique tool for a range of custom uses, including highlight reel construction, social media posting, and live updates for recruiters.
Alumni Profile | Making Connections

As Materials Innovation Director at The Minerals, Metals, and Materials Society (TMS), Warren Hunt (M.S. 1982, Ph.D. 1992) brings industry, government, and academic collaborators together to spur exciting materials developments. Though he has been with TMS since 2005—until recently as Executive Director—Hunt’s current role is a new one, created to foster connections that result in game-changing materials improvements.

Hunt began working at Alcoa Technical Center immediately upon graduating from Vanderbilt University in 1977. For the next 19 years, he worked in R&D and management positions focused on new product and process development—obtaining nine patents, publishing 50 papers, and editing three books. Hunt was recognized with two IR 100 Awards, the Alcoa Laboratories Merit Award, and the Alcoa A.V. Davis Award for Team Accomplishment. He also became an ASM International Fellow.

Incredibly, during this busy time period, Hunt earned both his M.S. and Ph.D. degrees at MSE. He and his wife Shawna were also raising two children: Erika and Jason. “I definitely didn’t have the typical experience that most graduate students have,” recalls Hunt. “Often, I would come over to the campus for a class, then go right back to work at Alcoa. It was a balancing act, but fortunately Alcoa was very flexible. I was even able to take time off for my residency and to finish my thesis.”

In 1996, Hunt started his own consulting firm, Aluminum Consultants Group, Inc., to provide technology services to clients in the primary metals, end product manufacturing, government, and legal sectors. “I discovered that a Ph.D. from Carnegie Mellon meant a lot in the business world,” says Hunt. “The reputation of the MSE Department certainly helped to establish my expertise and the value that I could deliver to clients across a broad range of research areas.”

Throughout his career, Hunt has worked with other alumni from MSE—and he enjoys being part of this close-knit community. “As a part-time student, I was at MSE for many years,” Hunt says with a laugh. “The benefit is that I was able to meet so many people and form great, lasting relationships that I still have today. When someone asks, ‘Were you at MSE when I was there?’ the answer is usually yes!”

Deck Party Reunites MSE Alums

The Department of Materials Science and Engineering hosted its third annual “Deck Party” on Friday, April 20, in conjunction with Carnegie Mellon’s Spring Carnival. This event, which grows in popularity each year, brings together a wide range of MSE alums and their family members. The weather was great, and the alums enjoyed the chance to reunite and share news with one another. We hope to see you in Spring 2013 for this MSE tradition!
Donations Keep MSE at the Forefront

Nearly 100 generous alumni and friends supported the Department of Materials Science and Engineering in fiscal year 2011, with donations totaling almost $54,000. The Department appreciates these contributions, which support ongoing innovations in our curriculum, facilities, and research that help Carnegie Mellon MSE to maintain its position as a global leader in materials science and engineering. We express our sincere gratitude to the donors listed below.

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Sophomore Tejank Shah, a member of the Carnegie Mellon student chapter of Engineers Without Borders, is leading an effort to install solar panels on a grade school in northern India. Along with fellow students and professional mentors, Shah has traveled more than 14,000 miles roundtrip in managing the project’s operations since its inception.

After the group’s first trip to the impoverished region of Rampur to visit the school in March 2011, Shah realized firsthand how much of a negative impact an old diesel generator system, coupled with an unpredictable power grid, were having on student learning. Replacing the generator with solar panels will improve conditions for more than 300 children in grades K–5 who have been enduring poor lighting and a humid study environment.

The effort was important to Shah on multiple fronts. “This project allowed me to reconnect with my Indian roots and give back to the country that nurtured my parents. I also appreciated the opportunity to work with great minds in both the U.S. and India in bringing this project to realization,” Shah explains.

“With the installation of this solar panel system, I hope this school will serve as the hub for future green energy endeavors and as motivation for others to release themselves from their reliance on these polluting diesel generators,” Shah says. “Personally witnessing how happy the school principal and students were is a memory I won’t ever forget.”

“It is simply amazing what these students are doing and how their work will impact both the Rampur grade school and the students,” says Kurt Larsen, Assistant Dean for Undergraduate Studies at the College of Engineering. “We have a service learning tradition at Carnegie Mellon, and this project has truly made this learning experience both global and borderless.”

Students Enjoy New Lab Space

As noted in the Spring 2011 issue of MSE News, the Department has been working hard to renovate its space on the A and C levels of Doherty Hall. The renovation of the C level—which housed the old Machine Shop—began last September and was completed in time for the start of Spring 2012 classes. The new facility consolidates three older labs that were spread out on the A level. The new C-level facility is able to accommodate all the undergraduate courses, while the A level undergoes its own makeover.

In Spring 2012, all the MSE labs were conducted in the new space. Undergraduate lab students can conduct tasks such as melting and casting, sample fabrication, heat treatment, mechanical testing, mechanical deformation, metallographic preparation, and optical microscopy.

The consolidation of the basic materials labs into this new facility will allow the development of more sophisticated labs in the newly renovated A-level space. Plans for the A-level space include a new soft materials lab, advanced material property testing, and advanced imaging and microstructural evaluation facilities. Watch future editions of MSE News for continuing news about this dramatic transformation!
In March, junior Anisha Bapna had a paper chosen for publication at the 38th Annual Northeast Bioengineering Conference (NEBEC). Bapna’s paper was titled “Relevance of PDMS Processing Techniques Used in Electricity Generating Muscle Energy Converter.”

Senior Emily Walker has received an Intel Foundation/SRCEA Fellowship from the Graduate Fellowship Program at Semiconductor Research Corporation. The fellowship provides tuition and fees, a stipend of $2,320 per month, and an annual unrestricted gift of $2,000 to the department in which students are enrolled. The award will support Walker’s graduate studies at the University of Texas/Austin under Professor Deji Akinwande.

Doctoral student Jihoon Choi is a finalist in the competition for the 2012 AkzoNobel Student Award in Applied Polymer Science. From more than 30 papers received, Choi’s has been selected as one of six finalists. Choi will present the paper at the AkzoNobel Student Award Symposium at the August national ACS meeting in Philadelphia, where the winner will be announced. Choi’s paper is titled “Particle Brush Systems for Flexible Photonic Coating Applications.”

Doctoral student Subhasis Sinha has received an award for research he conducted at Tata Steel in 2011. A Certificate of Honour was presented to Sinha in November for his research entitled “Development of Bainetic Steel Through Continuous Cooling With 1200 Mpa UTs and 20% Uniform Elongation.”

Doctoral student Li Li has been awarded two travel grants: one from The Minerals, Metals & Materials Society (TMS) and one from the Graduate Student Assembly (GSA) at Carnegie Mellon. Li has also been named Chair of the Carnegie Mellon Materials Advantage Group. The national Materials Advantage organization is a combined student program of four professional societies in the field of materials science: the American Ceramic Society (ACerS), Association for Iron & Steel Technology (AIST), ASM International, and TMS.

The Pittsburgh Golden Triangle Chapter of ASM International held its annual Young Members’ Night dinner meeting at the University of Pittsburgh on Thursday, February 16. Once again, MSE students had the opportunity to shine during the annual event, which brings students from local universities together with professional engineering groups.

In the graduate poster contest, Kelvin Cheung won first prize, Ben Anglin won second prize, and Xuan Liu placed third. Nathan Howell won first prize in the undergraduate division.

Madeline Cramer and Daniel Cardenas Rivera won the Past Chairpersons’ Educational Assistance Scholarship, while Robert Tisherman was presented with the Outstanding Senior Award.

Doctoral student Li Li was the Student Chair for the event and was also the student speaker. He presented a paper titled “Heterostructured Powders for Photocatalytic Hydrogen Production: Nanostructured TiO2 Shells Surrounding Microcrystalline (Ba, Sr) TiO3 Cores.”
MSE Celebrates Commencement

On May 20, the Department of Materials Science and Engineering celebrated its annual Commencement ceremony. The Department awarded 30 B.S. degrees and 30 M.S. degrees. An additional 24 students earned Ph.D. degrees. Some members of the Class of 2012 will go on to a variety of professional positions, while others will pursue additional degrees.

- The William W. Mullins Undergraduate Award Recipient: Andrew Tyler Polonsky
- The Hubert I. Aaronson Undergraduate Award Recipient: Dunyang (Rita) Wang
- The James W. Kirkpatrick & Jean Kirkpatrick Keelan Award Recipient: Morgan Heskett
- The William T. Lankford Memorial Scholarship Award Recipient: Parth Naidu
- The ASM Golden Triangle Chapter Outstanding College Senior Award Recipient: Robert Tisherman
- The Paxton Award for Best Doctoral Dissertation Recipient: Dr. Neerav Verma
- The Philbrook Prize in Engineering Recipient: Professor Lisa Porter
- 2012 Krivobok Brooks Award for Excellence in Metallography Undergraduate Recipient: Nathan Howell
- Graduate Recipient: Mina Abadier
Carnegie Mellon University does not discriminate, and Carnegie Mellon University is required not to discriminate, in admission, employment, or administration of its programs or activities on the basis of race, color, national origin, sex, or handicap in violation of Title VI of the Civil Rights Act of 1964, Title IX of the Educational Amendments of 1972, and Section 504 of the Rehabilitation Act of 1973 or other federal, state, or local laws or executive orders.

In addition, Carnegie Mellon University does not discriminate in admission, employment, or administration of its programs on the basis of religion, creed, ancestry, belief, age, veteran status, sexual orientation, or gender identity. Carnegie Mellon does not discriminate in violation of federal, state, or local laws or executive orders. However, in the judgment of the Carnegie Mellon Human Relations Commission, the Presidential Executive Order directing the Department of Defense to follow a policy of “Don’t ask, don’t tell, don’t pursue” excludes openly gay, lesbian, and bisexual students from receiving ROTC scholarships or serving in the military. Nevertheless, all ROTC classes at Carnegie Mellon University are available to all students. Inquiries concerning application of these statements should be directed to the provost, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, telephone 412-268-6684, or the vice president for enrollment, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, telephone 412-268-2056. Carnegie Mellon University publishes an annual campus security report describing the University’s security, alcohol and drug, and sexual assault policies, and containing statistics about the number and type of crimes committed on the campus during the preceding three years. You can obtain a copy by contacting the Carnegie Mellon Police Department at 412-268-2323. The security report is also available online.