Greetings! What you will find in this newsletter is a glimpse of the latest happenings in the Materials Science Program at UC, San Diego. The program is wide-ranging and is involved in engineering (Mechanical and Aerospace, Electrical, Structural, Nanoengineering, and Bioengineering), and the science (Physics, Chemistry and Biology) departments, and the School of Medicine. Indeed, our program is dynamic proof of the pervasiveness of materials science. Close to one hundred faculty are associated with the program, which is on a continual upward trajectory of growth and development.

You will find here samples of the work in the program, ranging from the mechanics of soft materials, the latest in perovskite solar cells and DNA biosensors, skin-inspired mechanoreceptors, to computational methodologies for novel material design.

We are glad to welcome more than 70 new graduate students with far reaching diversity and scientific and technological range. A seminal award named after a pioneering ex-colleague, the late Prof. Gareth Thomas (who worked at both UC, Berkeley and UC, San Diego), was given to Eric Hahn, whose work included seminal contributions in the molecular dynamics of materials. In addition to regarding the accomplishments of our students, we take pride in our alumni. Chi Nung Ni discusses aspects of how his doctoral training enabled him to navigate life in industry in Silicon Valley. Chiara Daraio, now a Professor in Caltech discusses fondly her time spent in the Materials Science program.

We hope you enjoy reading the newsletter and always welcome your feedback, support and good wishes.

Sincerely yours,

Prab R. Bandaru
Soft materials can be easily found in biological systems and daily life. However, the research on the mechanics of soft materials is still in a nascent stage. Dr. Cai’s group focuses on studying mechanics of a variety of soft materials such as electroactive polymers, liquid crystal elastomers, hydrogels and soft tissues. Dr. Cai’s group aims to understand large deformation, fracture, instability, and multifield coupling in those soft materials.

A recent study conducted in the Cai group has identified an important toughening mechanism in polydomain liquid crystal elastomer. The group’s research shows that a crack propagating in a polydomain liquid crystal elastomer may involve polydomain-to-monodomain transition of the material near the crack path (Figure 1), which results in a significant increase of its fracture toughness.

Another example is that, using polydomain liquid crystal elastomers, the Cai group has developed a simple and robust way to fabricate a reversible mechanochromic trilayer system as shown in Figure 2. The trilayer film can change its color through mechanical stretching or heating, and this process can be quickly reversed through releasing the stretch or cooling. Potential applications of such systems include the use as biomimetic camouflage and strain sensors.

Eversion-induced mechanical instability in an elastomer tube was reported several decades ago, but a satisfying explanation of the phenomenon has not been available until a combination of experiments and theoretical analysis conducted in the Cai group successfully resolved a long-lasting discrepancy between the theoretical predictions and experimental observations of surface instability in an everted tube as shown in Figure 3.

In response to a stimulus, soft materials, such as hydrogels and elastomers, can deform dramatically. This deformation provides most of their functions. Cai and his colleagues have formulated theories to better understand the interplay of mechanics and other fields, including chemistry, electric field and temperature, in soft materials. He has also studied several ways of using soft active materials to convert energy in different forms. Cai is currently investigating how to design and optimize structures made of soft materials to provide diverse functions, including harvesting energy, regulating fluid and desalinating salt water. He is also looking into using the mechanical instability phenomena associated with large deformation in soft materials to guide electromagnetic waves and provide other functions.
The hybrid organic-inorganic lead halide perovskites are an emerging new class of solar absorbers that show significant promise for revolutionizing solar by enabling solar cells made from earth-abundant materials at a fraction of the cost of current silicon-based solar cells. Recent advances have pushed the solar conversion efficiency from a few percent to 22.1% within several years, making perovskites already one of the most efficient solar technologies in existence. The materials have disruptive potential in solar cells and beyond, including other optoelectronic devices such as LEDs, lasers, and photodetectors due to their inexpensive fabrication cost and excellent optoelectronic properties.

Perovskite solar cells are made of hybrid materials, meaning that the active absorber layer consists of a mix of organic methylammonium (MA) halide and an inorganic lead halide in a 3D crystal structure. The properties and performance of the resulting MAPbX3 absorber, where X = Cl, I, or Br, is significantly influenced by spatial heterogeneities in elemental makeup. The all-iodide MAPbI3 chemistry has been the most extensively pursued for photovoltaic applications. Recently, researchers in the field have enhanced photovoltaic performance by introducing small amounts of Cl-containing precursors during the fabrication of the absorber layer. In our work, we use synchrotron-based nanoprobe X-ray fluorescence (NANO-XRF) to identify where chlorine is incorporated in the final device and characterize its heterogeneous spatial distribution in the MAPbI3-xClx films. We find that Cl can be introduced via the organic or the inorganic precursor and tends to reside at the boundaries of perovskite crystallites, indicating it likely plays a direct role in reducing defects and enhancing performance. This nanoscale investigation of the local chemistry of the emerging perovskite materials opens new directions toward understanding how minor amounts of additives such as chlorine can be harnessed to optimize and stabilize hybrid perovskite solar cells.

Professor Fenning’s research focuses on engineering materials for renewable energy conversion and storage, especially low-cost photovoltaics, direct photoelectrochemistry, and hybrid photovoltaic-electrochemical systems. Current research includes defect engineering in high-efficiency silicon solar cells, and coupling photovoltaics with electrochemistry for solar-to-fuel water splitting and CO2 reduction. His research emphasizes understanding and parameterizing defect/reaction kinetics and leverages a variety of synchrotron-based X-ray characterization, including in-situ synchrotron-based measurements of semiconductors, catalysts, and electrode interfaces. By developing a thorough understanding of the defects that dictate device performance, Professor Fenning’s research works toward the development of predictive models of material processing that enable accelerated material development and innovation.

**Revealing Nanoscale Variations in the Chemistry of Next-Generation Solar Cells**

(a) Nano-X-Ray Fluorescence (NANO-XRF) experimental set up for measuring full solar cell devices. (b) Spatial map of the chlorine-to-iodine stoichiometry in organic-inorganic lead iodide perovskite solar cell materials with nanoscale resolution. (c) Spatially resolved elemental maps indicating the preferential chlorine distribution at the boundaries of crystallites within CH3NH3PbI3-xClx perovskite films.

Single nucleotide polymorphisms (SNP) in a gene sequence are markers for a variety of human diseases. Current DNA sequencing, including SNP detection, primarily uses enzyme based methods or fluorophore-labeled assays that are time consuming, need lab-scale settings, and are expensive. Existing electrical charge-based SNP detectors have insufficient specificity and accuracy limiting their effectiveness. In the recent paper, we have demonstrated the use of a DNA strand displacement-based probe on a graphene field effect transistor (FET) for high specificity single nucleotide mismatch detection (Proc. Natl. Acad. Sci. 2016. Doi: 10.1073/pnas.1603753113). It will have wide applications in digital and implantable biosensors and high-throughput DNA genotyping with transformative implications for personalized medicine.

Gold-coated Magnetic Nanobowl Composite colloidal structures with multi-functional properties have wide applications in a targeted delivery of therapeutics and imaging contrast molecules and high-throughput molecular bio-sensing. Our goal is to develop drug carriers that we can direct to any part of the body, hold them there until they release their payload, and then direct them away—all done using a small magnet. This would enable us to control the release of drug payloads in our system. Our group has constructed a multifunctional composite magnetic nanobowl using the bottom-up approach on an asymmetric silica/polystyrene Janus template consisting of a silica shell around a partially exposed polystyrene core. The PEGylated magnetically-responsive nanobowls show size-dependent cellular uptake in vitro. (Nanoscale, 2016, 8, 11840)

Professor Lal is an authority on biomedical applications of atomic force microscopy (AFM) and nanoscale imaging of complex biological systems. Research in his lab involves the development of nanotechnologies for and multi-scale biophysical and system biology studies of channels and receptors. His lab also designs nanosensors and devices for biomedical diagnostics and therapeutics.
Biomimetic Tactile Devices for Neuro-Prosthetics: A Skin-Inspired Organic Digital Mechanoreceptor

A research frontier in thin-film device technologies is the transformation of conventional materials and fabrication processes to meet the demands of soft, pliant, and often easily damaged surfaces. Such research has created novel flexible electronics with tremendous impact on fields ranging from bio-electronics to energy sustainability. In the Flexible Printed Electronics Lab (http://flexible-electronics.ucsd.edu/), Professor Tina Tse Nga Ng and her group aim to push the boundary of how electronics are made and used, to potentially incorporate electronic control and power sources into any object, in order to realize seamless human-computer interfaces. Her group’s approach is based on scalable additive printing. This printing approach allows low-temperature patterning that is compatible with a wide range of materials, reduces wastes from mask steps, and enables rapid design changes and complex geometric or materials permutation. The group’s vision for flexible electronics is not only to create new stretchable objects and applications, but also to increase design and process versatility by taking advantage of printing fabrication techniques to engineer new material properties. The interplay between electronic and mechanical properties will enhance the functionalities of flexible actuators or sensors. They are working to discover fundamental materials principles and establish a fabrication platform with unprecedented design freedom.

In a collaborative project between Professor Ng and Professor Zhenan Bao at Stanford, the team demonstrated a biomimetic tactile device for neuro-prosthetics (Fig. 1, "A skin-inspired organic digital mechanoreceptor," Science, 350 (2015) 313–316). Through inkjet printing, Professor Ng realized organic ring oscillator circuits for a power-efficient analog-to-digital signal conversion scheme. As force was applied on the tactile sensor, the output frequency ranged from between 0 – 130 Hz to mimic slow-adapting skin mechanoreceptors. Then the sensor output was shown to successfully stimulate an optogenetically engineered somatosensory neuron in-vitro, achieving neural stimulations in accordance with pressure levels. This novel sensor design opens a new path to realize more sensitive prosthetics with touch feedback.

Professor Tina Tse Nga Ng’s research focuses on the development of flexible electronics. Her vision for flexible electronics is not only to create new stretchable objects and applications, but also to increase design and process versatility by taking advantage of digital fabrication techniques. Her work includes demonstration of bendable image sensors for x-ray medical imaging, complementary organic circuits and non-volatile memory for a sensor tape that monitors head concussions.
The Paesani group develops new theoretical and computational methodologies for molecular-level simulations of complex condensed-phase systems, ranging from porous materials to interfaces. Combining machine-learning techniques with modern quantum chemistry and statistical mechanics approaches, the Paesani group is interested in modeling proton conduction, ion transport, and magnetic properties of porous nanomaterials as well as interfacial chemical processes. Direct connection with experimental measurements are made through many-body molecular dynamics, a new simulation methodology developed by the Paesani group, which enables molecular-level computer simulations with unprecedented accuracy. For his contributions to the area of theoretical and computational chemistry, Prof. Paesani has received several awards, including the OpenEye Outstanding Junior Faculty Award from the American Chemical Society in 2014, the CAREER Award from the National Science Foundation in 2015, and the Early Career Award in Theoretical Chemistry from the American Chemical Society in 2016.

Current research focuses on modeling magnetic properties and proton conduction in metal-organic frameworks (MOFs). In a recent study, [J. Am. Chem. Soc. 138, 6123 (2016)], the Paesani group has reported the first theoretical analysis of the spin-crossover behavior of the [Fe(pz)[Pt(CN)4]] MOF upon water adsorption (Figure 1). Through computer simulations, the Paesani group was able to directly correlate the observed decrease of the spin-crossover temperature to the three-dimensional arrangement of the water molecules that induce a systematic expansion of the pore size. In collaboration with the Maurin group at the Université de Montpellier 2, the Paesani group applied its anharmonic Multistate Valence Bond (aMS-EVB) model to characterize water-mediated proton conduction in the UiO-66(Zr)-(CO2H)2 MOF [Angew. Chem. Int. Ed. 55, 3919 (2016)]. Combining the results of the aMS-EVB3 simulations with quasi-elastic neutron scattering (QENS) data, it was possible, for the first time, to determine individually the dynamics of both excess protons and water molecules (Figure 2).

Future work by the Paesani group will focus to develop an efficient theoretical/computational methodology for in silico modeling of multifunctional nanomaterials for applications in molecular sensing, catalysis, fuel cells, magnetic devices, and water desalination.

http://paesanigroup.ucsd.edu

Figure 1. Left: Temperature dependence of the magnetization curve calculated from MC/MD simulations as a function of the number of water molecules (NW) adsorbed per unit cell. Right: Average positions of the water molecules inside the MOF pores calculated for NW = 5. See J. Am. Chem. Soc. 138, 6123 (2016) for details.

Figure 2. Left: Illustration of proton conduction pathways (orange) mediated by water (blue) through the tetrahedral (A) and octahedral cages (B) of UiO-66(Zr)-(COOH)2 as predicted by aMS-EVB3 simulations performed at 450 K. Right: Arrhenius plot of the diffusion coefficient for excess protons (squares) and water molecules (circles) in the fully hydrated UiO-66(Zr)-(COOH)2. The QENS data are shown as open symbols while the aMS-EVB3 results are shown as filled symbols. See Angew. Chem. Int. Ed. 55, 3919 (2016) for details.

The Paesani group (http://paesanigroup.ucsd.edu) develops theoretical methodologies and algorithms at the intersection of quantum chemistry, statistical mechanics, and computer science to predict the behavior of complex molecular systems at different length and time scales for applications in materials research, energy, environmental chemistry, and biophysics.
CHIARA DARAIO
received her PhD in 2006 from the MATSE program (Advisor: Prof. V. Nesterenko and Prof. S. Jin) and is presently a professor at CalTech.

What was your thesis topic in UCSD? How did the related work impact your future career trajectory?
My thesis was focused on the “Design of materials configurations for enhanced phononic and electronic properties”. The idea was to use geometrical nonlinearities in materials to “tailor” macroscopic properties not found in conventional materials. The work had an enormous impact on my career, and has served as inspiration and guidance until today. The ability we have today to control the materials’ nano- and micro-structural geometry, allows materials to acquire unprecedented behaviors. The limits are mostly set by our imagination.

Could you briefly describe your career path - from UCSD to now?
As I was finishing to write my doctoral dissertation at UCSD, I was offered a position as Assistant Professor at the California Institute of Technology (Caltech). I completed my PhD in June 2006 and later I started my new academic adventure at Caltech. I became a full Professor in 2010, and I am still serving as a Professor there, in the Mechanical Engineering and Applied Physics departments. From 2013-2016, I spent ~3.5 years as a Chair of Mechanics and Materials at ETH Zürich (Switzerland), an experience that has widened my research interests and enabled new collaborations.

In retrospect, what were the highlights of the MATSE program?
The many opportunities given to the PhD students and the program’s flexibility to adjust to individual needs of each student. For example, I spent several months doing research for my dissertation at the Lawrence Berkeley National Lab (LBNL), to learn how to use the electron microscopes.

Any interesting memories (both good and bad!) of the MATSE program?
I have very fond memories of the MATSE program. It was the perfect fit for me, combining a stimulating academic program, a strong research training with a wonderful quality of life. The courses I have taken there as a student still serve as basic references for my own courses, and the friendships made while studying at UCSD are lifelong bonds. I loved the interdisciplinary training and the many exciting seminars. What I remember most, were my mentors: Prof. Nesterenko and Prof. Jin who were incredibly supportive, offering training, guidance, and many opportunities to succeed.

What are your suggestions/advice for MATSE students who would like to get into academia?
What has worked for me has been to pursue what I love, science, working hard but also learning to have fun with it, even when facing adversities. Also, to take advantage of the many opportunities MATSE offers, for collaborations and networking.

What was your thesis topic in UCSD? How did the related work impact your future career trajectory?
My master’s and PhD theses were on “Single Molecular Transistor” and “Carbon Nanotubes: Mechanical, Electrical, and Optical Properties”, respectively. They were still very advanced research topics in electronics at the time, and prepared me with the knowledge and skill sets for opportunities in the broad fields of electronics related research/engineering.

Could you briefly describe your career path - from UCSD to now?
I am a hands-on person and have great interests in engineering. I have moved from mechanical engineering focus to semiconductor processing to electronic device/circuit engineering. My career path has transitioned from being an individual contributor to project lead, and more (technology) managerial type of roles. I was initially hired at Applied Materials Inc. focusing on transistor reliability, as well as process integration and module development. I have recently moved to Maxim Inc. focusing on analog/power device technology development.

In retrospect, what were the highlights of the MATSE program?
I feel that MATSE offered a curriculum of broad as well as in-depth topics for graduate students. A class on electronic properties greatly strengthened my interests in electronics/solid state physics. I suggest that MATSE should encourage graduate students to intern during their school years to learn what the industry is doing and learn collaborative methods. I found that most of my colleagues who were able to adjust to company culture fast were the ones who had internships.

Any interesting memories (both good and bad!) of the MATSE program?
The memories of MATSE and the years in UCSD left with me are all good. The ones I found interesting are the ones related to team projects from which we experienced conflicts of ideas and required negotiation and we had to agree on a middle ground.

What are your suggestions/advice for MATSE students who would like to get into industry?
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CHI-NUNG NI
received his PhD in 2008 from the MATSE program (Advisor: Prof. P.R. Bandaru) and is presently a Principal Member of Technical Staff at Maxim Inc.

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What are your suggestions/advice for MATSE students who would like to get into industry?
Some of the following may be clichés (but I found clichés could be quite true): (1) It is not always easy to choose a research topic that is guaranteed to be a hot topic in the industry at the time you look for a job. Hence, it might be wise to put 100 (or 120%) of your efforts on your research topics and target to be the best, (2) Pay attention to the details but remember how one’s work relates to the overall big picture, (3) Make good connections- at the end of the day it’s about who you are and also who you know.
UC San Diego Joins the Redshirt in Engineering Consortium to Further Student Success

The National Science Foundation has awarded the University of California San Diego Jacobs School of Engineering just over $800,000 to implement a new scholarship program aimed at increasing the academic success of low-income (PELL-eligible) engineering students. The award is part of the “Redshirt in Engineering Consortium”.

Redshirt programs, in which a first-year college athlete is given a year to prepare to compete at the university level, are common in athletics. In 2009, the University of Colorado Boulder created the innovative concept of “redshirting” in engineering to offer students from underserved backgrounds an extra year of preparation for a college career in engineering.

Six universities including the University of California San Diego; Boise State University; University of Illinois Urbana-Champaign; University of Washington; Washington State University; and the University of Colorado, Boulder are now coming together to establish The Redshirt in Engineering Consortium. The six members will administer scholarships and academic support to a total of approximately 800 students across the program. While not all programs in the consortium are aiming for extra time for the degree, all programs will be providing support in math, study skills, professional development, time management, and career planning.

“There will be an emphasis on strengthening math skills,” said Pamela Cosman, Associate Dean for Students of the Jacobs School of Engineering, a professor in the Department of Electrical and Computer Engineering, and UC San Diego PI for the NSF award. “Engineering and computer science curricula are built on a foundation of math, but we’ve found that many students who are eager to become engineers or computer scientists need additional support initially to succeed. We don’t want calculus courses to be pushing talented students out of engineering.”

At UC San Diego, the funds will go toward scholarships, summer programs, faculty and industry mentorship, and other academic support programs for a cohort of 25-30 low-income students each year.

“There’s a big overlap with what we’re already doing to further student success,” said Cosman. “This grant gives us the opportunity to expand or create new programs within the IDEA Student Center, which is already providing comprehensive support to undergraduate engineering students.”
Describe your research interests.

My research interests lie at the intersection of computer science and materials science. Specifically, I am interested in studying the behavior of materials in extreme environments: pressure, temperature, strain rate, and radiation. By leveraging powerful laser facilities and massively parallel computing resources we can effectively investigate dynamic phenomenon ranging from inertial confinement fusion to planetary collisions. Next generation shock facilities and high performance computers are now being co-designed; I have a strong desire to make sure the scientific bridge between these projects is utilized to its maximum extent.

What have been your experiences in the MATSE program? How has your training in the MATSE program at UC San Diego helped your growth?

My experiences at UC San Diego in the MATSE program have been incredibly valuable; most of all, the ability to establish collaborations across departments and across institutions. Often the resources and expertise needed to successfully conduct laser experiments or massive computer simulations are quite dispersed. The support from my advisor, Dr. Marc Meyers, and the program enabled and encouraged many successful collaborations with Los Alamos National Laboratory, CalTech, General Atoms, and Lawrence Livermore National Laboratory.

Where do you see yourself in the future?

I see myself as a professor at a top tier university or a research staff member at a national laboratory. Each of these environments would allow me to conduct cutting edge research in addition to providing ample opportunities to mentor students. I would not be where I am today if not for the excellent teachers I have had along my way. I foresee myself in a position where I can help train future generations of researchers.

Figure 1. Molecular dynamics simulation of a ~50 GPa shock in a nanocrystalline tantalum sample. 20 million atom simulation run on 1024 cores of the Mustang high performance computer over 16 hours (Los Alamos National Laboratory, Institutional Computing, Exascale Codesign Center for Materials in Extreme Environments). Defective atoms are identified algorithmically and selectively colored. Atoms within each nanocrystal are then colored according to their local stress state: yellow: ambient, blue: compression, orange: tension. This simulation shows the formation of shock-induced defects (twins and dislocations) in the three uppermost frames followed by cohesive failure at the grain boundaries in the two most bottom frames as the shock wave is reflected from the rear surface.
Tina Tse Nga Ng
Electrical and Computer Engineering
Professor Tina Tse Nga Ng and her group aim to push the boundary of how electronics are made and used, to potentially incorporate electronic control and power sources into any object, in order to realize seamless human-computer interfaces.

Francesco Paesani
Chemistry and Biochemistry
The Paesani group develops new theoretical methodologies and algorithms at the intersection of quantum chemistry, statistical mechanics, and computer science to predict the behavior of complex molecular systems at different length and time scales for applications in materials research, energy, environmental chemistry, and biophysics.

Faik Akif Tezcan
Chemistry and Biochemistry
The Tezcan Lab is interested in using proteins as building blocks for the construction of new, evolvable biological machines and advanced, dynamic materials.

Ping Liu
Nanoengineering
Professor Liu’s research focuses on designing materials and architectures for electrochemical energy conversion and storage applications.

Alina Schimpf
Chemistry and Biochemistry
The Schimpf lab aims to develop and characterize inorganic materials with unique electronic or photophysical properties that can be accessed via inexpensive, solution-based techniques.

Kenneth Loh
Structural Engineering
Dr. Loh and the Active, Responsive, Multifunctional, and Ordered-materials Research (ARMOR) Lab focus on the design, manufacturing, and characterization of multifunctional nanocomposites and tomographic methods for various engineering applications.

Xiaohua Huang
Bioengineering
Professor Huang is currently working to create innovative bioanalytical technologies for high throughput genomics, proteomics and biomedical research - especially to develop technologies for the massive parallelization and miniaturization of biochemical reactions and biomolecule analyses.

Zheng Chen
Nanoengineering
Dr. Zheng Chen’s research focuses on development of novel nanostructured and polymeric materials for cutting-edge applications, including electrochemical energy devices (batteries, supercapacitors, and fuel cells), flexible and printable devices, and sustainable water and resources.
Gopesh Tilvawala from the Medically Advanced Devices Laboratory led by Prof. James Friend has produced 400 µm diameter steerable tip microcatheters and microguidewires suitable for minimally invasive neurointervention to navigate within the cerebrovasculature and treat aneurysms and strokes. A prototype device 15 cm in length has a steerable tip with sufficient precision to crudely write UCSD.