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2015 MRS Spring Meeting

2015 MRS Spring Meeting
April 6–10, 2015
San Francisco, California

2015 MRS SPRING MEETING & EXHIBIT

Meeting Day Four—Thursday

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The technical symposia continued in full swing throughout the day, topped off with the poster session in the evening. Highlights in between include presentations by **Karena W. Chapman** and **Ali Javey** who each received an Outstanding Young Investigator Award, and **Daniël Vanmaekelbergh** who discussed colloidal nanocrystals in Symposium X. We also include here news on **Samuel Stupp**'s plenary address from Wednesday.

Meeting Highlights

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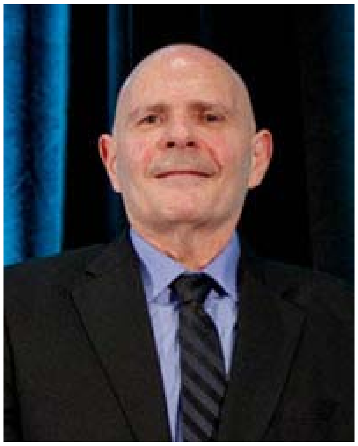
Plenary Session

Samuel Stupp, Northwestern University
Bio-Inspiration and Energy Landscapes in Soft Materials Design



Samuel Stupp began his presentation by noting that supramolecular materials—assemblies of molecular structures—are newcomers to the group of soft materials that traditionally have included polymers, organic and liquid crystals, and gels. He gave, as examples, the polar stacking of mushroom-shaped units via self-assembly to produce piezoelectric films and the vision of the self-assembly of device-like structures for photovoltaics with up to 1 million molecules per assembly. These materials can mimic the structures and physical properties of biological systems and therefore offer a rich platform for bio-inspired materials design, drawing on collagen matrices, protein complexes, ribosomes, chromosomes, and extracellular filaments—highly dynamic "parts" of cells that make life possible. Moreover, the biomimetic potential of supramolecular matter gives it the ability to reconfigure, adapt, order, and respond. Just as muscle responds to chemical fuels by contracting, a biomaterial could reconfigure to optimize signaling at a cell surface. Such dynamic materials offer the prospect of self-healing of defects, low energy recycling, fast biodegradation, directional charge transport, integration of multiple functions in a single material, and more.

Stupp provided examples of soft-matter design using supramolecular structures that integrate functions for energy applications or exhibit dynamic features of interest in bioactive materials. He began with a brief look at a room-temperature ferroelectric created from three-dimensional hydrogen-bonded networks of electron acceptors and donors. Moving on to supramolecular materials for photocatalytic and photovoltaic applications, he cited two examples: the development of supramolecular materials that mimic photosynthetic machinery by integrating light-harvesting components and catalytics systems, and the synthesis of a DuBois catalyst for photocatalytic production of hydrogen. Shifting to bioactive supramolecular materials, Stupp discussed cell signaling for biomedical targets, cell management with biomimetic supramolecular fibers, and regenerative medicine. It has been shown, for example, that supramolecular nanofibers can promote differentiation of neural stem cells into neurons, a possible strategy for neurodegenerative diseases, such as Parkinson's, Alzheimer's, and Lou Gehrig's (ALS). Then, citing the case of amphibians that regrow amputated limbs, Stupp asked "can we mimic such spatiotemporal control over bioactivity?" He then discussed computer-simulated free-energy surfaces for protein folding, where the structure and hence its function are determined by the folding pathway, and extending the principle to supramolecular materials, where a thermodynamically stable but non-bioactive material could become bioactive if it is kinetically trapped in a different structure.

In closing, Stupp took a brief look at the future prospects for supramolecular materials, emphasizing the need to draw on computational materials science to accelerate discovery of new supramolecular materials functions, such as materials that are reversibly responsive, dynamic, adaptable, or capable of integrating synergistic functions. These features emulate biological structures such as cells.

Outstanding Young Investigator Award

Karena W. Chapman, Argonne National Laboratory
Accelerating the Development of Energy Materials Through Advanced X-ray Tools

In her presentation, Karena Chapman described *in situ* (*operando*) measurements to directly probe critical processes during materials synthesis or operation by means of advances in pair distribution function (PDF) methods that can provide atomic-scale structural insights for systems that are beyond the limits of conventional crystallography (e.g., nanoscale, disordered, amorphous, and heterogeneous materials). Because they can penetrate materials under actual operating conditions, hard x-rays with energies 10 times higher than those in typical laboratory sources are an ideal tool. She uses the Advanced Photon Source at Argonne National Laboratory, whose intense and highly collimated beams allow the use of area detectors to record entire *in situ* spectra in a fraction of a second, thereby making time-resolved measurements of complex, heterogeneous materials feasible. Developing a reaction cell that allowed samples to be measured under realistic conditions was equally important.

Her first example of how to probe an energy material was unraveling complex reactions in nanoscale materials for advanced lithium-ion batteries with higher energy-storage capacities, faster charge and discharge rates, and longer cycling stabilities. For example, a time-resolved study of a starting electrode material containing iron oxyfluoride showed that it separated into a lithium salt and iron nanoparticles during discharge, but while charging did restore the storage capacity it did not restore the initial crystalline rutile structure but was instead a mixture of oxygen-rich rock salt and iron-rich amorphous rutile phases; that is, the iron and fluoride were partitioned. All in all, a single experiment was able to decouple electrochemistry, phase, oxidation state, particle size, and chemistry.

One candidate approach to advanced batteries beyond lithium-ion systems is the use of doubly charged magnesium ions because they have a doubled energy density. But the higher charge density means that the ions in the electrolyte are surrounded by more shells of tightly bound solvent molecules and these can impede ion movement between electrodes or prevent reactions at the electrode, suggesting that new electrolytes must also be identified. Chapman described the use of the PDF to probe the electrolyte structure by drawing on principle component analysis to provide the reference that allowed differential techniques to isolate the magnesium component. Switching gears, she showed how PDF could explore materials synthesis, using the example of zeolite-supported silver clusters for radiological gas capture and catalysis. Again, principle component analysis allowed species evolving separately to be distinguished, so that quantitative kinetics and reaction mechanisms were derivable from the evolution of the reaction products. In this case, infrared spectroscopy was used simultaneously with the x-ray measurements to provide information about low-atomic-number species, such as hydrogen.

Ali Javey, University of California, Berkeley
Emerging Materials for Future Electronics and Solar Cells

In accepting an Outstanding Young Investigator Award this evening, Ali Javey showcased a dazzling array of recent innovations from his research group at the University of California–Berkeley, before previewing some exciting new, unpublished data.

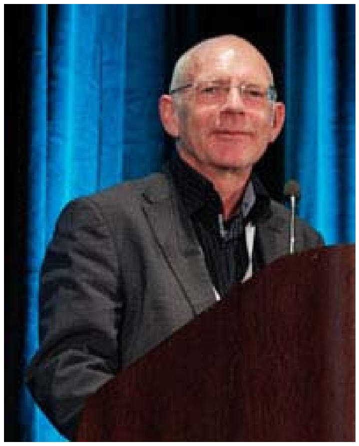
Materials innovation is at the core of all his research group's work, Javey said. The showcase he presented included monolayer doping of semiconductors, flexible interactive surfaces that emit light when pressed with a finger, electronic heterojunctions made of liquid-state components, and programmable materials that change their shape in response to temperature or light. Innovations like these are the reason why Javey was receiving the Young Investigator Award, but he flew through them to get to some recent data he was clearly excited about.

The vision driving Javey's newest work is to grow single crystalline semiconductor films on any substrate, like glass, plastic, or cloth, which no conventional growth method can do. If MOCVD or MBE are used—today's main thin-film growth techniques—to grow films on non-epitaxial substrates, the lateral size of crystalline domains is limited to roughly the thickness of the film. To achieve the large single-crystalline domains required for high-performance electronics, Javey turned to vapor-liquid-solid growth techniques (MOCVD and MBE use vapor-solid growth modes), fabricating templates that trapped a thin layer of liquid indium between a molybdenum foil substrate and a capping layer of silicon oxide. He then flowed phosphor vapor through the capping layer, into the liquid indium, to grow films a few nanometers thick with grain sizes greater than 500 µm.

Those findings were published in 2014, but Javey's excitement this evening was about new work in which he successfully used this method to grow single-crystalline indium-phosphide films on amorphous silicon oxide. To demonstrate the flexibility of their technique, Javey showed a single-crystal indium-phosphide film in the shape of a UC–Berkeley logo, about 70 µm across. He and his group have done *in situ* germanium doping of these films (in less whimsical geometries), achieving optoelectronic properties on par with state-of-the-art semiconductor films grown on epitaxial substrates.

Indium-phosphide films are a prototypical model system, but Javey says these techniques can be extended to many other materials systems. This latest innovation from the Javey group has exciting implications for low-cost solar cells and light-emitting diodes and three-dimensional electronics. The question, he asked, is just how far can we push it?

Symposium X: Frontiers of Materials Research



Daniël Vanmaekelbergh, University of Utrecht
Colloidal Nanocrystals: From Individual Quantum Objects to Building Blocks for Honeycomb Semiconductors Hosting Dirac Carriers

Freestanding crystalline honeycombs composed of semiconducting nanocrystals with graphene-like electronic properties: that's the punch line from Daniël Vanmaekelbergh's lunchtime lecture today in Symposium X, and to anyone interested in condensed-matter science, it's enough to make you forget you're missing lunch. Hailing from the University of Utrecht, Vanmaekelbergh presented a 30,000-foot view of research on colloidal semiconductor nanocrystals before zooming in on his work using those nanocrystals to create two-dimensional superlattices.

The history started in 1990 when colloidal nanocrystals (NCs) were first created at Bell Labs. These early NCs were synthesized at high temperatures to anneal out defects, and the resulting quantum dots ignited an explosion of research into the physical properties of these novel structures. In 1996, we saw the first core–shell NC systems and other heterostructures, with incredible chemical stability. Single-quantum-dot studies took off in 2000, when researchers starting interrogating individual NCs to better understand their electronic and optical properties, like photoluminescent blinking and Auger recombination.

At this point Vanmaekelbergh backtracked to mention that in the middle of that wild decade of discovery, around 1995, researchers starting using colloidal NCs as building blocks, assembling them into ordered superlattices as if each NC were a giant atom. These superlattices can be formed from a solution of NCs by simply allowing the solvent to evaporate slowly. Driven by entropy and van der Waals forces, the NCs come together in ordered structures, but they remain weakly bound and quantum-mechanically isolated from one another by surface-passivating ligands.

Another approach to making NC superlattices is reactive self-assembly, in which NCs bond facet-to-facet with atomic order across the interface. The process, known as oriented attachment, is controlled via evaporation temperature, capping ligands, and NC concentration—a process that Vanmaekelbergh describes as “miraculously simple.” Using this technique, Vanmaekelbergh and colleagues create freestanding two-dimensional structures, centimeters across but just a single NC-layer thick. These two-dimensional superlattices are exciting because they have both crystalline atomic order and long-range order, resulting in unusual combinations of electronic and optical properties.

Vanmaekelbergh discussed his work on PbSe NCs, which come together in either a square geometry (bonding at the {100} facets) or a honeycomb geometry (bonding at the {110} facets). Via cation exchange, the PbSe superlattices can be transformed into CdSe superlattices, which have particularly desirable semiconducting properties.

To verify this model of PbSe and CdSe NC assemblies, Vanmaekelbergh presented atomic-resolution TEM data, XRD, and EELS spectra. He collaborated with theorists to predict the electronic structure of these superlattices via tight-binding calculations and analytical models, which were then matched by data from four-point-probe transport measurements and optical absorption spectra.

Vanmaekelbergh noted that this was a “small historical moment,” his talk being the last MRS Symposium X—Frontiers of Materials Research lecture in San Francisco. (The MRS Spring Meeting moves to Phoenix next year.) This lucid talk proved a fitting conclusion

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Women in Materials Science and Engineering Breakfast

Kate C. Farrar, American Association of University Women
The Next Generation of Women's Leadership

Kate C. Farrar of the American Association of University Women (AAUW) challenged the attendees at the Women in Materials Science & Engineering Breakfast to come up with one thing they can each do today to support the next generation of women leaders. Farrar said the responsibility lies at the individual, workplace, and community levels. “Leadership,” Farrar finds, has numerous definitions.

When she asked the audience to name women leaders, one person shouted out "Millie" which received boundless applause as the audience recognized Mildred S. Dresselhaus of the Massachusetts Institute of Technology, who was also at the Breakfast. Millie is a leader, said this audience member, "because if I need information on graphene spectroscopy, she's the one to go to." Farrar said that leadership education is now being developed as a discipline. At AAUW, Farrar particularly works with students to develop leaders. "Stepping into leadership early is important for seniority," she said. She pointed to Princeton University and Harvey Mudd College as examples of campuses that have been successful in increasing the number of women leaders. Next comes changing the corporate culture to be more conducive to establishing a diverse leadership. In the meantime, on the ground level, individuals can begin with themselves and take The Implicit [Bias] Test created by Harvard. Once we are aware of our biases, we are better positioned to do something about it, Farrar said.

Government Funding Opportunities

At each MRS Meeting, the MRS Government Affairs Committee brings in representatives from several US government departments and agencies to describe programs that fund basic research in materials science. New this year was Teresa Axenson, Program Manager for the Director's Innovation Initiative (DII) within the National Reconnaissance Office (NRO). NRO supports defense and national communities, with the primary responsibility of collecting intelligence. In terms of funding research and development, the NRO establishes a risk-tolerant environment for conducting potentially high payoff projects that are revolutionary. Axenson showed a few examples of materials-related projects, including "robust GaN electronics," "novel nanostructured battery to reduce size and weight," and "membrane array antenna." The NRO goal is that 10-15% of the completed DII projects are further developed. The National Science Foundation, ARPA-E, and the Department of Energy (DOE) are traditionally represented at the MRS Meetings. This year, DOE's Harriet Kung—Director of Basic Energy Sciences (BES)—emphasized the importance of the federal government's support of basic research that enables breakthroughs leading to technology. Among the examples Kung reviewed are the BES's impact on photovoltaics technologies and trends in Lithium-ion batteries that saw their way to commercialization.

Technical Sessions

Symposium R: Photoactive Nanoparticles and Nanostructures

Photovoltaic Windows: Towards Energy-Zero Building
Sergio Brovelli, University of Milano Bicocca

Silicon photovoltaics (PVs) are optimized for use on rooftops. Large cities with skyscrapers and tall buildings preclude the use of Si PVs, since rooftop area is low. Applying PVs to the sides of building allows use of a much larger area, but this requires PVs to be integrated with windows, demanding transparency and thermal insulation. To address this, Sergio Brovelli designed PVs with a blend of chromophores in glass that absorb light and reemit it to be captured by PV cells at the edges of glass windows. However, these chromophores re-absorb their emitted light, which means much light is lost before being absorbed by the PV cells. To improve this device, Brovelli's group replaced the chromophores with core–shell quantum dots (QDs), with a thick copper indium selenide sulfide (CuInSeS) shell, used for light absorption, and a zinc sulfide (ZnS) core, used for light emission at a wavelength that the shell cannot absorb. This results in complete suppression of re-absorption of light, which was shown experimentally. The efficiency of these PVs is 3.2%, which may seem low, but calculations show that covering a skyscraper in these PVs and assuming that 50% of the incident sunlight is captured would generate 900kW of power—enough to power 300 apartments.

Symposium U: The Interplay of Structure and Carrier Dynamics in Energy-Relevant Nanomaterials

Full-Color Light-Emitting Diodes Based on Colloidal Quantum Dots for Next-Generation Displays
Changhee Lee, Seoul National University

From bulky cathode ray tubes (CRTs) to plasma screens to liquid crystal displays (LCDs) to light-emitting diodes (LEDs), the display industry has evolved dramatically in a mere 60 years. While LCDs currently dominate the market due to their affordability, Changhee Lee predicts OLEDs will soon overtake LCDs. OLEDs have matured since Lee established the first OLED team in Korea a little over 20 years ago; LG recently installed OLED lighting throughout Seoul National University's library. Historically, the ability to mass produce and the higher quality displays determined the future dominance of new display technologies. Beyond OLEDs, Lee prognosticates quantum dots (QDs) to be the next generation of display technology. The display quality is better because the emission band is narrow, yielding purer colors. The superior color gamut of QDs will produce images with more natural colors. Currently, quantum dot efficiency is low, but recent studies have improved it to 7% efficiency for red, 6% for green, and 2% for blue. Most importantly, QDs can utilize the manufacturing infrastructure of OLEDs.

Symposium W: Light-Matter Processes in Molecular Systems and Devices

Quantifying Electronic Transitions in Emitters through Computational Spectroscopy
Rashid Zia, Brown University

Researchers are interested in measuring absorption and emission properties to determine information about electronic transitions in materials, which Rashid Zia measured using Fourier-space imaging. Most materials operate within the electric dipole approximation, in which the wavelength of light is much smaller than the geometry of the particles being considered. However, when the wavelength of light is large compared to the geometry of the particles under study, the electric dipole approximation no longer applies, and the particle exhibits higher order multipolar resonances, such as magnetic dipoles (MDs) and electric quadrupoles (EQs). Zia uses emission measurements to identify EQ and MD behavior in lanthanides. He also revealed that lanthanides exhibit comparable emission rates by EQ and MD transitions. Finally, he uses wide-angle measurement to determine the multipolar composition of materials using only a single measurement, called "computational wide-angle spectroscopy, which leverages the natural basis of quantum emitters." This allows one to determine the multipolar composition of a material in the entire IR spectra using only one quick (10 second) measurement.

Symposium Z: Plasmonics and Metamaterials—Synthesis, Characterization and Integration

Electrically Tunable Metasurfaces and Metamaterials
Harry A. Atwater, California Institute of Technology

Harry A. Atwater is developing tunable metamaterials to modulate the resonant properties of such a material in a dynamic fashion. Current metamaterials are mostly tuned by static methods. In a metamaterial composed of gold colloids suspended in an electrolyte, sandwiched between two ITO resonances, Atwater showed experimental modulation of the extinction response by applying a voltage bias. However, the experimentally measured response did not match the theoretical predictions obtained from the Drude model fit for the dielectric function. As such, Atwater decided to look beyond the Drude model, and discovered that he needed to include the voltage dependence of the dielectric function, which affected the scattering rate of electrons that reside on the surface of the gold particle. By taking this into account, the simulated response matched the measured results very well. He also discussed plasmonic properties of graphene, in which the extreme mode confinement of graphene was shown to produce fantastic Purcell factors. By arranging graphene layers on silicon nitride with a gold backing layer, Atwater shows full absorption of an incident beam using the principles of a Salisbury screen. Since materials that exhibit strong absorption also exhibit strong emission, he decided to investigate the emissivity of graphene under bias, and demonstrated the plasmonic modulation of blackbody emission.

Symposium HH: Supramolecular Materials—Assembly and Dynamics

Functional Assemblies and Interfacial Dynamics with Cucurbiturils
Oren A. Scherman represented by Matthew Rowland, University of Cambridge

Oren A. Scherman was unable to attend the conference, so his talk was presented by a senior PhD student in his group. The researchers in Scherman's group have established their brand in materials science through the use of cucurbit[n]urils as aqueous hosts. The interior of these bowl-shaped molecules is very hydrophobic, which makes storing water inside the host system very high energy in aqueous systems. Instead, other hydrophobic molecules enter the cucurbit[8]uril host with extremely high association constants. Using this system, Scherman's group has created materials that form gels in water with self-healing properties. The guest molecules typically used for this gel contain viologen and naphthalene, which are considered too toxic for biomedical applications. Instead, the group found a combination of amino acids that enter the host cucurbit[8]uril and form the same kind of gel, opening the way for clinical work. Additionally, cucurbit[8]urils were placed on gold nanoparticles in water. The resulting surface enhanced raman spectroscopy investigation was sensitive enough to track the reaction progress of a single molecule.

Control on Morphology of Ligand Shell in Gold Nanoparticles
Francesco Stellacci, EPFL

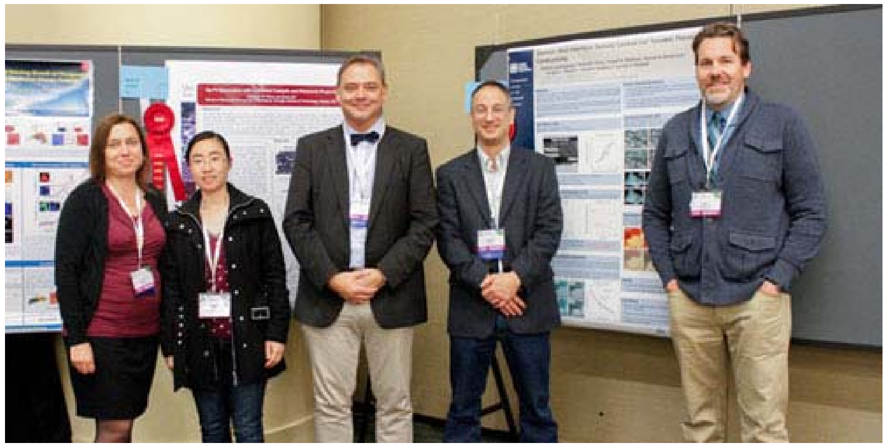
In his second lecture of the day, Francesco Stellacci explained how ligands adopt different morphologies on a gold nanoparticle. When two different ligands are mixed on a nanoparticle surface, one might expect two completely different phases due to entropy. Instead, the Stellacci Group has frequently observed the appearance of stripes along the nanoparticles. Is it possible to measure the size and arrangement of the stripes detected by STM? Taking the Fourier Transform of the image is not sufficient, so the group has been extracting information from the power spectral density of the images. Additionally, small angle neutron scattering has been employed to directly obtain information about the stripes found on the nanoparticles. In order to get this information, the team mixed deutero and proteo versions of hexanethiol and dodecanethiol. This allowed for the absolute determination of the nanoparticle surface morphology, confirming the presence of stripes. Ongoing theoretical work aims to explain the origin of this complicated phenomenon.

Symposium PP: Gold-Based Materials and Applications

Nanoparticles and Transmissible Diseases
Francesco Stellacci, EPFL

"I'm going to tell you about something today that's dear to my heart," Francesco Stellacci conceded. With a passion for eradicating diseases that disproportionately afflict poor countries, the Stellacci Group is engineering how nanoparticles interact with viruses. The team sees this as an opportunity to use nanoparticles as a learning tool, while simultaneously attacking some of the world's most terrible organisms like Ebola and Rotavirus. A key insight is that viruses need to latch onto a cell surface in order to infect the host. By attaching heparan sulfate proteoglycan (HSPG), a ligand involved in cell surface signaling, to gold nanoparticles, the team was able to specifically target pathogens. In this way, the virus was tricked into believing it had found a host cell, causing it to open its cell contents prematurely. Interestingly, HSPG by itself did not cause the viruses to rupture. It was only effective when attached to the nanoparticle. This should be a useful tool in the Stellacci Group's ongoing fight against viruses.

Thursday Poster Awards



Ag-Pd Nanocubes with Combined Catalytic and Plasmonic Properties
Jumei Li, Georgia Institute of Technology

Domain Wall Interface Density Control for Tunable Thermal Conductivity
David A. Scrymgeour, Sandia National Laboratory

Not shown: *Large-Area Heteroepitaxial Stacking and Stitching of Hexagonal Transition-Metal Dichalcogenide Monolayers*
Hoseok Heo, Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science (IBS), POSTECH

MRS TV Video of the Day

MRS Bulletin Special Issue on Propelling Innovation

Scanning the Meeting

About the Meeting Scene

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