

IMR Quarterly

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Probing High Frequency Acoustics with Light: Mechanical Properties of Submicron Structures

As the semiconductor industry strives to keep pace and sustain Moore's law, new materials are increasingly being introduced into micro/nano-electronic products. Among these material innovations are dielectrics with a dielectric constant (k) less than or greater than that of SiO_2 currently utilized in the high volume manufacturing of transistors and interconnect structures for advanced microprocessors. For example, a low- k SiOC:H interlayer dielectric (ILD) has been introduced at the 90 nm interconnect technology node. While materials with still lower dielectric constants will be needed for future technologies, they often introduce reliability concerns related to their mechanical robustness.

In a study supported by an IMR Industry Challenge Grant, OSU graduate student Sheldon Bailey and Professor Sooryakumar, in partnership with Intel Corporation's Logic Technology Development division, utilized the electric field of light waves to detect high frequency acoustic waves within ultra-thin low- k structures to non-destructively evaluate their mechanical properties. The reductions in k in these materials have often been through the introduction of various organic constituents into a SiO_2 matrix to make a carbon doped oxide or SiOC:H material. While the ensuing disruption in the connectedness of the SiO_2 network reduces electronic and ionic contributions to the dielectric function, it also leads to reduced mechanical properties of the material.



Sheldon Bailey, graduate student in Physics, and Professor R. Sooryakumar adjusting optics for the detection of high frequency acoustic waves.

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Faculty Spotlight: Michael Paulaitis, Chemical and Biomolecular Engineering



Dr. Michael Paulaitis joined the OSU Department of Chemical and Biomolecular Engineering in 2005, after faculty appointments at the University of Delaware and at Johns Hopkins University, where he also co-directed the Institute for Multi-Scale Modeling of Biological Interactions and the Burroughs Wellcome Fund Program in Computational Biology. He is currently an Ohio Eminent Scholar in Nanobiotechnology and Molecular Self-Assembly, and chairs the Executive Committee of the National Science and Engineering Center for Affordable Nanoengineering of Polymeric Biomedical Devices.

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Director's Note



Dear Colleagues,

With the ending of Ohio State's "quarter-based" academic calendar, the IMR Quarterly is closing an era with an issue that demonstrates the reach and relevance of materials research at OSU as we look forward to the semester schedule for 2012-13 and beyond.

As has been written in this space before, IMR has been focusing significant efforts toward building beyond what is already a very strong base of industry-relevant and industry-supported materials research through its Industry Challenge Grants program in a "grass-roots" style to encourage new and strategic directions of industry-relevant research and industry-university collaboration. This is becoming especially important as the national research paradigm continues to shift toward greater university-industry partnerships. Therefore, we are particularly proud to highlight the work led by R. Sooryakumar, a Professor in the Department of Physics, and his group, who with support from an IMR Industry Challenge Grant and Intel Corporation, have developed and applied a new, optically-based non-destructive method to characterize mechanical properties by probing acoustic waves within novel dielectric layers for next generation electronic devices. Based on this seed research, Prof. Sooryakumar was recently awarded a 3-year program funded by the Semiconductor Research Corporation to continue and advance this effort.

At the other end of the materials spectrum but at least as important, this issue reveals the cutting edge biomaterials research of Michael

Paulaitis, an Ohio Eminent Scholar in Nanobiotechnology and Molecular Self-Assembly and Professor in the Department of Chemical and Biomolecular Engineering, in our Faculty Spotlight. Prof. Paulaitis' research focuses on the multi-scale interfacial phenomena between biological systems and engineered surfaces appropriately analogous to the interface between materials and medicine that we are working to bridge through multiple IMR initiatives.

Inside you will also read about the exemplary efforts of Aimee Price, our IMR Member of Technical Staff in charge of the e-beam nanopatterning facility, who went above and beyond the call of nanolithography to mentor two local high school girls to success at this year's State Science Fair. Aimee's dedication to advancing science and technology is a true inspiration for all of IMR. You will also find the latest advancements in the Center for Emergent Materials, our NSF-funded Materials Research Science and Engineering Center that continues to define the forefront of spintronic materials, as well as updates on core facilities throughout the IMR constellation.

Wishing you all a fruitful and enjoyable summer; on to semesters!

Warm Regards,

Steven A. Ringel, Ph.D.

Neal A. Smith Chair Professor

Director, The Ohio State University Institute for Materials Research

Achievement was given to Steven Ringel, IMR Director and Neal A. Smith Chair Professor of Electrical Engineering, and the Faculty Diversity Excellence Award went to Betty Lise Anderson, Electrical and Computer Engineering. The Harrison Faculty Award for Excellence in Engineering Education was given to Andre Palmer, Chemical and Biomolecular Engineering. The Innovators Award, to recognize scientists who best demonstrate innovation in the development of a product and/or technology originating from the OSU research enterprise, was awarded to Liang-Shih (L.S.) Fan, Chemical and Biomolecular Engineering. The Lumley Research Award, which recognizes the research contributions of faculty and research scientists, was given to 17 people, including IMR members L. James Lee, Michael Paulaitis, Wolfgang Windl, Roberto Myers, Siddharth Rajan, and Boian Alexandrov. The Lumley Interdisciplinary Research Award, which recognizes the interdisciplinary research contributions of faculty and research staff was awarded to Thomas Blue and Wolfgang Windl, and to the Battery Research Group: Giorgio Rizzoni, Suresh Babu, Bharat Bhushan, Marcello Canova, Lei Cao, Terry Conlisk, Yann Guezennec, Mike Mills, Simona Onori, Wolfgang Windl, and Stephen Yurkovich.

IMR Member News



Sheikh Akbar, Professor of Materials Science and Engineering, has been selected to receive the Electrochemical Society Sensor Division Outstanding Achievement Award, which is given "to recognize outstanding achievement in the science and/or technology of sensors; and to encourage excellence of work in the field."



Malcolm Chisholm, Distinguished University Professor of Chemistry and IMR Associate Director, is the 2012 recipient of the American Chemical Society Edward W. Morley Award. This award is given "to recognize significant contributions to chemistry through achievements in research, teaching, engineering, research administration and public service, outstanding service to humanity, or to industrial progress."

The OSU College of Engineering held its annual award banquet on May 15th, honoring many IMR members with faculty awards. The Clara M. and Peter L. Scott Faculty Award for Outstanding Academic

Materials Centers Updates : Center for Emergent Materials (CEM) Update

The Center for Emergent Materials is a National Science Foundation (NSF) Materials Research Science and Engineering Center (MRSEC) at The Ohio State University.

CEM Industry Seminar with LakeShore Cryotronics



CEM Industry Seminar speaker Dr. David Daughton of LakeShore Cryotronics

On March 14, the Center for Emergent Materials welcomed Dr. David Daughton from LakeShore Cryotronics for a CEM Industry Seminar. Dr. Daughton's talk was attended by 43 graduate students and postdoctoral researchers across 9 departments and 3 centers. Topics including best practices for networking, finding and targeting jobs, and how to stand out to recruiters were discussed and dissected. In addition, Dr. Daughton gave a short overview on the research leading to an Ohio Third Frontier grant and collaboration between LakeShore and OSU.

CEM Member Wins Award

In April, the California Nanosystems Institute (CNSI) at University of California Santa Barbara announced that CEM Postdoctoral Researcher Dr. Adam Hauser has been awarded this year's Elings Prize Fellowship in Experimental Science. The fellowship, open to applicants in any area of the physical sciences, biology, or engineering, provides funding for two years of research and is renewable for a third year. Dr. Hauser, who currently works in Professor Fengyuan Yang's group in the Physics Department, will begin work this summer with Professor Susanne Stemmer in the UCSB Materials Department.

IRG-2 Discovers a High-Temperature Ferrimagnetic Semiconductor

The main barrier to spintronic applications to date has been finding a semiconductor that can exhibit ferromagnetic ordering well above room temperature. Such a material would provide sufficiently high spin polarization for next generation technologies such as half-metallic spin injectors. Unfortunately, efforts have largely stalled due to the low Curie temperatures (< 300K) of developed material classes such as dilute magnetic semiconductors.

In April, the Interdisciplinary Research Group dedicated to Double Perovskite interfaces and heterostructures (IRG-2) published a breakthrough in the Rapid Communications section of *Physical Review B*, detailing the semiconducting nature of Sr₂CrReO₆ when

films are grown to high order. This result, when coupled with a Curie temperature (508 K), could open the way for application advances in spintronics. In addition, this work represents a new level of thin film growth mastery, as the semiconducting nature of Sr₂CrReO₆ only exhibits itself when the Cr-Re ordering is far better than anything reported before. The work was also selected as an Editor's Suggestion by the *Physical Review* editorial staff.

IRG-2 is now pursuing collaborations with Ohio State's world leaders in device fabrication, such as Ezekiel Johnston-Halperin (Physics) and Siddharth Rajan (Electrical and Computer Engineering), to bring to bear next-generation spintronic device prototypes. In addition, the group is aggressively seeking out new collaborations to explore the fascinating science inherent in this highly correlated complex oxide. Interested groups should contact Professor Fengyuan Yang at fyang@physics.osu.edu.

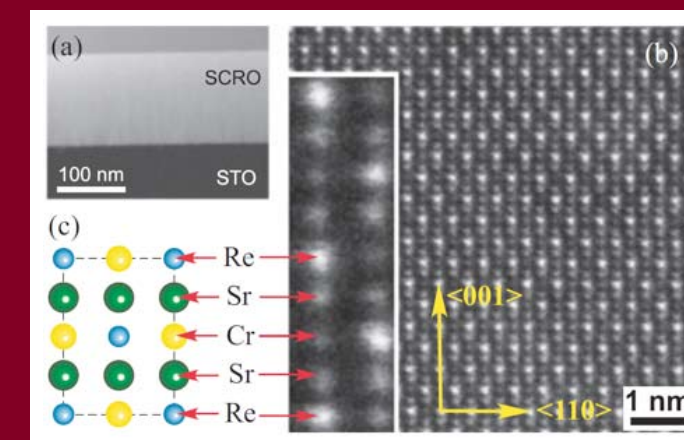


Figure 1: HAADF STEM images of a 134-nm-thick Sr₂CrReO₆ (001) film grown on SrTiO₃ viewed along the <110> direction (a) at low magnification showing a uniform film and (b) at high magnification revealing the clear contrast of Sr, Cr, and Re atoms. The inset in (b) highlights the atomic contrast, which matches (c) the schematic projection of DP lattice along the <110> direction. *Phys Rev B* 85, 161201(R) (2012)

For more information about the Center for Emergent Materials, visit their website at cem.osu.edu.

Probing High Frequency Acoustics with Light: Mechanical Properties of Submicron Structures

(continued from page 1)

Moreover, low-k dielectrics also exhibit intrinsic tensile stresses and increased thermal expansion relative to SiO₂ leading to serious thermal-mechanical reliability concerns. It is anticipated that the continued reduction in dielectric constant will eventually lead to the formation of various levels of nano-porosity that will likely further degrade the mechanical properties. Thus, as industry moves to 22 nm and beyond, the porous low-k ILD thickness will approach 100 nm or less and reliable, non-destructive techniques capable of measuring the elastic constants, Young's modulus and Poisson's ratio of materials at these thicknesses are needed.

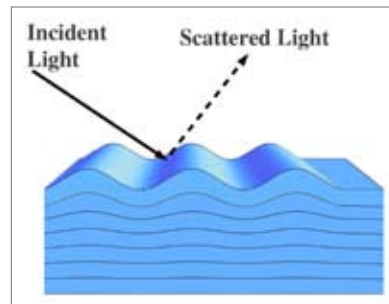


Figure 1. Surface ripple scattering as used in Sooryakumar's research

In the present study velocities of acoustic vibrations within the material - which are related to its elastic constants - are measured through laser based methods. Expansions and contractions created within the material by high frequency acoustic waves that are present at ambient temperature, including those akin to resonances in an organ pipe, result in spatial and time dependent changes of the electromagnetic characteristics, such as the material refractive index. These modulations underlie the coupling of light to the acoustic waves. Conversely, the electric field of an incident light wave can induce spatially varying and temporally periodic elastic strains and initiate acoustic waves in materials. Coupling of light to the acoustic waves is also achieved through the surface ripples

(created by the sound waves) that function as a moving grating (Figure 1). The corresponding loss of energy from the light wave to the material results in a downshift of the scattered photon frequency, while the transfer of energy from acoustic waves to the incident light wave results in a light frequency up-shift. These energy transfers modulate the scattered light wave with discrete sum and difference frequencies impressed upon the frequency of the incident light wave. From the measured frequencies the acoustic wave velocities are determined rendering the Young's modulus and Poisson's ratios which are central parameters for a complete characterization of the mechanical properties of low-k interconnects. Results from this study were recently published in the *Journal of Applied Physics* in an article co-authored by Prof. Sooryakumar, Mr. Bailey, and Intel Corporation researchers ("Elastic properties of porous low-k dielectric nano-films," J. Appl. Phys. 110, 043520 (2011); <http://dx.doi.org/10.1063/1.3624583>)

The Industry Challenge Grant provided by IMR were critical to establish the feasibility of this non-destructive method used to assess mechanical properties of these materials at the submicron and nanometer scale, which are leading contenders to become central components of future electronic devices. As a direct result of this support from IMR, the research has now been funded over the next three years by the Semiconductor Research Corporation (SRC), which brings together industry and academic researchers to create unique collaborations. Dr. Sooryakumar continues to work on expanding this technique to biological membranes such as the eye lens and the cornea.

For more information about Dr. Sooryakumar's work, visit <http://www.physics.ohio-state.edu/~soory/> or contact him at soory@mps.ohio-state.edu.

Encouraging Young Women in Science: Nanotech West Scientist Aimee Price Helps Local Teens' Project Reach State Science Day

Aimee Price, Senior Research Associate at Nanotech West Laboratory, can usually be found in the cleanroom lab working on micro and nanometer scale lithography projects. However, Aimee also takes time out of her busy schedule to share her passion for science with young women interested in engineering. Most recently, Price mentored two local high school students with an optics project that progressed to the state-level science competitions.

Maddie Miller and Disha Shidham, 9th grade students at Upper Arlington High School, conducted all of their work at IMR's Nanotech West Laboratory for their science project "The most effective material and color in offsetting the effects of 446-477 nanometers of wavelengths of light on the circadian rhythm." The girls were interested in the fact that blue light, like that from LED backlighting on computers, smart phones, and televisions disrupts the body's natural sleep cycle. They found that blue light specifically changes the timing of secretion of melatonin, the "sleep hormone," and makes it difficult to fall asleep. Since many teenagers are working later into the evening on devices with blue light, Maddie and Disha believe that finding a way to minimize exposure to blue light while still enabling use of the electronics is critical. At Nanotech West, Aimee taught Disha and Maddie how to measure the transmission of an LED light across the visible spectrum with an Ocean Optics spectrometer, typically used by researchers in the PVIC Wright Center. The girls looked at how the various materials and colors act as filters by reducing certain wavelengths of light, while still allowing others to pass through.

At their District Science Day competition in March, the Freshmen team's project received a superior rating, ranked first in the Engineering category, and received a special award in the optometry/

optics category. In May, they advanced to Ohio's State Science Day where their project was rated Excellent and won the Interdisciplinary Research Award for best team project, an award sponsored by OSU's chapter of the scientific research society Sigma Xi.

Price first became interested in science in eighth and ninth grades, and she also had a successful science fair project herself as a young woman. She has also helped judge at the State Science Day for the American Chemical Society. "When I went to the International Fair, I said that one day I'd help however I could and I finally had the opportunity," shares Price. "Kids who have good experiences at these fairs and in the process in general really seem to enjoy science going forward, which is a huge win in the battle to keep them interested." She was involved from the very beginning of the project, spending many hours with the girls in brainstorming project ideas and ensuring good understanding of the scientific method. Price notes that her Nanotech West colleagues also helped the team with their research project over several months by sharing lab space, lending tools, and transporting the girls' optics table numerous times, making this a true team effort.



IMR Member of Technical Staff Aimee Price (center) with science teacher Wendy Pinta and mentees Disha Shidham and Maddie Miller at an award banquet where the girls were recognized for their work.



Shidham and Miller aligning a flashlight with a spectrometer as part of their science experiment.

IMR Industry Challenge Grants Program – Promoting Industrial Collaborations with Ohio State's Materials Researchers

The Institute for Materials Research (IMR) engages in a wide variety of programs and activities to support the advancement of materials-allied research at Ohio State. IMR's Research Enhancement Program has been one of its most popular and successful initiatives, providing several research funding opportunities to OSU researchers. Since 2010, IMR has provided \$100,000 to support industry collaborations through Industry Challenge Grants, which provide cost share to strengthen new collaborations between OSU researchers and private industry partners in materials-allied research.

IMR Industry Challenge Grants provide one-to-one matching funds up to \$20,000 per year to allow OSU researchers to conduct new, innovative materials-allied research in collaboration with

private industry partners that will lead to major external proposal development. Industry Challenge Grants are eligible for renewal for a second year of funding and proposals are accepted on a rolling basis, year-round, with no deadline.

The Industry Challenge Grants program is intended to facilitate securing new industry contracts by providing one-to-one cost share funding from an internal source. As with all IMR funding programs, these funds are not subject to indirect costs (F&A) and all of the IMR funds can be used for direct costs, giving the OSU researcher maximum leverage of financial resources contributed to the collaboration.

IMR Industry Challenge Grants Program - How it works

Research negotiations are fluid and do not always follow a specific timeframe or step-by-step process. Below is an example of how we envision a typical Industry Challenge Grant coming about; however, we recognize that each collaboration is unique and IMR can be somewhat flexible with the order of these steps.

- An OSU researcher begins discussions with an industry collaborator about potentially engaging in a new research project. Once the preliminary details are agreed upon, the researcher contacts the Office of Sponsored Programs and works with them to begin the industry contract process.
- The OSU researcher contacts IMR to notify us of their intent to submit an Industry Challenge Grant proposal for additional financial support for this research project and provides some preliminary information about the industry collaboration.
- The OSU researcher submits an Industry Challenge Grant proposal to IMR. Proposals include a two-page write up of the intended research, a short statement of planned external proposals, industry partner information, a budget, and CVs for each investigator. Full proposal instructions are available online in a Request for Proposals.

- IMR internally reviews the proposal and evaluates it based on the NSF-style review criteria listed in the RFP.
- If IMR determines the research project merits funding, an award letter is sent to the Principal Investigator indicating that IMR will provide matching funds when the related industry contract is active.
- The OSU researcher continues to work with the Office of Sponsored Programs and the industry collaborator on the formal industry contract. Once the contract is approved and set up through the Office of Sponsored Programs, IMR transfers the Industry Challenge Grant funds to an internal OSU account to be used as documented cost share to the industry contract.
- The OSU researcher engages in research as planned, formally documents cost share using the Industry Challenge Grant funding, and provides a brief technical and financial report at the end of the year.

For more information about IMR Industry Challenge Grants, visit IMR's website at <http://imr.osu.edu/research/programs/industry-challenge-grants/> or contact IMR Program Manager Layla Manganaro at 614-247-4685.

Faculty Spotlight: Michael Paulaitis, Chemical and Biomolecular Engineering (continued from page 1)

Research in the Paulaitis group is focused on the central role protein interactions play in the hierarchy of complex interactions underlying self-assembly in aqueous environments and at the interface between biological systems and engineered surfaces. The overall goal of the lab is to relate protein interactions to the chemical, biophysical, mechanical, and topographical features of those interfaces, and ultimately to biological functions that are governed by interfacial properties on length scales of nanometers to microns. The lab's primary interest is on the role of hydration in these relationships. The lab's approach is to develop quantitative molecular thermodynamic models based on statistical mechanical principles and molecular simulations to predict protein interactions and self-assembly in aqueous solutions and at interfaces. The molecular modeling and simulation efforts are supported by experimental characterizations of protein interactions and self-assembly using primarily small angle neutron scattering (SANS) and light scattering.

supported by the remarkably similar effects temperature has on protein denaturation and on the transfer of hydrocarbons from an organic phase into water. The pressure dependence of protein unfolding is, however, at odds with this model. The volume change for unfolding is positive at low pressures but negative at pressures on the order of a few kilobars, while hydrocarbon transfer into water shows exactly the opposite pressure dependence. Using an information theory model of hydrophobic interactions coupled with molecular simulations on simple hydrophobic solutes, Dr. Paulaitis and collaborators at Los Alamos National Labs (LANL) proposed that proteins are destabilized at high pressures due to water penetration into the hydrophobic core, rather than the transfer of nonpolar groups from the hydrophobic core into water.

Dr. Paulaitis and his graduate students tested this model prediction through extensive molecular simulations of the unfolding transition for the protein, staphylococcal nuclease, and demonstrated that their simulations captured structural features

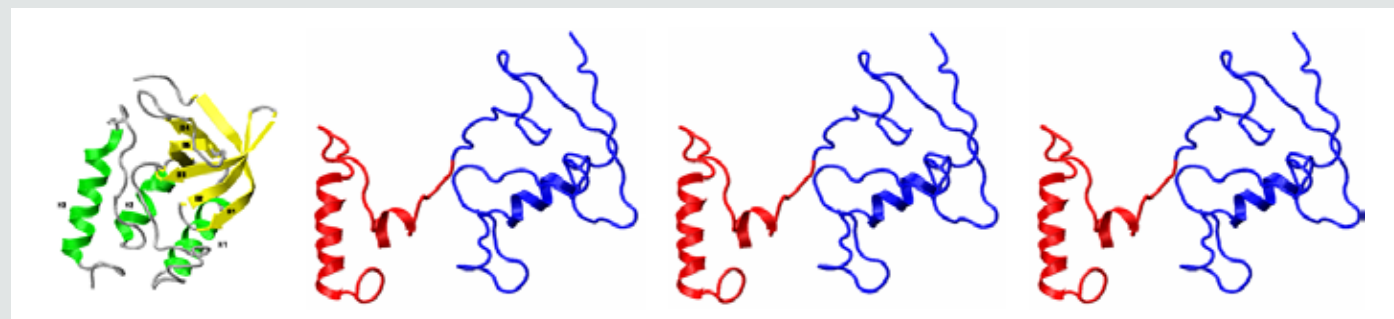


Figure 1. Representative structures of staphylococcal nuclease during the initial stages of the pressure-induced unfolding transition derived from molecular simulation. From left to right: the structure in the folded state at 1 bar, and structures at 8 kilobars at time intervals of several nanoseconds. The two sub-domains are shown in red and blue.

Hydrophobic interactions provide the principal non-specific thermodynamic driving force for protein self-assembly and stability in aqueous media and at interfaces. Dr. Paulaitis and his group have developed thermodynamic models of molecular hydrophobic phenomena that enable detailed descriptions of protein unfolding mechanisms, and have applied these models to determine conditions under which proteins can become unstable, which can be a critical issue in many bioengineering applications. Protein unfolding in aqueous solution at elevated pressure stands out as an example of this work.

Although a variety of forces stabilize folded proteins, the formation of a hydrophobic core is thought to be a dominant factor. The hydrophobic-core model of protein folding is

of the protein folding-unfolding transition observed in their high-pressure SANS measurements (Fig. 1). The simulations further showed that unfolding was initiated by destabilization of a few, specific hydrophobic contacts between two sub-domains of this protein as a result of water insertions at high pressures. Most importantly, these specific contacts define key indicators and/or targets of interest for assessing or even controlling the stability of staphylococcal nuclease over a wide range of conditions well beyond aqueous solutions at elevated pressures. Identifying these targets using their molecular models and simulations coupled with high-pressure SANS measurements for other proteins is a current focus of the lab.

Hydrophobic interactions are also implicated in the microscopic

structure and thermodynamic properties of fluid-like, oil-water interfaces. The biological importance of a molecular description of oil-water interfaces arises in modeling biomembrane formation, partitioning of small molecules into these membranes, and the intermembrane organization of membrane protein assemblies. Dr. Paulaitis and his LANL collaborators simulated an oil-water interface common in reversed phase liquid chromatography, consisting of n-C18 alkyl chains tethered to a planar support in contact with water, the mobile phase in the column (Fig. 2). The simulations showed that the interfacial water density profile is determined by the local hydration water structure around the constituent hydrophobic methyl and methylene groups of the alkyl chains in the interfacial region, which results in water penetration into the interfacial region on the molecular scale. The finding suggests a thermodynamic model that emphasizes local molecular fluctuations in the interfacial region relative to the adjoining bulk phases, which improves upon primitive models of depletion forces in macroscopic hydrophobic interactions that invoke collective effects of a drying transition at the oil-water interface on length scales larger than molecular as the hydrophobic force driving self-assembly in aqueous media.

While non-specific hydrophobic interactions drive the formation of macromolecular assemblies, the specific shapes that are adopted result from a complex balance of specific interactions

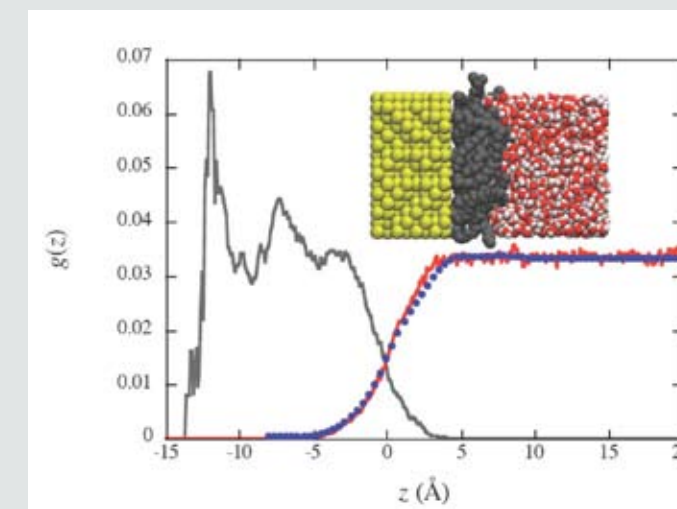


Figure 2. n-C18 alkyl carbon and water oxygen interfacial densities. The gray and red lines indicate the carbon and oxygen densities, respectively, at 300 K determined from molecular simulation. The blue points indicate the oxygen densities reconstructed from the carbon-oxygen radial distribution function averaged over alkyl chain conformations sampled in the molecular dynamics simulation. The interfacial mid-point ($z=0$) is set at the point where the alkyl carbon and water oxygen densities are equal. The inset shows a configuration of several layers of water in contact with the alkyl chains anchored to a gold substrate. Approximately twice as many water molecules were included in the calculation than are shown. The water interface on the right side is a free liquid-vapor interface.

between constituent charged and polar groups in addition to molecular geometric constraints. Some of the essential features of self-assembly governed by these interactions can be captured using continuum solvent models of hydration. However, explicit water molecules interacting with specific, solvent accessible sites on macromolecules can have an enormous impact on macromolecular structure, and biological function as a consequence, and these contributions are not taken into account in continuum models of hydration. To address the issue of the specific hydration of proteins, Dr. Paulaitis and his group have developed a quasi-chemical model of hydration in which explicit water molecules and other molecular constituents of the solvent that are localized at specific protein sites are naturally viewed as part of the protein. Protein interactions are thus described in terms of quasi-components consisting of the protein along with "bound" water and other constituents, immersed in a continuum solvent. An advantage of the quasi-chemical model of hydration is in its ability to describe at the molecular level the preferential partitioning of ions or other solvent constituents at specific sites on the protein surface or in the interfacial region between the protein and aqueous solution. Another consideration is the reduced computational demands for simulations that do not need inordinately large numbers of explicit water molecules to hydrate the protein as a whole. Comparing model predictions with osmotic second virial coefficient measured for several well-characterized proteins in aqueous solution as a function of solution pH and ionic strength, Dr. Paulaitis and his graduate students have shown that the pH and ionic strength dependences of protein-protein interactions are accurately predicted when specific hydration is taken into account. Their model also led to the mechanistic interpretation that specific hydration reduces short-range attractive interactions by eliminating a number of highly complementary protein-protein configurations. Their current focus is on extending this work to develop a molecular model for protein solvation that can identify specific protein sites as targets for chemical modifications or simply adding co-solvents that can further stabilize or destabilize protein interactions as desired.

Protein self-assembly and protein stability in aqueous media in which metal ions are present as cofactors or active participants presents by far the greatest challenges for molecular thermodynamic modeling. Metals mediate energy and information flow in biological systems, and by virtue of their energetically strong interactions with the medium, are exceptional agents of chemical change, and thus the self-organization of the system itself. Over half of all proteins are believed to use metals for their structure and function, and aberrant metal-protein interactions have been implicated in many protein misfolding and aggregation neurodegenerative diseases.

Faculty Spotlight: Michael Paulaitis, Chemical and Biomolecular Engineering (continued from page 7)

Metals interact with biological materials and with aqueous media with strengths rivaling those of covalent bonds. Thus, quasi-chemical models of hydration are ideally suited to describe the role of these local, chemically intricate interactions in protein self-assembly and protein stability.

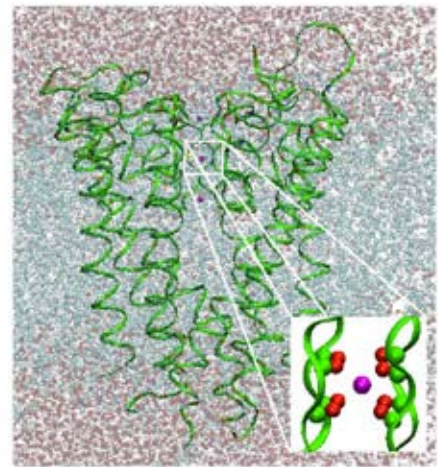


Figure 3. A configuration of the potassium ion channel generated from simulation. Inset shows a potassium ion (purple) in the S2 site, and carbonyl groups of the peptide backbone that ligate the ion.

Dr. Paulaitis, his graduate students, and collaborators have begun extending their quasi-chemical models to metal ion solvation and metal ion binding to proteins. Recent modeling and simulation efforts have been aimed at describing the K⁺/Na⁺ selectivity of the KcsA potassium ion

channel. This selectivity is attributed to the favorable partitioning of K⁺ relative to Na⁺ in a narrow selectivity filter of the channel (Fig. 3). Carbonyl oxygens in each binding site of the filter coordinate an ion. The proposed mechanism for selectivity, based on the crystal structure of the channel, invokes the size difference between K⁺ and Na⁺, and the molecular complementarity of the selectivity filter with the larger K⁺ ion. However, this ion size-based selectivity mechanism does not account for thermal fluctuations and the conformational flexibility of the binding sites of the selectivity filter, which are greater than the size difference between these two ions. Dr. Paulaitis and his collaborators showed that the binding sites of the selectivity filter conform to efficiently bind both ions, but must pay an entropy penalty to bind the smaller Na⁺ ion. This entropy penalty corresponds to the loss of conformational flexibility in the case of Na⁺ binding. The results suggest an evolutionary process in which high K⁺ selectivity is selected for by optimizing protein conformations to favor K⁺ binding in the selectivity filter.

For more information about Michael Paulaitis' research, visit <http://www.chbmeng.ohio-state.edu/people/paulaitis.html> or email him at paulaitis@chbmeng.ohio-state.edu.

IMR Colloquia Series Brings National Solar and Laser Research Updates to OSU Campus

The Institute for Materials Research completed its 2011-2012 IMR Colloquia Series with two additional seminars by esteemed members of the international materials research community.

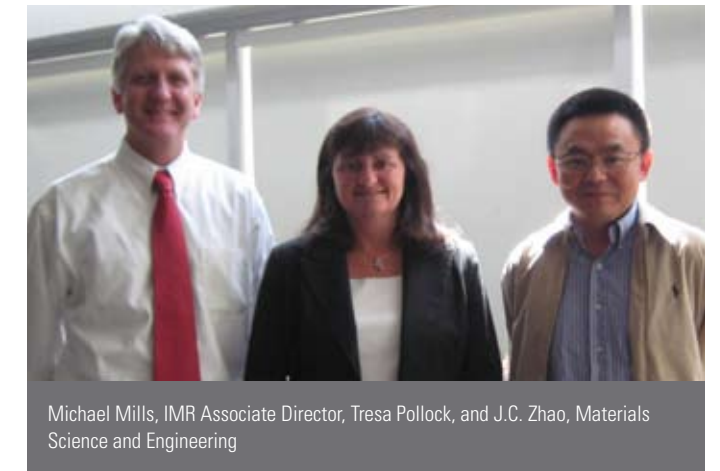


Steve Ringel, IMR Director, and John Benner

John Benner, Executive Director of the Bay Area Photovoltaic Consortium (BAPC), conducted a colloquium on March 6 to introduce the BAPC which brings

photovoltaic industry members together with leading university research teams to select and support research improving manufacture of photovoltaic modules. His presentation, titled "Made in the U.S.A. – Photovoltaic Energy Solutions," reviewed the history of the American solar industry and new research funding planned by the Bay Area Photovoltaic Consortium. A copy of his presentation is available on IMR's website.

On May 12, IMR welcomed Dr. Tresa Pollock, Alcoa Professor of Materials and Department Chair of the Materials Department at the University of California Santa Barbara. Dr. Pollock's colloquium "Materials Tomography and Femtosecond Lasers" discussed a "TriBeam" approach that combines the femtosecond laser within a focused ion beam platform to permit high resolution imaging, as well as crystallographic and elemental analysis. Early 3D datasets from the TriBeam system demonstrate acquisition rates 4 to 6 orders of magnitude faster than focused ion beam systems.



Michael Mills, IMR Associate Director, Tresa Pollock, and J.C. Zhao, Materials Science and Engineering

ME Students and Faculty Meet President Obama

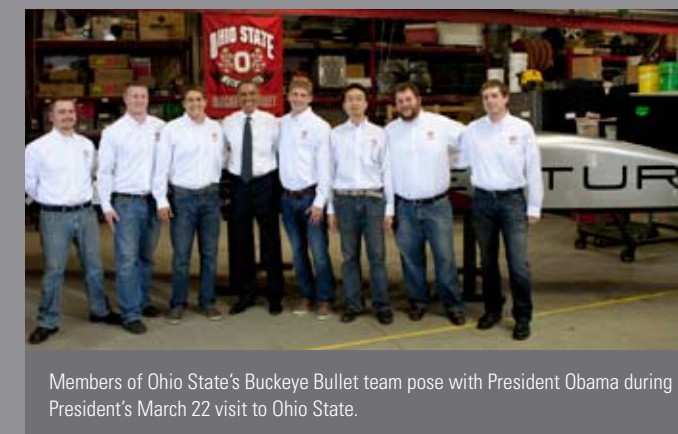
From the OSU Mechanical and Engineering Department website - this article originally appeared online at mae.osu.edu

Several Department of Mechanical and Aerospace Engineering students and faculty couldn't help but feel a bit "revved-up" when President Barack Obama took time during his visit to Ohio State on March 22 to drop by Ohio State's Center for Automotive Research. In an assembly later that day at Ohio State's RPAC, the President declared, "This school is a national leader in developing new sources of energy and advanced vehicles that use a lot less energy. I just had a chance to take a tour of the Center for Automotive Research. I admit, the best part of it was seeing the Buckeye Bullet, which has gone over 300 miles an hour and is now shooting for 400 miles an hour. The Buckeye Bullet is the fastest electric car in the world. It is a testament to the ingenuity

here at Ohio State and what is essential to American leadership when it comes to energy – our brain power. We've got to look at renewable energy as the key to our future and we've got to build cars and trucks that get more miles to the gallon . . . and we'll do it by harnessing the same type of American ingenuity and imagination that's on display right here at Ohio State."

For undergraduate and graduate students alike, not to mention faculty advisors including Giorgio Rizzoni, Marcello Canova, and Shawn Midlam-Mohler, getting the chance to shake the President's hand and explain their work on a variety of motorsports projects was the thrill of a lifetime. Evan Maley, an undergraduate in mechanical engineering and one of the Buckeye Bullet team leaders commented, "It was an honor to explain our project to the President and show how we are trying to advance alternative

energy transportation." The Buckeye Bullet holds the land-speed record for a battery-powered electric vehicle, more than



Members of Ohio State's Buckeye Bullet team pose with President Obama during President's March 22 visit to Ohio State.

307 miles per hour; Maley said breaking the 400 miles-per-hour barrier is next. In addition to the Buckeye Bullet team, Obama met students and faculty working on EcoCAR2, an international student competition focused on fuel efficiency. (In June 2011, Ohio State placed second in the first EcoCAR competition.) He also met Formula SAE and Buckeye Electric Motorcycle team members.

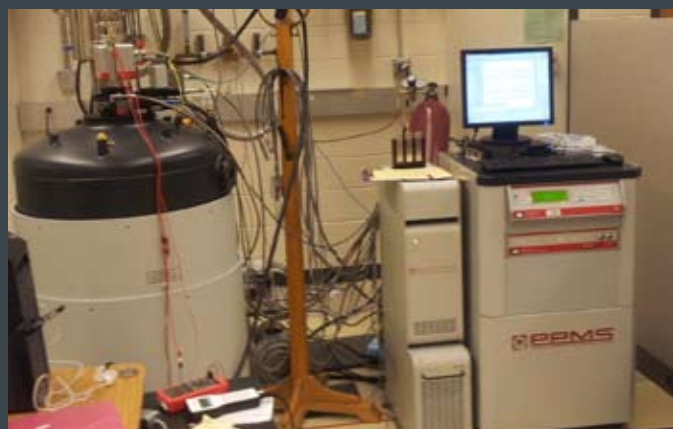
"I'm excited that President Obama is turning to some of the youngest and most innovative minds here at OSU's Center for Automotive Research to learn about advancements in renewable and efficient energy," said Julia Hare, a Buckeye Electric Motorcycle team member and undergraduate in electrical and computer engineering.

Materials Facilities Updates

In each issue of our newsletter, IMR provides updates on our three core materials research facilities, the ENCOMM NanoSystems Laboratory (ENSL), Center for Chemical and Biophysical Dynamics (CCBD), and Nanotech West Laboratory. More information on these facilities and over a dozen other open user materials research facilities on OSU's Columbus campus, visit our website at: imr.osu.edu/research/facilities.

ENCOMM NanoSystems Laboratory (ENSL) – ensl.osu.edu

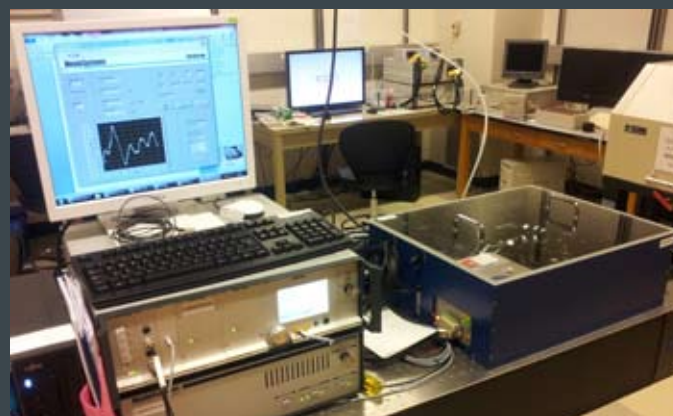
The newly acquired Physical Properties Measurement System (PPMS) by Quantum Design USA has been installed in room 0177 Physics Research Building, and the instrument is now operational and available to users. The PPMS is capable of conducting resistivity, AC transport (ACT), AC magnetic susceptibility (ACMS), Vibrating Sample Magnetometry (VSM) and torque magnetometry measurements. The VSM capability of the PPMS comes with both large and small bore coil sets and a high temperature oven option with the capability for sample heating up to 1100 K. All measurements can be conducted in magnetic fields of up to 14 T and over the temperature range between 1.9 K and 400 K (1100 K if VSM oven is used). To reduce the costs of system operation, the instrument is equipped with a helium reliquifier that dramatically reduces liquid helium consumption. The instrument has proven to be very popular with users. In order to schedule training, please contact ENSL Administrative Assistant Rachel Page at page.257@osu.edu or (614)688-1158.



Physical Properties Measurement System (PPMS) by Quantum Design USA installed at ENSL in room 0177 PRB.

An additional component of the PPMS is the cryogenic Atomic Force Microscope/Magnetic Force Microscope (AFM/MFM) delivered by ION-TOF GmbH. The instrument will allow scanned probe microscopy surface studies of samples in magnetic fields of up to 14 T and over the temperature range between 1.9 K and 400 K. Such a capability is unavailable on most commercial AFM/MFM instruments. This microscope is currently undergoing installation tests and is expected to become available to users in May 2012.

ENSL has recently acquired a new TerraHz time domain spectrometer (THz-TDS) for the study of solid state materials. The instrument has been provided by Lake Shore Cryotronics, Inc. as a part of a collaborative effort between Lake Shore Cryotronics and the OSU NSF Center for the Emergent Materials (CEM) to develop a commercial THz spectrometer. This collaboration is funded by an Ohio Third Frontier award. The current instrument is capable of conducting THz spectroscopy at room temperature under ambient conditions. In the future this instrument will be replaced with a prototype of low temperature THz spectrometer that is currently being developed by Lake Shore Cryotronics, Inc. The instrument is expected to arrive at ENSL in August of 2012.



TerraHz time domain spectrometer (THz-TDS) provided by Lake Shore Cryotronics, Inc. as part of a collaborative effort between Lake Shore Cryotronics and the OSU NSF Center for the Emergent Materials (CEM) to develop a commercial THz spectrometer.

Center for Chemical and Biophysical Dynamics (CCBD) – ccbd.chemistry.ohio-state.edu

CCBD has several updates to share regarding instrument upgrades and testing and current research projects conducted in the lab.

- A 35-femtosecond Mantis laser was recently serviced by the manufacturer to resolve an optics contamination issue. This upgrade will ensure the consistent day-to-day operation of the femtosecond stimulated Raman setup that is planned to be the focus of CCBD research for the next several months.
- Debugging and tests are under way for the 512-pixel InGaAs array detector – based near IR range (1100 – 1300 nm) transient absorption setup. Flexible mathematics of data collection allows one to use the spectrometer both in transmission and reflection mode for materials-related experiments.
- Single-wavelength near IR (1500 nm) transient absorption experiments are under way to study relaxation dynamics of GaN nanowires on Si at various excitation wavelengths. This unique data will also help to test the InGaAs array detector-based experimental setup.
- A project is under way to use CCBD femtosecond UV/visible and femtosecond infrared transient absorption spectrometers to study the carrier recombination dynamics in p-type dye sensitized solar cells. The experiments will be performed by Drs. Evgeny Danilov and Zhiqiang Ji of Chemistry under the guidance of Profs. Terry Gustafson and Yiying Wu.
- And finally, CCBD Director Prof. Terry Gustafson recently resumed his duties after spending several months on sabbatical leave in Auckland, New Zealand. He is back and better than ever focusing on multi-dimensional femtosecond infrared and Raman spectroscopy.

Nanotech West Laboratory – nanotech.osu.edu

The Nanotech West Lab has just completed the installation of a new Diener Pico® plasma asher. The asher vacuum system is completely oil-free, being pumped by a dry scroll pump. It fills a need of many users for a low-damage oxygen plasma clean of critical surfaces, especially for pre-metallization (gate and ohmic contact) semiconductor process steps. This is in part due to the fact that photo or electron beam lithography processes often leave small amounts of organic residue even in channels that appear (in optical microscopy) completely clean and developed. The tool is powered by a 13.56 MHz RF generator (0-50 W) and has two input gas channels, but at the moment is only plumbed with pure

oxygen. The asher, designated “ASH01” in the Nanotech West tool database, is located in Bay 3 of the cleanroom. While the tool is very easy to operate, a short training session is required; interested users should contact Pete Janney (janney.9@osu.edu) for a session.



Nanotech West's Lab Coordinator Pete Janney with the new Diener Pico® plasma asher instrument

Nanotech West will also soon complete the installation of a Plasma Therm 790 plasma-enhanced chemical vapor deposition (PECVD) tool. Gases plumbed to the tool will enable the deposition of high-quality, low-temperature silicon nitride and silicon oxide. Nanotech West users will receive a broadcast email when the tool is available.

The asher and PECVD were both purchased with capital funds from the Ohio Wright Center for Photovoltaics Innovation and Commercialization (PVIC), which in turn is funded by the Ohio Third Frontier Program of the Ohio Department of Development.

OSU Materials Week >>>>>>>>

>>>>>>>> May 7 – 10, 2013, Ohio Union

Materials Week is moving! Due to The Ohio State University's academic calendar changing from quarters to semesters in 2012, the next OSU Materials Week will be scheduled for Spring 2013.

Materials Week speakers and registration information will be posted on IMR's website: imr.osu.edu and in future issues of IMR Quarterly newsletter.

A program planning committee has been created and has begun planning technical sessions for the next Materials Week. If you would like to share feedback on past Materials Week conferences or suggestions of topics, speakers, or events for 2013, please send your ideas to Layla Manganaro, IMR Program Manager, at manganaro.4@osu.edu

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