THIS ISSUE: COMING OF AGE DURING THE MOLECULAR ENGINEERING REVOLUTION

CONTENTS

Director's Remarks
New Structures, New Connections 1

Feature Story
Coming of Age 2

Science News
Water 6
Nanoscale Materials 11
Energy 13
Arts, Sciences, and Tech. 16
Quantum Information 18
Immuno-engineering 21
Q&As 23–24

Honors & Awards 26

Community
Outreach 28
Development 30
Molecular Science and Engineering of Water

“I’ve never taught this course before. I don’t believe this course has ever been taught before anywhere,” Skinner states. His students learn about the bewildering variety of states in which water manifests itself, both as a liquid and as a solid. They learn about liquid water and supercritical water (water under high temperature and pressure). They study the astonishing variety of ices, from amorphous ices to glassy ices to super-cooled water that somehow remains liquid even below freezing. They learn how to apply quantum mechanics, statistical mechanics, and thermodynamics to water. And in the engineering area, they learn about water treatment and purification; water and energy; water’s role in the atmospheric, oceanic and geosciences; and water in biology, human health, and medicine.
There are institutions that have required decades to arrive at a clear sense of their strengths and their mission. They began in response to a specific need, then years later reached a level of organizational coherence and maturity that enabled them to focus and impact a field of work.

The IME has taken a 21st century approach—what the business community calls a “green field” start up—and began with a clear mission, clear requirements, and unambiguous University of Chicago support. With planning and implementation, we have been continually taking form—and then modifying that form—during our brief five-year existence.

The IME has been able to aggressively assemble a team of top engineering scientist-teachers. We have built world-class facilities and equipped them with all the right technologies. We have recruited researchers and champions in quantum, bio, materials, and water research.

We have fused human resources and knowledge platforms to build innovative graduate and undergraduate education programs that take advantage of our world-class university with its liberal arts core curriculum. Beginning with our partnership with Argonne National Laboratory, we have designed a host of institutional alliances and networks of experts across the globe. An advisory council of accomplished supporters and distinguished alumni was formed to advise us and advocate for the IME. And an industrial affiliates program is now up and running to create those vital avenues and opportunities for our researchers and students to work on real problems in conjunction with advanced technology companies.

We cultivate connections to the arts in order to direct left- and right-brain processes toward innovation. At key moments in this rapid institutional formation, the IME has reset its administrative structures to match the new requirements of growth. Without these timely adjustments to how we operate, the IME would have lost momentum and been unable to move forward into new stages of development.

In the last several months we have reconfigured our administrative team and created a Chief of Staff position, now occupied by Carolyn Williams Meza. The faculty leaders in our areas of responsibilities are now deputy directors who serve on an executive committee along with Meza and with Rovana Popoff, recently elevated to senior associate dean. We regularly meet as a group to further integrate the IME’s far-flung activities, initiatives, alliances, responsibilities—and keep us focused on the prize: Find solutions to some of society’s most pressing problems, and raise up new generations of committed, collaborative, and innovative molecular engineers and engaged leaders. Sharon Feng, who has been so instrumental in shaping the Institute’s first several years of rapid development, is now Senior Associate Dean and Special Assistant for External Initiatives, focusing her energies on the IME’s opportunities in the innovation sphere. We are also exploring numerous international initiatives.

This maturing structure at the IME is reflected in another aspect of our work—communications. You are reading our inaugural quarterly report. The Institute is now producing four quarterly reports to trigger a more rapid news cycle, create content that is responsive to major developments, and encourage deeper faculty and researcher input as stories take shape.

The IME continues to be a leader and influencer in molecular engineering technologies and their impact on society. This year, several IME faculty were called upon to testify, in their areas of scientific expertise, before U.S. Congressional committees. The Institute will take the opportunity to use future quarterly reports as a vehicle for this leadership voice. So, enjoy this inaugural issue and let us know what you would like to see in upcoming editions.
Coming of Age during the Molecular Engineering Revolution

Highlights of IME’s progress thus far in 2017

By all accounts, the Institute for Molecular Engineering has reached an important turning point in developing its capacity to fulfill an ambitious educational, scientific and technological mission.

With nearly a full complement of 21 faculty members, IME now has a critical mass of teaching and research specialists focusing on areas that promise concrete advances in important technology sectors. Collaborating across disciplines, they are exploring innovative and potentially game-changing approaches to molecular scale design and engineering—putting into practice IME’s mantra: “We will make significant contributions to solving society’s most pressing problems” in areas such as energy storage and harvesting, immuno-engineering and cancer, water resources, and quantum information technology.

The Institute’s tireless faculty expansion of recent years continues in 2017, now shifting its focus toward filling five new positions to accelerate activities in IME’s Water Research Initiative under the leadership of its inaugural director and Crown Family Professor in Molecular Engineering, James Skinner.

“This truly is an interdisciplinary effort,” states Skinner. “Engineering, chemistry, biology, physics: It is no stretch to say that you have to bring all these disciplines to bear on these problems. It’s exciting to be involved in something that’s so cross-cutting.” (see Water Research Initiative, p. 8)

Timing is right to create a quantum technology ecosystem

One of the most exciting developments that signals IME’s coming of age is the launch of the Chicago Quantum Exchange (CQE) in June. CQE’s founding has brought material support to a vision first glimpsed in 2013. Discussions about establishing a trailblazing quantum engineering initiative began soon after Awschalom joined the UChicago faculty in 2013 when he proposed this concept, and is being developed through the recruitment of faculty and the creation of state-of-the-art measurement laboratories.

“We are at a remarkable moment in science and engineering, where a stream of scientific discoveries are yielding new ways to create, control and communicate information between quantum states of matter,” said Awschalom, who directs the exchange. “Efforts in Chicago and around the world are leading to the development of fundamentally new technologies, where information is manipulated at the atomic scale and governed by the laws of quantum mechanics.”

The launch of this intellectual hub will advance academic, industrial, and governmental efforts in the science and engineering of quantum information, further fostering UChicago’s leadership in the field. It has become possible through UChicago’s extraordinary investments in hiring faculty members who specialize in quantum research and in building the associated laboratory and incubator infrastructure on campus, at Argonne National Laboratory, and at the Polsky Center for Entrepreneurship and Innovation.

“The combination of the University of Chicago, Argonne National Laboratory, and Fermi National Accelerator Laboratory, working together as the Chicago Quantum Exchange, is unique in the domain of quantum information science,” said Matthew Tirrell, dean and Founding Pritzker Director of IME and Argonne’s deputy laboratory director for science. “The CQE’s capabilities will span the range of quantum information, from basic solid state experimental and theoretical physics, to device design and fabrication, to algorithm and software development. CQE aims to integrate and exploit these capabilities to create a quantum information technology ecosystem.”

Gearing-up for water research

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The new quantum ecosystem will provide a collaborative environment for researchers to invent technologies in which all the components of information processing—sensing, computation, storage, and communication—are kept in the quantum world. This contrasts with today’s mainstream computer systems, which transform electronic signals from laptop computers into light for internet transmission via fiber optics, transforming them back into electronic signals when they arrive at their computer destinations, finally to become stored as magnetic data on hard drives.

Eight IME faculty members conduct research in quantum information and technology, one of the institute’s six major themes. Three members of that group are new hires: Professor Aashish Clerk and assistant professors Alex High and Tian Zhong.

Trio add expertise to quantum group

Aashish Clerk comes to IME from McGill University in Canada, where he served as a professor of physics. A theoretical physicist, Clerk pursues broad research interests in the quantum phenomena of engineered artificial systems. His work has applications in quantum information processing and quantum sensing. He plans to teach undergraduate...
“I’m confident that the Chicago Quantum Exchange will...”
Interdisciplinary Water Research Rises at the IME

The Institute's research in water is expanding, reaching from agriculture to medicine, basic science to product development.

In 2013 the IME launched the Water Research Initiative with Argonne National Laboratory and Ben-Gurion University of the Negev. Its focus: using molecular engineering to find new methods of water production, purification and preservation. The initiative’s first projects examined challenges in providing abundant, clean water around the world.

James Skinner arrives, accelerates the Water Research Initiative

That initial stream of research and innovation will become a torrent in the years ahead. In January, distinguished theoretical chemist James Skinner became the inaugural director of the initiative. As one of his first steps, he is hiring five scientists or engineers to launch research projects in a range of water-related areas.

“Water, and especially the energy-water nexus, is an important area to deploy IME’s bridge from the campus to Argonne,” said Matthew Tirrell, the Pritzker Director and Dean of IME. “Molecular ideas appropriate for the University can be deployed at scale through a national laboratory.”

Four areas of focus

The new projects will address four areas:

• producing clean water for people, industry and agriculture;
• using water to help meet the planet’s energy demands through finding efficient technologies to separate and capture hydrogen as a clean fuel;
• examining the role water can play in mitigating climate change; and
• understanding water’s role in biology and medicine and using that information to design new therapies.

Scientists and engineers working in these areas will develop new catalysts and advanced membranes for filtration, as well as new proteins and bio-compatible materials for use in medicine.

“This truly is an interdisciplinary effort,” Skinner said. “Engineering, chemistry, biology, physics: It is no stretch to say that you have to bring all these disciplines to bear on these problems. It’s exciting to be involved in something that’s so cross-cutting.”

The work of the past few years has created a foundation for the initiative’s expansion. About 30 scientists have participated in initial collaborations in which the three original institutions to include World Business Chicago, a government, research institutions and the investment community to leverage Chicago’s water assets to create new jobs and technologies.

The challenge of fouling

The team led by Seth Darling, an Argonne scientist and an IME Fellow, has been addressing the challenge of “fouling” – a problem in which membranes used to filter out contaminants from water clog and become unusable.

“When stuff ganks up those pores, it is harder to get water to go through,” Darling said. “That means it consumes more energy or you just have to replace or clean the membranes. It’s a universal problem in the industry and currently there’s really little you can do about it.”

Darling and his colleagues developed a novel coating that can be applied to membranes meant to filter out material, ranging from large dust particles to ions a few nanometers in diameter. The coating, deposited in a layer a few hundreds of atoms thick, makes it harder for organic and biological materials to stick to the pores and destroys them if they do. The compound also renders out organic pollutants in the water when exposed to sunlight.

“Micro-pollutants like pharmaceuticals end up in our waste water, and there aren’t especially good technologies today for taking them out,” Darling said. “This technology may be able to help.”

Creating a water research and technology hub

Research may be the heart of the Initiative, but its work also branches into government and industry. IME, for example, is a member of a new citywide initiative called Current that brings together water-intensive industries, government, research institutions and the investment community to leverage Chicago’s water assets to create new jobs and technologies.

The water initiative’s partners have grown from the three original institutions to include World Business Chicago, a public-private non-profit; the Illinois Department of Commerce and Economic Opportunity; UChicago’s Polsky Center for Entrepreneurship and Innovation; and the Energy Policy Institute at UChicago.
Analyzing the effects of dissolved salts on water structure

What is the extent to which dissolved salts modify water’s molecular structure? The important implications of this intriguing question include explaining the origin of the Hofmeister series, which ranks different salts on their ability to increase or decrease the solubility of large biomolecules in water.

Galli group simulations

IME’s Alex Gaduk, a fellow of the Natural Sciences and Engineering Research Council of Canada, and Giulia Galli, Liew Family Professor in Molecular Engineering, explored the question last March in the Journal of Physical Chemistry Letters.

Using state-of-the-art first-principles simulations of a sodium chloride solution in water, they determined that the constituent ions affect the liquid in different ways. The sodium ion Na+ has a strong local but a weak long-range effect on water structure. The chloride ion Cl−, meanwhile, has a weak local but a noticeable long-range effect on the hydrogen bond network of water.

Even though the effect of Cl− extends far from the ion, it is too weak to affect solubility of large biomolecules in water, suggesting that the Hofmeister series likely arises due to direct interaction of proteins with salts.

Pioneering a water quality sensing network in one of India’s longest rivers

An innovative combination of sensors in the water, networking in the Cloud, and change management on the ground promise potential solutions to age-old water quality problems along the River Godavari.

Sixty million people live within the Godavari River basin that drains into the Bay of Bengal on India’s east coast. The river’s water quality affects everyone, and the region stands to benefit from this first-of-its-kind sensor network installation and change management initiative. The Bill and Melinda Gates Foundation supports this work through a grant to the Administrative Staff College of India’s program to provide city-wide sanitation improvements for urban populations in the state of Andhra Pradesh. ASCI and UChicago experts collaborate to deliver innovative systems to assess water quality, gauge its impact on the local environment, and create more informed practices.

Two UChicago schools lead the way

The project is a tale of two UChicago schools—the IME and Harris Public Policy—addressing a real-world problem through very different fields of inquiry and knowledge. Together they are building connections that will elevate the research initiative beyond science.

IME Professor Supratik Guha, a specialist in sensing technologies and cyber-physical sensing networks, has partnered with UChicago law Professor Anup Malani, who leads the Chicago Harris School of Public Policy’s International Innovation Corps (IIC), a global collaboration program. They are investigating new systems for assessing, mapping, and positively impacting the water conditions at towns along India’s second-longest river system.

Sensing, collecting, mapping

By combining readily available, remote, in-the-water sensing technologies, with Cloud-based data collection and real-time mapping systems, the research and implementation teams intend to demonstrate the importance and value of detecting and anticipating pollutants that enter the river as human waste, organic materials, or chemical contaminants. This approach will uniquely use a boat-based mobile sensing platform that carries out streaming measurements, enabling water-quality maps (graphical color representations of the data known as heat maps) to be obtained in desired sections of the river.

By instantly measuring multiple quantifiable parameters and using data-analytics techniques, investigators expect to identify trends in pollution levels that are not easily or cheaply measurable on-site, such as microbial content. The multiple parameter heat mapping should also enable them to pinpoint sources of pollution entering the river.

Guha describes the IME’s role in terms of innovative engineering and systems building. “We will use two-to-five commercial mobile sensor platforms installed on boats moving through various points in the river to map water quality with high resolution and over time. The platform will be configured with an array of sensors, a power source, an onboard processor, a GPS and a cellular link for data communications.

“With these sensing installations, the IME will survey a section of the Godavari River and develop a Cloud-based data curation platform with the ability to push data about river conditions to mobile phones using visualization applications, making the data about pollutants publicly available and more accessible.”

Guha highlighted the novelty of this research: “Very little work has been done to date in this area, where large systems of sensors are combined with Big Data and physics models to create cyber-physical sensing systems for large water bodies. The work will be one of the first serious pilot programs to demonstrate the scalability, viability, and utility of this approach. The innovation will be in integrating this as an entire system.”

Malani, IIC co-founder and faculty director, explained the IIC’s contribution: “We work to identify and implement scalable, sustainable, high-impact interventions that make great leaps in solving pressing development challenges. This water-sensing project is a good example—leveraging top global talent here at UChicago and in India, and implementing the research through intensively trained IIC Fellows operating on the ground with the public sector in Andhra Pradesh. So this work is very much about connections—in technology and people.”

On the ground in Andhra Pradesh

Five IIC Fellows working in Andhra Pradesh are engaging with ASCI to channel the water-sensing results through cultivated government and civic relationships to bring new and actionable insights to the attention of local and regional authorities, agrarians, health professionals, and social agencies. The collected, curated, and visualized data should help assess benchmark levels of contamination and inform regulatory measures aimed at mitigating the pollution. IIC Fellows also will use the data analyses to optimize the sanitation program to maximize health and environmental benefits from interventions.

IIC Fellow Priyank Hirani and Srinivas Rao Balivada, a water quality expert who has recently joined the project, are driving the local implementation of the water-sensing research in Andhra Pradesh. This involves coordinating the technical aspects of the project for Guha while simultaneously advancing Malani’s vision of intervention—forming relationships and preparing the civic groundwork for meaningful change in local mindsets, water quality regulations, and infrastructure. Hirani enthusiastically views the challenge.

“This river monitoring project puts in motion a set of steps that can have a real impact on the condition of populations residing in the Godavari River basin,” he said.

In India, Guha has enlisted additional help on the Godavari water-sensing project from IBM Research, where he was director of physical sciences before joining the IME and Argonne National Laboratory.

“IBM is in the arena of the area of technologies related to the Internet-of-things and we are collaborating with a strong research group at IBM Bangalore who have been working in the area of analytics for water,” Guha said.

Toward the end of the project, the IME will also help evaluate the environmental impact of ASCI’s interventions and develop a prototype for more accessible water-sensing technology. The work will run through August 2018.
Water

Mapping the research landscape toward carbon-free energy from water splitting

At the University of Chicago, IME scientists and collaborators are fine-tuning the mechanisms required to generate hydrogen from water and sunlight.

Hydrogen production offers a promising approach for producing scalable and sustainable carbon-free energy. The key of a successful solar-to-fuel technology is the design of efficient, long-lasting and low-cost photo-electrochemical cells (PECs), which absorb sunlight and drive water-splitting reactions.

First-principle explorations of interfaces

Giulia Sallì, Liew Family Professor in Molecular Engineering, together with her former students T. Anh Pham, Lawrence Fellow at Lawrence Livermore National Laboratory; and Yuan Ping, assistant professor at the University of California, Santa Cruz, reviewed the use of first-principles methods to understand the interfaces between photo-absorbers, electrolytes and catalysts in PECs. Their work appeared in the Jan. 9 edition of *Nature Materials*.

The key to building an efficient PEC relies on the availability of abundant semiconducting photo-electrode materials that absorb sunlight and drive water-splitting reactions.

"Despite steady efforts and some breakthroughs, no single material has yet been found that simultaneously satisfies the efficiency and stability required for the commercialization of PEC hydrogen production technology," Pham said.

The team showed that with growing complexity of PEC architectures, understanding the properties of the interfaces between its components is key to predicting novel, better-performing materials, and eventually, to optimizing device performance.

In the *Nature Review* article, the team discussed open challenges in describing PEC interfaces using first-principles techniques, focusing on the interplay between their structural and electronic properties.

The scientists also reviewed first-principles techniques relevant for the study of solid-liquid interfaces, the structural and electronic properties of photo-electrode-water and photo-electrode-catalyst water interfaces and open theoretical challenges in the simulation of PEC interfaces.

The work was funded by a grant from the National Science Foundation Centers for Chemical Innovation and the Lawrence Fellowship.

Nanoscale Materials

Revealed: Inner workings of liquid crystals

Liquid crystals are used in everything from tiny digital watches to huge television screens, from optical devices to biomedical detectors. Yet little is known of their precise molecular structure when portions of such crystals interact with air.

New research led by Juan de Pablo, Liew Family Professor at the IME, uncovered previously unknown features that develop from the interface between air and certain widely studied liquid crystals.

"Liquid crystals are high-fidelity reporters of molecular events, and their effectiveness relies on controlling their molecular orientation at an interface," de Pablo said. "The precise understanding of this interface gained from our research will enable the design of better liquid crystal sensors and displays."

Teams collaborate, facilities deliver

For the research published Feb. 8 in the *Journal of the American Chemical Society*, de Pablo worked with a team of scientists at UChicago, including Binhua Lin and Benoit Roux, and at the University of Illinois at Chicago and the University of Wisconsin. They used synchrotron X-rays at Argonne National Laboratory and large-scale simulations to reconstruct the molecular details.

Liquid crystals exist in a state between liquids and solids, allowing them to flow like a liquid but also having some properties of a solid. Their molecules have a rod-like structure that can be organized in various ways. Certain liquid crystals go through phase transitions in response to changes in temperature. In the nematic phase, the rod-like molecules line up in a disorderly yet parallel fashion. In the smectic phase, they also line up in parallel—but in organized layers.

"Our research revealed a number of previously unknown features," de Pablo said. "For example, our findings indicate that the interface imprints a highly ordered, solid-like structure into the liquid crystal material. This structure then propagates well into the bulk of the liquid crystal, particularly for nematic and smectic phases."

The research found similar characteristics between the widely studied liquid crystals nematic 4-pentyl-4'-cyanobiphenyl and smectic 4-actyl-4'-cyanobiphenyl. Both align perpendicularly at the air-liquid crystals interface and exhibit well-defined, surface-induced layers at the interface. When both were heated to a fully liquid phase, only a single layer of structured molecules formed at the interface between the liquid and the air.

"THE PRECISE UNDERSTANDING OF THIS INTERFACE GAINED FROM OUR RESEARCH WILL ENABLE THE DESIGN OF BETTER LIQUID CRYSTAL SENSORS AND DISPLAYS."

— JUAN DE PABLO

The researchers plan to study the interfaces of liquid crystals and aqueous electrolytes to understand the effects of electrostatic interactions and the liquid crystal molecular structure.

"These results will be particularly important in guiding the design of responsive liquid crystal interfaces for sensing chemicals and biological molecules," the researchers concluded. 
Materials

Form predicts function? Tuning the electronic properties of organic semiconducting glasses

Research studies conducted over the last few years have shown that organic glass films formed by physical vapor deposition exhibit enhanced stability relative to those formed by conventional liquid cooling and aging techniques. Recently, experimental and computational evidence has emerged indicating that the average molecular orientation can be tuned by controlling the substrate temperature at which these “stable glasses” are grown. Reporting new findings in ACS Central Science on the structure of vapor-deposited organic glasses were IME graduate student Lucas Anthony, Argonne postdoctoral fellow Nick Jackson and Juan de Pablo, Liew Family Professor in Molecular Engineering. The co-lead authors of both papers were IME postdoctoral researchers Xiao Li and Jose Martinez-Gonzalez.

Breaking through blue-phase boundaries

Blue-phase liquid crystals usually consist of randomly oriented polycrystalline magnetic domains, a feature that has limited their performance for emerging electro-optical and sensing technologies. The team recently developed a new strategy to direct the self-assembly of blue-phase specimens and produce, for the first time, macroscopic single crystals of blue phases with a desired lattice orientation. This advance in appeared in Nature Communications.

“[These findings open up the possibility to fully exploit the optical features of blue phases, which until now have been hampered by the formation of grain boundaries, which could be particularly useful for design of a new generation of biological sensors, photonic materials, and liquid-crystal displays],” de Pablo said.

In the Proceedings of the National Academy of Sciences, the team explored another intriguing aspect of blue phases. The IME researchers found that they exhibit martensitic transformation, which involves concerted atomic motion but no intermingling of the constituent particles. Under precise conditions, the team discovered, regions of blue phases that encompass billions of molecules can behave like atomic scale processes.

To analyze the transformation between blue phases, the researchers developed a strategy to control their nucleation and growth. Once they achieved the ability to manipulate and produce a macroscopic single crystal, they studied the structural and dynamic details of the transformations.

A first: Self-assembly of macroscopic single blue-phase liquid crystals points toward better sensors, photonics, displays

Blue-phase liquid crystals are states of matter that are neither quite solid nor quite liquid. IME researchers published papers on these exotic substances in two high-profile journals earlier this year: the Proceedings of the National Academy of Sciences and Nature Communications.

Both papers were collaborations between the research groups of Juan de Pablo, Liew Family Professor in Molecular Engineering, and Paul Nealey, the Brady W. Dougan Professor in Molecular Engineering. The co-lead authors of both papers were IME postdoctoral researchers Xiao Li and Jose Martinez-Gonzalez.

Scientists make atoms-thick “Post-It” notes for solar cells and circuits

Over the past half-century, scientists have shaved silicon films down to just a wisp of atoms in pursuit of smaller, faster electronics. For the next set of breakthroughs, though, they’ll need novel ways to build even tinier and more powerful devices.

In a study published Sept. 20 in Nature, IME and Cornell University researchers described an innovative method to make stacks of semiconductors just a few atoms thick. The technique offers scientists and engineers a simple, cost-effective method to make thin, uniform layers of these materials, which could expand capabilities for devices from solar cells to cell phones.

Stacking thin layers of materials offers a range of possibilities for making electronic devices with unique properties. But manufacturing such films is a delicate process, with little room for error.

“The scale of the problem we’re looking at is: Imagine trying to lay down a flat sheet of plastic wrap the size of Chicago without getting any air bubbles in it,” said IME Professor Jiwoong Park, who led the study. “When the material itself is just atoms thick, every little stray atom is a problem.”

In their work, the team presented a comprehensive all-atom simulation study of ethylbenzene, a canonical stable-glass former, using a computational film formation procedure that closely mimics the vapor deposition process.

Energy

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Today, these layers are “grown” instead of stacking them on top of one another. But that means the bottom layers have to be subjected to harsh growth conditions such as high temperatures while the new ones are added—a process that limits the materials with which to make them.

Park’s team instead made the films individually. Then they put them into a vacuum, peeled them off and stuck them to one another, like “Post-It” notes. This allowed the scientists to make films that were connected with weak bonds instead of stronger covalent bonds—interfering less with the perfect surfaces between the layers.

High quality thin films, stacked

“The films, vertically controlled at the atomic-level, are exceptionally high-quality over entire wafers,” said Kibum Kang, an IME postdoctoral associate and the study’s lead author.

Kan-Heng Lee, an IME graduate student and the study’s co-lead author, then tested the films’ electrical properties by making them into devices and showing that their functions can be designed on the atomic scale, which could allow them to serve as the essential ingredient for future computer chips.

The method opens a myriad of possibilities for such films. They can be made atop water or plastics; they can be made to detach by dipping them into water; and they can be carved or patterned with an ion beam. Researchers are exploring the full range of the method’s potential, which they said is simple and cost-effective.

“We expect this new method to accelerate the discovery of novel materials, as well as enabling large-scale manufacturing,” Park said.
Energy technologies to benefit from predictions for liquid electrolytes

Liquid electrolytes are essential components in a variety of emerging energy technologies, including batteries, supercapacitors and solar-to-fuel devices. Now, IME’s Marco Govoni and Giulia Galli have presented an experimentally validated simulation strategy for computing the electronic properties of aqueous electrolytes.

“To predict and optimize the performance of these devices, a detailed understanding of the electrolytes, particularly their electronic properties such as the ionization potential and electron affinity, is critical,” said Lawrence Livermore National Laboratory’s Anh Pham, the lead author of a paper that reported the simulation strategy in the June 23 edition of Science Advances.

Simulations pinpoint solar cell atomic-level defects, possible solutions

Understanding a complex material with specific functions, and then engineering ways to improve its properties requires that scientists study its smallest parts. In the ongoing effort to improve solar cell energy conversion efficiencies, researchers have in some cases begun digging to the atomic level to identify material defects that can undermine the conversion process.

Heterogeneous nanostructured materials are widely used in a variety of optoelectronic devices, including solar cells. Due to their heterogeneous nature, however, these materials contain nanoscale interfaces exhibiting structural defects that can affect the performance of these devices. To identify these defects in experiments, researchers at IME and Argonne National Laboratory ran a series of atomistic calculations at Lawrence Berkeley National Laboratory’s National Energy Research Scientific Computing Center (NERSC). The goal was to find the root cause of defects in two commonly used semiconductor materials—lead selenide (PbSe) and cadmium selenide (CdSe)—and provide design rules to avoid them.

Energy

“We are interested in understanding quantum dots and nanostructures and how they perform for solar cells,” said Giulia Galli, co-author of a paper published in Nano Letters that presents the findings. “We are doing modeling, using both classical molecular dynamics and first-principle methods, to understand the structure and optical properties of these nanoparticles and quantum dots.”

Tuning quantum dots, sunny-side-up

For this study, the team focused on heterostructured nanoparticles—in this case a colloidal quantum dot in which PbSe nanoparticles are embedded in CdSe. This type of quantum dot—also known as a core-shell nanoparticle—is like an egg, said Márton Vörös, Aneesur Rahman Fellow at Argonne and co-author on the paper. A “yolk” made of one material is surrounded by a “shell” made of the other material. “Experiments have suggested that these heterostructured nanoparticles are very favorable for solar energy conversion and thin-film transistors,” Vörös said.

Contributing to the work along with Govoni, a visiting scientist; and Galli, Liew Family Professor in Molecular Engineering, were three other scientists from the Livermore Lab and the University of Southern California.

Pham noted that proper energy alignment at the electrode-electrolyte interface of photoelectrochemical (PEC) cells is key to achieving efficient hydrogen production.

The team demonstrated that the coupling of its simulation strategy with advanced spectroscopy techniques provides a powerful tool for the identification of chemical species and reactions that occur in solutions.

The new method makes it possible to predict the electronic response in complex electrolytes for a range of applications. For example, the research provided a theoretical foundation for understanding and engineering the electronic properties of liquid electrolytes in PEC cells for hydrogen production and ionic liquid for batteries.

“The proposed computational framework is general and applicable to non-metallic liquids, offering great promise in understanding and engineering solutions and liquid electrolytes for a variety of important energy technologies,” Pham said.

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Energy

“We are interested in understanding quantum dots and nanostructures and how they perform for solar cells,” said Giulia Galli, co-author of a paper published in Nano Letters that presents the findings. “We are doing modeling, using both classical molecular dynamics and first-principle methods, to understand the structure and optical properties of these nanoparticles and quantum dots.”

Tuning quantum dots, sunny-side-up

For this study, the team focused on heterostructured nanoparticles—in this case a colloidal quantum dot in which PbSe nanoparticles are embedded in CdSe. This type of quantum dot—also known as a core-shell nanoparticle—is like an egg, said Márton Vörös, Aneesur Rahman Fellow at Argonne and co-author on the paper. A “yolk” made of one material is surrounded by a “shell” made of the other material. “Experiments have suggested that these heterostructured nanoparticles are very favorable for solar energy conversion and thin-film transistors,” Vörös said.

While colloidal quantum dot energy conversion efficiencies currently hover around 12 percent in the lab, “we aim at predicting quantum dot structural models to go beyond 12 percent,” said Federico Giberti, postdoctoral research scholar at IME the lead author of the Nano Letters paper. “If 20 percent efficiency could be reached, we would then have a material that becomes interesting for commercialization.”

To make this happen, however, Vörös and Giberti realized they needed to better understand the structure of nanoscale interfaces and whether atomic defects were present. So, along with Galli, they developed a computational strategy to investigate, at the atomic level, the effect of the structure of the interfaces on the materials’ optoelectronic properties. Their framework allowed them to build computational models of these embedded quantum dots. Using this model as the basis for a series of simulations run at NERSC, the research team characterized the PbSe/CdSe quantum dots and found that atoms that are displaced at the interface and their corresponding electronic states—what they call “trap states”—can jeopardize solar cell performance. They then used the model to predict a new material that does not have these trap states and that should perform better in solar cells.

“Using our computational framework, we also found a way to tune the optical properties of the material by applying pressure,” Giberti said. “We believe that our atomistic models, when coupled with experiments, will bring a predictive tool for heterogeneous nanostructured materials that can be used for a variety of semiconducting systems. We are very excited about the possible impact of our work.”

This research, which was funded by the U.S. Department of Energy’s Office of Science, used four million supercomputing hours at NERSC. Looking ahead, the research team plans to use this new computational framework to investigate other materials and structures.
Arts, Sciences, and Technology

Professional artists and scientists working together in the STAGE lab

Attempting to create theatrical pieces using research methodologies of experimental science has been the mantra at the STAGE lab since its inception. Traditional story development in the professional theatre world typically does not allow ample room for exploration, as the process tends to be result-driven. This year, in a series of two workshops, the STAGE lab collaborated with more than twenty scientists and artists, including actors, writers, dramaturgs and designers from various regions of the country. The group spent their time prototyping and improvising within a highly collaborative, research-oriented work process. Under the guidance of Nancy Kawalek, Professor and Distinguished Fellow in the Arts, Sciences and Technology at the IME, this exploration led to the development of a new theatre piece, The Art of Questionable Provenance.

Exploring critical themes

The Art of Questionable Provenance is both a mystery story and a tale of perception that parallels the functions of the brain. It explores critical themes emerging from modern neuroscience and examines how we piece together the stories—real or illusory—of ourselves. Do the firings of neurons in particular patterns ultimately determine who we are?

STAGE uses scientific experimentation and research as a model for its creative process, starting with a hypothesis (a central premise) and ending with a “publication” (a fully-scripted performance). Initial research for Provenance led to themes of perception, the science of consciousness, and connectomics (the study of maps of neural connections in the brain). Following this line of research gave rise to the idea of a museum as a perfect setting for a play about perception, and an art diagnostician—who uses multispectral imaging to examine great works of art—as the main character. Through improvisation, a play developed: the scientific analysis of artwork and the science of human thought are woven into a complex story about people who, through a series of misperceptions, have metaphorically lost their way in life, and what they go through to get back on course.

As in all of the STAGE lab’s work, technology plays an integral role in the story telling. For example, as Provenance deals with the science of consciousness, one of the grad student collaborators used Google Deep Dream software to prototype the video imagery for a particular scene. Employing an artificial neural network to convey the workings of the brain’s neural network gave rise to projections that echoed the theme of Provenance on multiple levels.

THE MAIN CHARACTER, AN ART DIAGNOSTICIAN, DISCUSSES HER WORK ON A LATE-NIGHT TALK SHOW IN A SCENE FROM THE ART OF QUESTIONABLE PROVENANCE.

Premiere at the STAGE lab

The first public performances of The Art of Questionable Provenance were held in the STAGE lab’s theatre space in May, at the end of a developmental workshop of the play. They received overwhelmingly positive responses from the more than 150 audience members who attended: students, faculty, and staff, as well as scientists and artists from different parts of the country. The play—imbued with humor, depth, and stunning visual imagery—gave the audience the visceral experience that STAGE believes is key in engaging the public’s interest in science and technology, and to having a broader impact in that endeavor.

ERC art installation promotes inquiry, dialogue

On October 3, 2017, the William Eckhardt Research Center lobby became the temporary home for the installation/sculpture by Chicago-based artist Dan Peterman, MFA’86: Slipping and Jamming: Variable Installation of Z-Forms.

Peterman’s work explores the tension between structural stability and instability. It is composed of thousands of “Z-Forms”—post-consumer reprocessed plastic elements (each cut in the form of a Z) that, when assembled into large sculptural installations, embody a counter-intuitive idea: the possibility of creating load-bearing, stable forms not by orderly arrangement of the individual elements, but by random, disordered configurations (held together through friction and gravity) that structurally resemble a liquid with the potential to flow.

Assembled on site by Peterman, the sculpture was facilitated by the Arts, Science & Culture Initiative at UChicago as an aspect of the Chicago Architecture Biennial, and was supported by the University of Chicago’s Public Art Committee.

THE END OF THE PLAY.

GOOGLE DEEP DREAM PROTOTYPED USING SEQUENCE THAT WAS REVEALED IN A VIDEO SUBSCONSCIOUS IS FAR LEFT: IN PROVENANCE, THE ART DIAGNOSTICIAN’S SUBSCONSCIOUS IS REVEALED IN A VIDEO SEQUENCE THAT WAS PROTOTYPED USING GOOGLE DEEP DREAM SOFTWARE. LEFT: A SCENE FROM THE END OF THE PLAY.
Quantum Information

Researchers use atomic-scale defects to communicate quantum states in semiconductor material

An international team led by IME has discovered how to manipulate a weird quantum interface between light and matter in silicon carbide along wavelengths used in telecommunications.

The work advances the possibility of applying quantum mechanical principles to existing optical fiber networks for secure communications and geographically distributed quantum computation. The IME’s David Awschalom and his 13 co-authors announced their discovery in the June 23 issue of Physical Review X.

“Silicon carbide is currently used to build a wide variety of classical electronic devices today,” said Awschalom, Liew Family Professor in Molecular Engineering. “All of the processing protocols are in place to fabricate small quantum devices out of this material. These results offer a pathway for bringing quantum physics into the technological world.”

International collaboration facilitates discovery

The findings are partly based on theoretical models of the materials performed by Awschalom’s co-authors at the Hungarian Academy of Sciences in Budapest. Another research group in Sweden’s Linköping University grew much of the silicon carbide material that Awschalom’s team tested in experiments at UChicago. And another team at the National Institutes for Quantum and Radiological Science and Technology in Japan helped the UChicago researchers make quantum defects in the materials by irradiating them with electron beams.

Exploiting Entanglement

Quantum mechanics governs the behavior of matter at the atomic and subatomic levels in exotic and counterintuitive ways as compared to the everyday world of classical physics. The new discovery hinges on a quantum interface within atomic-scale defects in silicon carbide that generates the fragile property of entanglement, one of the strangest phenomena predicted by quantum mechanics. In entanglement, two particles can be so inextricably connected that the state of one particle can instantly influence the state of the other, no matter how far apart they are. “This non-intuitive nature of quantum mechanics might be exploited to ensure that communications between two parties are not intercepted or altered,” Awschalom said.

The findings enhance the once-unexpected opportunity to create and control quantum states in materials that already have technological applications, Awschalom noted. Pursuing the scientific and technological potential of such advances will become the focus of the newly announced Chicago Quantum Exchange, which Awschalom will direct.

An especially intriguing aspect of the new paper was that silicon carbide semiconductor defects have a natural affinity for moving information between light and spin (a magnetic property of electrons).

“A key unknown has always been whether we could find a way to convert their quantum states to light,” said David Christie, a former IME postdoctoral scholar and lead author of the work. “We knew a light-matter interface should exist, but we might have been unlucky and found it to be intrinsically unsuitable for generating entanglement. We were very fortunate in that the optical transitions and the process that converts the spin to light is of very high quality.”

The defect is a missing atom that causes nearby atoms in the material to rearrange their electrons. The missing atom, or the defect itself, creates an electronic state that researchers control with a tunable infrared laser.

Extracting information from electron spins in commercial silicon carbide

“What quality basically means is: How many photons can you get before you’ve destroyed the quantum state of the spin?” said Abram Falk, a researcher at the IBM Thomas J. Watson Research Center in Yorktown Heights, N.Y., who is familiar with the work but not a co-author on the paper.

The IME researchers found that they could potentially generate up to 10,000 photons, or packets of light, before they destroyed the spin state. “That would be a world record in terms of what you could do with one of these types of defect states,” Falk added.

Awschalom’s team was able to turn the quantum state of information from single electron spins in commercial wafers of silicon carbide into light and read it out with an efficiency of approximately 95 percent.

The duration of the spin state—called coherence—that Awschalom’s team achieved was a millisecond. Not much by clock standards, but quite a lot in the realm of quantum states, in which multiple calculations can be carried out in a nanosecond, or a billionth of a second.

The feat opens up new possibilities in silicon carbide because its nanoscale defects are a leading platform for new technologies that seek to use quantum mechanical properties for information processing, sensing, and communication using light.

“The defect is a missing atom that causes nearby atoms in the material to rearrange their electrons. The missing atom, or the defect itself, creates an electronic state that researchers control with a tunable infrared laser.”

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Quantum Information

NSF grant:IME, Harvard launch nation’s first university-industry quantum graduate research program

The Institute for Molecular Engineering and the Chicago Quantum Exchange (CQE) have partnered with Harvard University to launch the nation’s first university-industry research and education program in quantum information science and engineering (QISE) with a grant of nearly $1.6 million from the National Science Foundation.

“The intent is to develop a tightly integrated university-industry network focused on QISE,” said David Awschalom, Liew Family Professor in Molecular Engineering and CQE director. QISE-NET will pioneer a new approach to graduate education as it assembles three-person teams of university faculty, industrial researchers, and graduate students who will serve as pivotal components of the collaborations.

Students selected for QISE-NET will benefit from the mentorship of both academic and industrial advisors on QISE research topics that will pursue leading-edge science and engineering along with longer-term industrial goals. The students will serve as the principal communicators in residence at both the universities and in industry, translating ideas into research results. Approximately 16 students will receive four years of funding under the program.

Awschalom will develop QISE-NET in collaboration with Evelyn Hu, Harvard’s Tarr-Coyne Professor of Applied Physics and of Electrical Engineering.

“I AM TREMENDOUSLY EXCITED BY THE DRAMATICALLY DIFFERENT EDUCATIONAL FORMAT OF THE QISE-NET PROGRAM, WHICH ALLOWS GRADUATE STUDENTS TO PLAY THE PIVOTAL ROLE IN A NEW, CONVERGENT APPROACH LINKING INDUSTRY, NATIONAL LABS AND ACADEMIA IN PUSHING FORWARD THE FRONTIERS OF QUANTUM SCIENCE.”

— EVELYN HU

Double agents: Vessels that enable cancers can also boost immune therapies

In a surprise finding, an international research team from the IME, the University of Lausanne, and the Swiss Federal Institute of Technology in Lausanne has discovered that the lymphatic vessels, often blamed for enabling cancer cells to spread from a primary location to many other sites, have a flipside.

Lymphatics can expand around and into a tumor—a process known as lymphangiogenesis. This process has long been associated with a cancer’s ability to spread to new locations. But a team led by IME’s Melody Swartz found that in patients being treated with checkpoint inhibitors—drugs that help activate an immune response against the tumor—lymphangiogenesis can strongly enhance the effects of cancer immunotherapy. It boosts the immune system’s primary anti-cancer tool, T cells, enabling them to infiltrate tumors and kill cancer cells.

The study, published in the Sept. 13 issue of Science Translational Medicine, suggests that physicians may predict—with a simple blood test before starting treatment—which patients are most likely to benefit from cancer immunotherapy, at least in melanoma patients. Currently, only a minority of patients actually benefit from such therapies. Moreover, it has the potential to lead to new therapeutic strategies to make cancer immunotherapy more effective for more patients.

Our study presents a completely unexpected role for the lymphatic system in cancer therapy,” explained Melody Swartz, William B. Ogden Professor in Molecular Engineering. Lymphatic vessels “play on both teams,” enabling both metastasis and T-cell invasion. Lymphangiogenesis is driven in part by a chemical messenger, vascular endothelial growth factor-C (VEGF-C), which has long been associated with metastasis and poor patient prognosis, and can also promote immune suppression in tumor microenvironments.

“IT WAS EXCITING TO GET SUCH SURPRISING RESULTS. AND THE TRANSLATIONAL IMPLICATIONS ARE EVEN MORE EXCITING THAN IF OUR HYPOTHESIS HAD BEEN CORRECT.”

— MELODY SWARTZ

“VEGF-C was always considered bad for cancer patients,” said Swartz. “We thought that blocking VEGF-C would help boost immunotherapy by removing some factors that suppress the abilities of T cells to kill tumor cells. That was our original hypothesis.” But their studies in mice, followed by human data obtained from two clinical trials for melanoma patients, changed their thinking.

“It was exciting to get such surprising results,” Swartz said. “And the translational implications are even more exciting than if our hypothesis had been correct.”

A possible biomarker for immunotherapy candidates

In both trials, the results showed that VEGF-C levels in the blood before immunotherapy “not only predict the magnitude and quality of immune responses raised by a cancer vaccine but also stratifies long-term patient responses to combined checkpoint blockade and further strengthens the case for investigating the use of serum VEGF-C as a predictive biomarker for immunotherapy candidates,” the authors wrote.
Immuno-engineering

The authors noted several limitations, including the T cell infiltration into metastatic tumors and resulted in the difference was striking. Almost all patients with understanding the immune microenvironment said. “We measured dozens of factors, but nothing else correlated, not VEGF-A, VEGF-D or other growth factors, only VEGF-C.”

The difference was striking. Almost all patients with higher-than-average VEGF-C levels in their blood responded to immunotherapy. This not only resulted in eradication of the primary tumors, it also encouraged T cell infiltration into metastatic tumors and resulted in long-term protection. This could become a useful biomarker, Swartz suggested. “It’s easy to measure from a blood sample. And it can predict who is likely to respond. If VEGF-C is low, immunotherapy is much less likely to be effective.”

Understanding the immune microenvironment

The authors noted several limitations, including the potential effects of VEGF-C on other immune cell subsets. This study “brings into focus a more comprehensive understanding of the immune microenvironment,” Swartz said.

“We now appreciate the numerous mechanisms of immunosuppression that a T-cell-inflamed tumor develops to survive, including lymphangiogenesis,” the authors conclude. “But when the scales are tipped toward activating factors dominating over suppressive ones, as is the case with immunotherapy, these T cells become robust participants in antitumor immunity.”

The study was funded by the Swiss National Science Foundation, the European Research Council, SwissTransMed, and Fonds Pierre-François Vittone.

Tirrell Group Targets Heart Disease with Nanoparticles

Imagine deploying billions upon billions of nanoparticles to serve as diagnostic and therapeutic agents for battling heart disease which claims approximately 600,000 lives annually in the United States alone. In a series of recent studies, Matthew Tirrell and his colleagues have begun pioneering such a strategy.

“We think we actually have a legitimate, workable therapy,” said Tirrell, the Institute for Molecular Engineering’s Pritzker Director, Professor and Dean. A great deal of work remains to be done, however, to translate a promising material into deployed treatments.

“When you can land the particle at the plaque—helping you to see it—that’s good. But if you can simultaneously deliver something that has a beneficial effect, that’s even better. And we have that now,” Tirrell said.

The Tirrell group’s nanoparticles spontaneously assemble themselves through chemical reactions, and can carry peptides—protein fragments—that foster a desired biological activity such as homing to blood cells. “These nanoparticles are modular,” Tirrell noted. “You can plug in different functionalities very easily, just by making different molecules and then allowing them to assemble.”

Some, for example, could have a targeting effect, while others could help with diagnostics by improving contrast for any of several medical imaging techniques.

NIH grant funds further investigation

In his most recent work, Tirrell has collaborated with Yun Fang, an assistant professor of medicine at the University of Chicago. “He pointed out to us that maybe the best therapeutic agents would be certain kinds of nucleic acid inhibitors of certain activities in the endothelial lining of blood vessels, which is where this heart disease occurs,” said Tirrell. “This led them to make a different kind of nanoparticle that carries nucleic acids in its core. These nucleic acids promote various activities that reduce inflammation and that help transport fats out of the endothelial lining.

“THE NIH GRANT ALLOWS US TO TEST THE EFFECTIVENESS OF THESE NEWLY ENGINEERED NANOPARTICLES IN TREATING MAJOR VASCULAR DISEASES SUCH AS HEART ATTACK AND STROKE IN ANIMAL MODELS.”

— YUN FANG

“The most promising nucleic acid inhibitor that we’ve been looking at is one that reduces inflammation,” Tirrell said. And now he and Fang have received a $1.9 million grant from the National Institutes of Health (NIH) to develop nanoparticles to treat serious conditions where inflammation is a factor.

Jeffrey Hubbell discusses his entrepreneurial research career, materials science and immunology, and tissue engineering

Jeffrey Hubbell collected two noteworthy honors this year. In April he earned the Society for Biomaterials’ 2017 Founders Award, which goes to individuals who have made long-term, landmark contributions to the discipline of biomaterials. Two months later he was named the inaugural Eugene Bell Professor in Tissue Engineering. Hubbell develops biomaterials of many sorts, especially for regenerative medicine and for delivery of various therapeutic agents. His work includes molecular and materials-engineering approaches to immunotherapy for infectious disease and cancer.

Q: You’ve co-founded five companies, three of which relate to your research at IME. What should we know about the most recent, Clostrabio, co-founded with Cathryn Nagler, the Bunning Food Allergy Professor at UChicago?

A: That company relates to delivering microbial metabolite molecules to the gut to try to re-establish gut barrier function. The gut becomes leaky in allergy. We want to re-establish gut barrier function in patients with dis-regulated microbiome and associated food allergy. We’re using some materials chemistry in our laboratory and animal models in immunology in Cathryn’s laboratory to try to ameliorate allergies to foods like peanuts.

Q: How did this effort evolve out of your research program?

A: It was motivated by a publication of Cathryn’s showing what kind of dis-regulation in the gut resulted in loss of gut-barrier function. Based on what microbes were absent one can make reasonable guesses about what metabolites those missing microbiomes would have produced. We weren’t working in that area before. After a conversation with her we decided to try to make materials that could indeed produce and release those metabolites.

Q: How did your entrepreneurial activities evolve?

A: It’s something I started trying to do intentionally. I very much wanted to be able to prove that ideas work. We develop new therapies and I didn’t find it very satisfying to do something in the laboratory and then conclude that it works when the final test is whether or not it works in humans. So we try as quickly as we can to move to realistic animal models of disease in a laboratory. But another approach is to start a company around the technology and then to build a whole team to move toward humans. It was an intentional desire to prove whether ideas had validity or not and thereby have impact in society.

Q: Do the entrepreneurial activities impact your students?

A: These entrepreneurial exercises are very much a two-way street, where the start-up collaborates with the academic lab, and the academic lab collaborates with the start-up. This provides a great way for trainees to get exposure to different styles of doing research. I find it a really important part of the lab training for students and postdocs. They get to see much more than the goal of publishing a paper; it’s a paper that’s got legs to go on and have impact beyond the publication.

Q: You work in the relatively new field of immune-modulating materials. How big is that research community today and what is its growth potential?

A: There are probably 20 labs working in materials science and immunology now around the world. If you go back 10 years, it would’ve been just two or three labs working in that field. So yes, it’s a growing area where people realize that instead of only making drugs to modulate immunity, one can also make materials to modulate immunity. We’re focusing on that kind of material-drug interface.

Q: You also work in tissue engineering. What’s the status of your work in that arena?

A: We’re asking questions about how you deliver growth factors–biomolecules in the body that induce morphogenesis–in the most effective way. They induce tissue-repair processes. Chronic wounds are a target of ours. Diabetics especially develop chronic wounds in their feet, which can lead to limb amputation and loss of productivity and quality of life. We’ve shown in mouse models of autoimmune diabetes that we can indeed accelerate wound healing.
Seth Darling discusses the IME’s status, his work, and his artistic interests

Seth Darling’s perspectives on the origin and evolution of the Institute for Molecular Engineering are deeply rooted in the University of Chicago and in Argonne National Laboratory. He received his doctorate in chemistry from UChicago in 2002, when he joined Argonne as a postdoctoral researcher. A scientist at Argonne’s Center for Nanoscale Materials, he became an IME Fellow in 2013. In August he was appointed IME’s director at Argonne.

Q: From your various perspectives at UChicago and Argonne, what stands out in your mind about the origin and evolution of IME at the University?

A: It’s easy to forget that a few years ago there was no IME, no building, no labs, no faculty, no students. And I can remember the days, which were not that long ago, when engineering might be considered a bad word in certain company at the University. In a remarkably short period of time since then, the IME has built a thriving organization with exciting science and engineering bubbling up all over the place. The University certainly made one of its best decisions in my 20-or-so-year experience with UChicago when it hired Matt Tirrell as IME’s founding director. His leadership and vision seeded the IME with an inaugural cohort of faculty who brought instant credibility and recognition to the organization and created an environment that has continued to grow and foster excellence since that time. And evolution of IME at the University?

Q: What are your responsibilities as IME director for Argonne?

A: Broadly speaking, I’m charged with providing scientific vision, technical guidance, and leadership to IME at Argonne. A big piece of this includes facilitating connections between IME students and Argonne and Argonne researchers. Students are the most effective glue between these two institutions and really between most pairs of research institutions that try to work together. Another big piece is being a program integrator here at the Laboratory. The purview of molecular engineering as we envision it is broad. It covers chemistry and some biology and physics and materials science and also process engineering and technology transfer. To stitch that all together into an integrated program is the role of the Institute for Molecular Engineering at Argonne.

Q: Your own research interests span a range of fields of research, including materials for solar energy and water treatment, plus, you’ve co-authored a book on climate change. Do they have some underlying commonality?

A: A lot of things interest me, but it’s not a random walk through science. The vast majority of what I do is ultimately motivated by trying to make society better. I don’t have the skill set to heal sick people or address fiscal inequalities. I’m a scientist and so the best tool I have for making a difference is science. Climate disruption and the water crisis are certainly two of the biggest challenges we face as a society. Those are great examples both of massive global need and an area in which science can help. And so I try my best to steer my research effort in those directions.

Q: You have a fairly longstanding interest in the interplay between science and art. How did this interest come about?

A: I’ve always had an interest in the aesthetics of science and aesthetics in general. I do mosaic art on the side, for example. I enjoy the aesthetic side of life, not just the technical side. There’s great aesthetic to science, which is often overlooked. More broadly, though, it’s part of my interest in science communication. Art is a tool that can help with that. We’re in a time, probably more than ever in our history, when scientists have an obligation to communicate with non-scientists, with the public. It’s an enormously important thing to do and it’s something I enjoy doing.

Q: What are you working on now in your research?

A: These days I’m excited about working on advanced materials for cleaning up water. It’s the prospect of coming up with things that can impact the next Deepwater Horizon disaster or the next Flint, Michigan, or providing safe water to the developing world. It’s fun to come to work, even when it’s hard, when making that kind of difference is the light at the end of the tunnel. There’s a remarkable void in this space of advanced materials for water, relative to, say, energy. Many research institutions have a collection of researchers working on energy. The same is not true for water and yet the scale of the problem is just as massive.
IME RECOGNITION

Honors & Awards

David Awschalom chairs AAAS section on physics, named Vannevar Bush Faculty Fellow

David Awschalom, Liew Family Professor in Molecular Engineering, in January was elected Chair of the Section on Physics of the American Association for the Advancement of Science. The world’s largest multidisciplinary scientific society and a leading publisher of cutting-edge research through its Science family of journals, AAAS has individual members in more than 91 countries worldwide.

Awschalom also was selected as a 2017 Vannevar Bush Faculty Fellow in March. The Department of Defense fellowship provides $3 million dollars for bold and ambitious “blue sky” research that may lead to extraordinary outcomes such as revolutionizing entire disciplines, creating entirely new fields, or disrupting accepted theories and perspectives.

Jun Huang receives National Science Foundation CAREER Award

Jun Huang, assistant professor in molecular engineering, brought the prestige of a Faculty Early Career Development (CAREER) Award from the National Science Foundation to UChicago last February. His research project, “Single-molecule Imaging of T-cell Recognition and Signaling,” will receive $500,000 in funding over a five-year period.

T-cells are a type of white blood cell that scans the human body for cellular abnormalities and infections. Huang’s goal is to understand the molecular mechanism of T-cell recognition and signaling, which determine the selection, development, fate, and function of a T cell.

Juan de Pablo delivers polymer science plenary lecture at national meeting

Juan de Pablo, Liew Family Professor in Molecular Engineering, presented the 2017 Polymers and Polymer Science Plenary Lecture at the American Chemical Society National Meeting last April in San Francisco. His talk, “Directed Assembly of Hierarchical Polymeric Materials,” focused on his group’s recent work on DNA-based polymeric materials and described some of the design principles that are emerging from such efforts. He also received the 2017 Polymeric Materials Science and Engineering Plenary Lecture Award at the event.

Jeffrey Hubbell becomes inaugural Eugene Bell Professor, earns Biomaterials Founders Award

Jeffrey Hubbell, the MacLean Professor of Molecular Engineering Innovation and Enterprise, in April received the Society for Biomaterials’ 2017 Founders Award, presented to individuals who have made long-term, landmark contributions to the discipline of biomaterials.

In June, Hubbell became the inaugural Eugene Bell Professor in Tissue Engineering at UChicago. The Bell Professorship promotes innovative work at IME and the Marine Biological Laboratory in Woods Hole, Mass.

American Institute of Chemical Engineering names Eun Ji Chung to 35 under 35 in bioengineering

Former IME postdoctoral scientist Eun Ji Chung is one of 35 notable young professionals under the age of 35 who was honored in August by the American Institute of Chemical Engineering. Chung, the Gabilan Assistant Professor in Biomedical Engineering at the University of Southern California, was honored based on her achievements in bioengineering.

David Awschalom chairs AAAS section on physics, named Vannevar Bush Faculty Fellow

Juan de Pablo delivers polymer science plenary lecture at national meeting

Jeffrey Hubbell becomes inaugural Eugene Bell Professor, earns Biomaterials Founders Award

Eun Ji Chung receives National Science Foundation CAREER Award

American Institute of Chemical Engineering names Eun Ji Chung to 35 under 35 in bioengineering
IME students among 15 who present “Science Cafés” at Chicago’s Museum of Science and Industry

The Junior Science Café program at the Museum of Science and Industry creates a series of events that awaken in primary and high school students scientific curiosity. Through dynamic demonstrations and hands-on activities, they experience scientific processes and thought-provoking results.

Two IME grad students rose to the challenge of hosting Science Cafés in the last several months. In support of STEM (Science, Technology, Engineering, and Math), the IME students talked with attendees about their career paths and their personal journeys into science.

The Future of Solar Power

In December, 2016, the IME’s Arin Greenwood discussed with students the importance of renewable energy, especially solar energy—the subject of her own research. She explained how nanoparticles can be used to make inexpensive and versatile solar cells. She brought to the classroom three different types of 3D-printed nanoparticles to show the students how they can be made in different shapes and sizes. Through a connect-the-dots activity the students also learned how electrons travel through nanoparticle solar cells as compared to a typical commercial silicon solar cell.

“Through the experience I received the opportunity to learn how to express my own research in terms that would be understandable by a group of middle school students, and really just learn how to teach a young audience,” Greenwood said. “I especially loved seeing the excitement on the students’ faces.”

From Tiny Particles to Planets and Gene Therapy

In April, 2017, IME grad students Hao Wu and Jiuyan Li conducted experiments and computer simulations during their presentation to show participants how tiny charged particles attract oppositely charged particles via electrostatic interaction, a universal phenomenon of everyday life. They extended this phenomenon to explain how planets form in the same manner. They also discussed how small particles can be used to encapsulate small gene segments to treat deadly diseases.

“The Junior Science Café experience was one of the best moments that I had during the two-year MSI program,” Wu said. He added that he came away amazed at his audience’s curiosity and willingness to learn, at the broad spectrum of scientific knowledge that the students possessed, and at the interest and aspiration they expressed in contributing to scientific advancement.

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“Through the experience I received the opportunity to learn how to express my own research in terms that would be understandable by a group of middle school students, and really just learn how to teach a young audience,” Greenwood said. “I especially loved seeing the excitement on the students’ faces.”

Embracing the start-up culture in one of Google’s strategic initiatives

Klimov, PhD’16, has tackled such varied projects that one might say his specialty is intellectual agility. He can pick up a complex problem that he knows nothing about, analyze, understand, and distill it into its fundamental aspects; and then solve those aspects quickly and precisely.

“Usually this process requires teamwork, which gives me the opportunity to understand the problems from different perspectives and learn far more than would be possible solo,” said Klimov, who earned his doctoral degree from the Institute for Molecular Engineering in 2016 as a member of David Awschalom’s group. “In many ways, my IME training taught me to think and work in this way and got me excited about this type of work.”

Since June 2016, Klimov has honed his intellectual agility as a quantum electronics engineer on the Google Quantum AI team, which is building a quantum computing platform and applying it to artificial intelligence and machine learning. The Quantum AI unit is designing hardware and software that replaces Boolean logic by quantum law at the algorithmic level. For certain computations such as optimization, sampling, search, or quantum simulation this promises dramatic speedups. Many tasks in these areas rely on solving hard optimization problems or performing efficient sampling.

“We embrace the start-up culture, in which each member wears several hats,” Klimov said. “As a result, I’ve had the opportunity to contribute to many interesting projects.”

IME ALUMNUS Profile

PAUL Klimov

Quantum Electronics Engineer, Google Quantum AI, Santa Barbara, California

Embracing the start-up culture in one of Google’s strategic initiatives

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Water for the World: A Crown Family Celebration

On February 13, 2017, The University of Chicago celebrated the arrival of James L. Skinner as Crown Family Professor of Molecular Engineering and director of the Water Research Initiative at the William Eckhardt Research Center.

The event highlighted the IME’s water research partnership with Ben-Gurion University of the Negev, which began in 2013, and the potential impact that UChicago can bring to developing water research technology with support from the Crown Family’s investment. The initiative—originally charged with using nanotechnology to create new materials and processes for making clean, fresh drinking water more plentiful and less expensive by 2020—is broadening its scope.

The Crown Family Professorship was made possible by an endowment from UChicago Trustee James S. Crown, who was among the distinguished guests. Other trustees attending were Steven Kersten, president of WaterSaver Faucet Co., and his wife Priscilla; and Michael Polsky, founder, president, and CEO of Invenergy, LLC. Also attending the event were UChicago President Robert Zimmer, University of Chicago Deputy Mayor Steven Koch, Joining them were Chicago University officials, IME and chemistry faculty members and guests from Argonne National Laboratory and Ben-Gurion University.

Delivering the keynote address was Seth Siegel, author of the acclaimed, Let There Be Water: Israel’s Solution for a Water-Starved World. Following the address was a panel discussion led by Matthew Tirrell, Pritzker Director, Professor, and Dean of the IME. In addition to Skinner and Siegel, the panel consisted of Elion Adar, director of the Zuckerberg Water Research Institute at Ben-Gurion University; and Seth Darling, director of IME at Argonne National Laboratory. Darling led the Argonne team that developed the Oleo Sponge, a highly effective new technology for recovering oil and other petroleum products from water bodies. (See pp 25–26 for Darling Q&A)

Skinner spoke of the potential use of nanotechnology in creating new materials and processes for water purification based on hydrogen bonding. Tirrell provided perspective on the broad range of the Institute’s research projects that have the potential to impact technological challenges facing society.

Seattle, Washington, May 4

David Awschalom and Andrew Cleland addressed a group of Seattle alumni on IME’s basic and applied research in the emerging field of quantum engineering. They outlined the big picture of the physics involved, and described the highlights of each of their team’s work in quantum computation, quantum communication, and quantum sensing.

Harper Lectures update alumni on the impact and potential of IME’s mission

Scottsdale, Arizona, March 23

Matthew Tirrell and James Skinner provided UChicago alumni with overviews of the IME’s ongoing pursuits within the Water Research Initiative. Launched in 2013 in collaboration with researchers at Ben-Gurion University of the Negev and Argonne National Laboratory, the initiative covers a broad range of issues, including water availability, potability, climate change, and energy.

Support for the IME continues

From its founding through the fall quarter of 2017, the IME has benefited from the vision and generosity of many:

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Development

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