Jan 10, 2011 10:40 AM 1011 EB1

Dr. Jesse Q. Bond University of Wisconsin, Madison

Pathways to energy-dense bio-fuels

We will show that γ -valerolactone (GVL) is a promising platform molecule for the sustainable generation of transportation fuels and specialty chemicals from lignocellulosic biomass. Our recent studies have demonstrated the selective production of energy-dense transportation fuels from GVL in a two-stage catalytic process.

In the first stage, GVL undergoes ring opening and subsequent decarboxylation to quantitatively yield butene monomers over an acidic SiO2/Al2O3 catalyst. In the second stage, butene units are coupled at low temperatures over acidic catalysts, such as Amberlyst-70 and H-ZSM-5, for selective production of higher olefins, with yields in excess of 95%. This integrated, two-stage process has demonstrated high yields (>80%) of fuel range hydrocarbons from GVL in stable, continuous operation at the laboratory scale, potentially providing a new route for cost effective conversion of lignocellulosic biomass to transportation fuels at commercial scale.

It is imperative that future research address the major challenges in the production of GVL from lignocellulosic biomass. Accordingly, we will consider the major impediments to cost effective production of GVL and present recent advances toward mitigating these challenges.

Jan 26, 2011Dr. Lauren F. Grenlee10:40 AMNational Institute of Standards and Technology, Boulder, CO

1011 EB1

Zero valent iron nanoparticles: Synthesis, characterization & applications

There has been a growing interest in using iron-based nanoparticles in water treatment due to their catalytic properties. Monometallic and bimetallic iron nanoparticles are reactive in an aqueous system and can be designed for targeted removal of specific organic and inorganic water contaminants.

This research investigates aqueous-based synthesis and characterization of monometallic iron nanoparticles and bimetallic iron-palladium nanoparticles. Several organic stabilizers are compared in their ability to control particle aggregation and size during nanoparticle synthesis, as well as control particle oxidation over time.

Dynamic light scattering is used to evaluate nanoparticle size distributions. Techniques such as zeta potential measurement, thermogravimetric analysis, and electron microscopy are used to evaluate particle morphology and stabilizer surface coverage on the nanoparticles. Finally, electron paramagnetic resonance (EPR) and quartz crystal microbalance techniques are used to evaluate changes in particle magnetism and particle mass, respectively, during surface oxidation in an aqueous environment.

Jan 28, 2011 10:40 AM 1007 EB1

Parag Banerjee

University of Maryland, College Park, MD

Strategies for building nanostructured energy devices

Controlled and well-ordered nanostructures present an opportunity to build a). traditional devices with improved performance and enhanced functionalities or b). novel devices exploiting entirely new phenomena. An added advantage can be realized by invoking facile fabrication techniques thus providing benefits of simplicity, low cost and scalability as well. In this talk, I will present a design scheme based on self-assembled nanotemplates and a material set deposited using self-limiting and self-aligned processing principles to develop 1). novel metal-insulator-metal (MIM) nanocapacitors for energy storage and 2). oxide-based heterojunction diodes for energy harvesting.

The initial part of my talk will focus on the process development aspects of each of the individual processes. Our template for building nanostructures is a highly self-ordered, porous, anodic aluminum oxide (AAO) film.

The latter part of my talk will focus on the process integration aspects of the actual devices. Here, I will talk about process integration strategies we have used to build MIM capacitors and oxide-based heterojunction diodes. I will present characterization and performance data from our current 'star' devices and the challenges we face as we iron out integration issues and improve on the quality and reliability of these devices.

Jan 31, 2011 10:40 AM 1011 EB1

Dr. Abhinav A. Shukla Bristol-Myers Squibb Co.

Bioseparations - Quo Vadis?

Bioseparations – the art and science of purifying biological macromolecules - has changed in radical ways since the first use of chromatographic separation processes over a century ago. However, a number of forces are re-shaping the biopharmaceutical arena.

These factors include a significant increase in the number of biopharmaceutical products and drug candidates due to enhanced interest from both biotech and big pharma, the advent of monoclonal antibodies as a key product class requiring larger production scales and higher productivity, a heightened focus on drug safety at the FDA, and the advent of personalized therapeutics and increasing competition – both from innovator companies and from the looming threat of biosimilars.

This presentation shares a perspective on how these forces will shape the field of bioseparations.

Particular emphasis will be paid to monoclonal antibody (mAb) downstream processing and how some of the separations challenges unique to this product class are being overcome. The presentation will also highlight some recent trends in process validation and the implementation of the Quality by Design (QbD) framework for biopharmaceutical manufacturing processes. Finally, the presentation will share a vision for how academic research can play a key role in helping this dynamic field evolve in the coming years.

Feb 2, 2011 10:40 AM 1011 EB1

Dr. William A. Tisdale MIT - Organic and Nanostructured Electronics Lab

Hot Electron Transfer from Semiconductor Nanocrystals

Solar cells have had limited impact in meeting energy needs because of their high cost and low power conversion efficiencies. Semiconductor nanocrystals, or quantum dots, offer new possibilities because they are predicted to have novel optoelectronic properties that could enable ultra-efficient solar power conversion.

In conventional semiconductor solar cells, absorption of photons with energies greater than the semiconductor band gap generate "hot" charge carriers that quickly "cool" before all of their energy can be captured. However, the discretization of electronic energy levels in quantum dots can slow down this cooling process, which might enable the harvesting of photogenerated charge carriers before their excess energy is lost as heat.

In this talk, I will demonstrate the transfer of hot electrons from PbSe nanocrystals to conduction band sates of bulk TiO2 and the concomitant excitation of coherent surface vibrational modes associated with this ultrafast process. In order to make these measurements, we developed the use of optical second harmonic generation (SHG) for femtosecond time-resolved studies of interfacial charge separation.

I will discuss information we obtain from this technique as well as the effect of temperature, nanocrystal size, and surface chemistry, and how these observations inform our understanding of the way charge and energy move across interfaces between nanoscale and bulk materials.

Feb 7, 2011 10:40 AM 1011 EB1

Dr. Derek W. Bartlett

Cal Tech - Cancer Immunotherapeutics & Tumor Immunology

Barriers to Delivery: Cancer-Targeted Delivery Vehicles

Transport across artificial or natural biological barriers plays a central role in biomedical applications ranging from pharmaceutical production to drug delivery. These barriers can include artificial membranes used in filtration devices for hemodialysis or the purification of pharmaceutical products.

Alternatively, these barriers can include naturally occurring physiological barriers such as the vascular endothelium or the glomerular basement membrane that influence the pharmacokinetics of administered therapeutic molecules. Quantitative analysis of transport across these artificial or natural barriers can facilitate the rational design of novel therapeutics, purification processes, or biomedical devices.

In this seminar, the utility of such an approach will be illustrated with examples from research conducted on the development of targeted small interfering RNA (siRNA) nanoparticles and the production of antibody-chelate conjugates for radioimmunotherapy. These examples will also highlight the utility of mathematical models in the design, production, and preclinical evaluation of cancer-targeted delivery vehicles.

Feb 14, 2011Dr. Jonathan Z. Sexton10:40 AMDepartment of Pharmaceutical Sciences - NC Central University1011 EB1

Engineering Solutions for Drug Discovery and Bioseparations

There is an increasing need for engineering solutions coupled with multivariate data modeling in both biomanufacturing and drug discovery to yield better process quality and understanding. Here we present applications to bioseparations and high-throughput screening that integrate FPLC, LC/MS, automated microscopy, and multivariate data analysis to provide engineering solutions in these areas.

In downstream processing, the evaluation of protein purification process health is largely ignored and protein purification columns are typically retired after a static number of purification cycles. This approach ignores lot-to-lot variation in chromatographic media and operator influence on the packing of individual columns. We have developed a bench-scale model for the optimization and evaluation of compressed-bed protein purification columns and a multivariate Transition Analysis (TA) framework for real-time monitoring of process health.

In drug discovery, we present a high-throughput drug discovery pipeline for the discovery of small molecules that increase peroxisome biogenesis in human cells for therapeutic value in Type-II Diabetes (T2D) and Metabolic Syndrome (MetS). Development of a principal component analysis scoring system for compounds effects has led to several promising lead compounds with demonstrated therapeutics in a rodent model for T2D and MetS.

Mar 2, 2011	Professor Jason Locklin
2:00 PM	University of Georgia
2018 EB1	
Making Surfaces Smart	

Surface-initiated polymerization reactions are rapidly developing as methods to prepare functional, high-tech coatings. This is a technique based on the growth of polymer molecules at the surface of a substrate in situ from a surface bound initiator, which results in the covalent attachment of polymer molecules to this substrate.

Polymer layers in which the polymer chains are irreversibly immobilized to the substrate are especially attractive for a wide variety of applications, as these layers have excellent long-term stability, even in rather adverse environments. In addition to improved stability, the arrangement of stretched polymer chains allows for high densities of functional groups to be obtained in a limited area.

We are currently developing new polymerization methodologies using surface initiated polymerization for the following applications: Light induced mechanical motion, orthogonal click-chemistry, colorimetric sensors, and enzymatic biofuel cells made from conjugated polymers.

Apr 4, 2011Dr. L. Louis Hegedus, Visiting Distinguished Fellow10:40 AMRTI International1011 EB1

America's Energy Future in Three Dimensions

Energy is one of the grand challenges of mankind, a conundrum that has mobilized huge and global technological, economic, and societal forces, and upon which much of the future of our society will depend. Energy issues also tend to be dynamic and complex; the complexity comes in part from the fact that the key dimensions (technology, economics, and societal considerations) are intertwined, inseparable, and interactive.

RTI has mounted an interdisciplinary effort to breach the boundaries between the disciplines and analyze the energy grand challenge in the context of all three of its key dimensions. This talk will review energy technologies in their economic and societal contexts, energy economics in their technological and societal contexts, and the societal aspects of energy in their technological and economic contexts.

It will highlight the insights gained from such analysis, and point to research needs, primarily in the societal domain, to enable or create the necessary and sufficient conditions for optimizing the US energy infrastructure.

Apr 18, 2011 10:40 AM 1011 EB1

Dr. Emmett Crawford Eastman Chemical Company

Development of Tritan Copolyesters

Over the last two decades, there have been very few examples of the successful commercialization of 'new to the world' polymer products derived from new monomers. Tritan copolyesters are the trade name of Eastman Chemical Company's new family of copolyesters based on 2,2,4,4-tetramethyl-1,3-cyclobutanediol (TMCD).

The unique chemistry of Tritan provides a higher glass transition temperature (Tg) than traditional copolyesters, translating into superior heat resistance. In conjunction with the material's exceptional toughness, chemical resistance, and hydrolytic stability; molded products can withstand the harsh dishwasher environment without crazing, cracking, or hazing from continual exposure to high heat, humidity, and aggressive cleaning detergents and sanitizers.

In addition, Tritan is manufactured without bisphenol-A. This combination of properties makes the Tritan family of materials well suited for packaging, house wares, and medical applications. The Tritan copolyester family has enjoyed remarkable early commercial success.

Apr 25, 2011	EB1 Dr. Stanley C. Ahalt, RCI Director
10:40 AM	Department of Computer Science at UNC-Chapel Hill
1011	
The LINC System's Panaissance Computing Institute (PCI)	

The UNC System's Renaissance Computing Institute (RCI)

This talk will provide an overview of the current activities at RENCI, including both our traditional, HPC-centric Computational Science and Engineering (CSE) collaborations, but also our work that is more broadly based on a wholistic cyberinfrastructure (CI). CI problems include examples drawn from both life and environmental sciences that are characterized by requirements that span simulation, data management, workflow, analytics,

and decision support, and which ultimately are aimed at producing actionable information.

May 10, 2011 Dr. Timothy J. Bunning

11:30 AM

1007 EB1

Air Force Research Laboratory - Georgia Tech

Dynamic coloration from polymer/liquid crystal architectures

A variety of stimuli can be utilized to introduce dynamic optical properties of thin films. Introducing polymeric structures into these systems enables nanocomposite structures whose responsiveness can be mitigated by surface elasticity and area.

Cholesteric liquid crystals (CLCs) are highly promising in a myriad of photonic-based applications. Unfortunately, the helical nature that defines CLCs inherently limits their reflection to 50% of unpolarized light. In addition, CLCs are typically considered 'binary' where an electric field switches the colored state 'off' from a stable, reflective planar state. Over the past few years, we have investigated a variety of photosensitized versions of CLC systems, where light is used to tune the color instead of turning it on and off. We have recently demonstrated light induced tuning of more than 2000 nanometers (compared to 150 nanometers), fast tuning and relaxation on the order of minutes (compared to hours and days), autonomous cueing (self-limiting of output light intensity), photoinversion of the pitch handedness, and coupled electro-optic and photo-optic behavior.

We have also recently utilized anisotropic photopolymerization to enable high reflectivity in a single cell through the formation of a chiral templated polymer network grown from one substrate. This so-called hyper-reflectivity can be turned on or off or tuned using light or heat.