Welcome to the 8th Annual

Amgen-Clorox Graduate Student Symposium

Friday, October 02, 2015

Department of Chemical Engineering

University of California, Santa Barbara

Program and Abstracts

UCSB ChE's 8th Amgen-Clorox Grad Student Symposium

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This symposium is generously supported by educational donations from Amgen and Clorox.

8th Annual Amgen-Clorox Graduate Student Symposium

Friday, October 02, 2015

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Industry guests, faculty and presenters are all welcome		
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UCSB Chemical Engineering's 8th Annual
Amgen-Clorox Graduate Student Symposium

Oral Presentation Abstracts

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Nikolai Petsev — *Dow Lecture*: Multiscale from molecular to continuum: a hybrid simulation method for multicomponent systems

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Lauren Huyett — *Schlinger Lecture*: Impact of sensing and actuation characteristics on artificial pancreas design

Session I: Transport and Methods

Multiscale from molecular to continuum: a hybrid simulation method for multicomponent systems

Nikolai D. Petsev, L. Gary Leal, and M. Scott Shell

Department of Chemical Engineering, University of California Santa Barbara

Numerous problems in molecular and interfacial physics involve processes spanning many different length scales, a feature that poses major challenges in applying traditional simulation techniques such as molecular dynamics (MD). This difficulty has motivated efforts in recent years to develop "multiscale" simulation techniques that allow for a detailed treatment of select regions where atomistic resolution is required, and a more coarse-grained description for other parts of the problem. Previously, we developed a multiscale simulation strategy using a stochastic particle-based technique called "smoothed dissipative particle dynamics" (SDPD). SDPD is a thermodynamically consistent particle method for solving the fluctuating hydrodynamic equations of Landau and Lifshitz. Using our multiscale approach, it is possible to couple a MD region to a hierarchy of SDPD domains featuring different characteristic length scales.

While there have been a number of hybrid simulation strategies for single-component fluids proposed in the last few years, extending these types of approaches to multicomponent systems remains a major challenge. In this talk, we describe a novel generalization of our multiscale methods to systems that involve one or more dissolved species. First, we develop a new multicomponent formulation of SDPD for a binary mixture through a particle discretization of the diffusion equation with fluctuations in the concentration field. This opens the possibility for a wide range of applications in biological and drug delivery problems. Next, we generalize this multicomponent approach for multiscale simulation and discuss how it can be reconciled with our MD-continuum techniques. Finally, we consider several simple equilibrium and non-equilibrium case studies and discuss future applications to nanodroplet dissolution and formation under flow.

Probing the influence of flow-induced breakage on the rheology and kinematics of micellar solutions

Peng Cheng, L. Gary Leal, and Matthew E. Helgeson

Department of Chemical Engineering, University of California, Santa Barbara, CA 93106 USA

Wormlike micelles (WLMs) – polymer-like surfactant aggregates – are ubiquitous in various industrial processes and consumer products including enhanced oil recovery, personal care products, etc. Rheology of WLMs is critical to these applications, and so it is necessary to understand how micellar architectures respond to, and in turn influence, the flows they are subjected to. Specifically, WLMs are known to exhibit a number of nonlinear flow instabilities, such as shear thickening, flow-induced structure, and shear banding. The latter is observed across a wide range of material systems, and involves spontaneous development of distinct regions with widely differing velocity gradient in a number of different flow geometries, and is typically attributed to mechanical instability due to a non-monotonic constitutive curve. The broad goal of this work is to identify the molecular processes that could possibly give rise to this non-monotonic behavior, and test them for a range of micellar architectures and types of flow.

The physics of WLMs have been characterized in the framework of “living” polymers, in which bonds between monomers are impermanent and the assemblies undergo dynamic scission and reformation. These processes lead to a broad equilibrium distribution of micelle lengths, which could be influenced by flow in a non-trivial fashion. Here, we report a combination of rheology, flow velocimetry, and small angle neutron scattering (SANS) measurements in Taylor-Couette flow to probe the influence of flow on the micelle scission process, and its potential role in the rheology and kinematics of shear banding WLMs. Experimental data are quantitatively compared to the predictions using the Vasquez-Cook-McKinley (VCM) constitutive model, which incorporates a phenomenological model for the kinetics of dynamic scission and reforming of WLM chains under flow. We find that the VCM model successfully captures both the WLM rheology and flow kinematics at steady state. However, as with other models for shear banding, the predicted time scale to achieve steady state banding is at least an order of magnitude smaller than what is observed experimentally. Moreover, we carry out SANS measurements of the local length distribution of micelles with systematically varying average contour length, and compare this with coarse-grained distributions predicted by the VCM model. Given with significant discrepancies between the experimental data and the model predictions, we propose adaptations to the model to better reflect the underlying equilibrium and non-equilibrium length distributions of micelles.

Design of a tip-enhanced Raman spectroscopy system with a novel total internal reflection illumination geometry

Alexander Heilman and Michael J. Gordon

Department of Chemical Engineering, University of California Santa Barbara

Tip-enhanced Raman spectroscopy (TERS) is a hybrid microscopy technique that combines the high spatial resolution of atomic force microscopy (AFM) with the chemical specificity of vibrational (Raman) spectroscopy to achieve label-free chemical imaging with sub-diffraction-limited resolution. In TERS, a metal-coated AFM tip acts as an optical antenna, coupling with incident laser light to generate a strong, confined electric field at the tip apex; this field is used to locally enhance Raman scattering from a nanometer-scale volume. Both the nature of the tip-laser coupling, and the intensity of the confined field in the tip-substrate gap, strongly influence the capabilities of any TERS instrument, but these factors are difficult to measure or quantify in most systems. In this work, a home-built TERS system is presented, with emphasis on its unique total internal reflection illumination geometry, which enables direct interrogation of tip-laser coupling, tip-surface interactions and other near-field optical phenomena. Experimental studies of tip-laser coupling efficiency, as a function of both tip-surface distance and laser wavevector, were in excellent agreement with FDTD simulations and were used to optimize the excitation conditions for TERS experiments. The instrument was used to demonstrate tip-enhanced Raman imaging of a nanopatterned array of phthalocyanine on Au and exhibited a spatial resolution much better than the diffraction limit.

Session II: Biomolecules and Biosurfaces

Elucidating the functional and structural consequences of adenosine A2a receptor oligomerization

Nicole Schonenbach, Monica Rieth, Songi Han, Michelle O'Malley

Department of Chemical Engineering, University of California Santa Barbara

G protein coupled receptors (GPCRs) are integral membrane proteins that play a crucial role in cellular signaling, and have long been popular drug targets. Their localization at the cell surface makes them easily accessible for small molecule therapeutics to trigger or block particular intracellular reaction cascades. The human adenosine A2a receptor is well known for its role in cardioprotective functions, but it can tune its function by forming oligomers with itself as well as other GPCRs, such as the dopamine D2 and D3 receptors. In addition to cardioprotection, these oligomers are potential targets for treatment of central nervous system disorders such as schizophrenia and Parkinson's disease. However, design of structurally-inspired pharmaceuticals to target specific oligomers has been limited by experimental difficulties associated with obtaining structural data for membrane proteins. These problems stem from low abundance of GPCRs in native tissues, as well as a poor understanding of functional consequences of homo- and hetero-oligomerization.

To elucidate structure-function relationships of GPCR oligomers, we have developed a system to overexpress the full-length adenosine A2a receptor in the yeast *Saccharomyces cerevisiae,* and purify functional receptor for biophysical study of homo-oligomers with size exclusion chromatography coupled with multi-angle light scattering (SEC-MALS) and spin label electron paramagnetic resonance (EPR). We have observed that A2a tends to form homo-oligomers in mixed micelles, and that these oligomers are able to bind to ligand, indicating properly folded receptor. By employing site-directed spin labeling (SDSL) and EPR we have explored the relationships between ligand binding and structural rearrangement within the receptor oligomers. EPR can provide information about the distances between certain positions of each receptor within a dimer, helping to identify the oligomer interface. Such information is crucial for the rational design of therapeutics targeting specific oligomers. Additionally, the application of this approach to A2a-containing heteromers and other GPCR complexes, will lead to a better understanding of the role oligomers play in modulating ligand response.

Ionic liquids as antimicrobials, solvents, and prodrugs for treating skin disease

Michael Zakrewsky and Samir Mitragotri

Department of Chemical Engineering, University of California Santa Barbara

The skin is the largest organ in the body. It provides a compliant interface for needle-free drug delivery, while avoiding major degradative pathways associated with the GI tract. These result in improved patient compliance and sustained and controlled release compared to other standard delivery methods. Concurrently, for the treatment of skin related diseases (e.g. bacterial infection, skin cancer, psoriasis, atopic dermatitis, etc.) cutaneous application provides targeted delivery to the diseased site, allowing the use of more potent therapeutics with fewer systemic side effects. Unfortunately, the outer layer of the skin – the stratum corneum (SC) – presents a significant barrier to most foreign material. This is particularly true for large hydrophilic molecules (>500Da), which must partition through tortuous lipid channels in the SC to penetrate deep tissue layers where the majority of skin-related diseases reside. Interestingly, over the last few decades ionic liquids (ILs) have emerged as a burgeoning class of designer solvents. ILs have been proven beneficial for use in industrial processing, catalysis, pharmaceuticals, and electrochemistry to name a few. The ability to modulate either the cation or anion individually presents an advantageous framework for tuning secondary characteristics without sacrificing the primary function of the IL. Here, we report the use of novel ILs for cutaneous drug delivery. Specifically, we demonstrate their potential as potent, broad-spectrum antimicrobials, as solvents for topical delivery of hydrophilic and hydrophobic drugs, and as prodrugs to enhance delivery of macromolecules and reduce toxicity of drugs that cause skin irritation.

Adaptive and synergistic interactions of amino acids in underwater bio-adhesives

Michael V. Rapp

Department of Chemical Engineering, University of California Santa Barbara

In physiological fluids and seawater, adhesion of synthetic polymers to solid surfaces is severely limited by high salt, pH, and hydration, yet these conditions have not deterred the evolution of effective adhesion by many marine organisms. In particular, mussels secrete protein glues that robustly adhere underwater; the amino acids within the glue adapt and bind to a variety of chemically heterogeneous surfaces through specific side-chain/surface interactions [1]. Additionally, the abundance and proximity of catecholic Dopa (3,4-dihydroxyphenylalanine) and lysine residues hint at a synergistic interplay in adhesion. Certain siderophores—bacterial iron chelators—consist of paired catechol and lysine functionalities, thereby providing a convenient experimental platform to explore molecular synergies in bioadhesion. These siderophores and synthetic analogs exhibit robust adhesion energies ($E_{\mathrm{ad}} \geq$ -15 mJ/m^2) to mica in saline pH 3.5 to 7.5 and resist oxidation. The adjacent catechol-lysine placement provides a "one-two punch," whereby lysine evicts hydrated cations from the mineral surface, allowing catechol binding to underlying oxides [2].

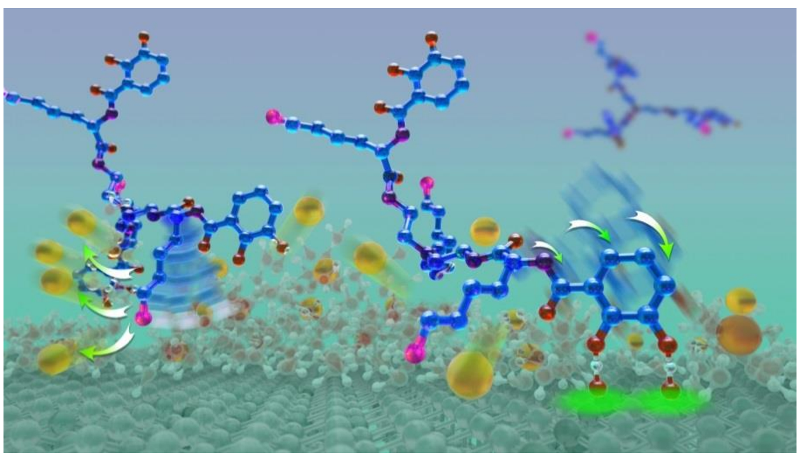

Figure 1: Wet adhesion of the catechol-amine compound, Tren-Lys-Cam, to a mica surface. The cationic lysine residue (the cationic amine is shown in pink) is depicted as penetrating through the hydration layer and evicting potassium ions (gold balls), preparing the mica surface for catechol hydrogen bonding (highlighted by the green aura). Illustration by Peter Allen.

References:

[1] Yu, J; Kan, Y; Rapp, M; Danner, E; Wei, W; Das, S; Miller, D. R.; Chen, Y; Waite, J. H.; Israelachvili, J.N. *Proc. Natl. Acad. Sci. USA* **2013**, *110*, 15680-15685.

[2] Maier, G. P.*; Rapp, M. V.*; Waite, J. H.; Israelachvili, J. N.; Butler, A. *Science* **2015**, *349*, 628-632

Session III: Materials and Complex Fluids

Saccharide-mediated hydration and crystallization of inorganic structural materials

Rahul P. Sangodkar, Michael F. Doherty, and Bradley F. Chmelka

Department of Chemical Engineering, University of California Santa Barbara

Competitive adsorption of dilute quantities (<1 wt%) of certain organic molecules and water at inorganic oxide surfaces strongly influences the rates of dissolution, hydration, and/or crystallization of inorganic species. Organic molecules, such as saccharides or phosphonic acids, adsorb on heterogeneous low-surface-area (ca. 1 m^2/g) oxide particles to inhibit hydration reactions in technologically important cement-water mixtures and also in biominerals. Such competitive adsorption of organic species in place of water slows the formation of hydration products that are responsible for the development of mechanical strength in synthetic and naturally occurring structural solids. For example, certain saccharide molecules adsorb at inorganic oxide (or biological) surfaces in place of water and thereby inhibit hydration processes. The surface-adsorption efficacies of different saccharide molecules depend on their molecular compositions and interactions at solid-liquid interfaces. Detailed molecular-level information regarding the surface-adsorbed saccharide species can be obtained by using powerful methods of nuclear magnetic resonance (NMR) spectroscopy, and correlated with electron microscopy, X-ray diffraction, X-ray fluorescence, and mechanical strength analyses. Examples will be presented for silicate-aluminate cementitious solids and carbonates of synthetic and biological origin, where hydration and crystallization processes are influenced by low absolute quantities of adsorbed saccharide or phosphonic acid molecules. The results show that closely related saccharides exhibit surprisingly different adsorption behaviors and the corresponding hydration influences are established to arise from their distinct surface interactions vis-à-vis water. The adsorption behaviors of such saccharides have been shown to depend on the relative extents and types of surface interactions, including hydrogen-bonding and electrostatic interactions, which consequently depend on the molecular architectures, stereochemistries, and chemical reactions of the saccharide molecules. Overall, the insights provide criteria for the rational design and use of organic adsorbates to mediate hydration and crystallization processes at silicate, aluminate and carbonate particle surfaces, which are fundamentally and technologically important for oilwell cementing, carbon capture, and development of mechanical strength in biominerals, several of which will be highlighted.

Understanding the dynamics and rheology of polymer-colloid mixtures using temperature-sensitive nanoemulsions

Juntae Kim and Matthew E. Helgeson

Department of Chemical Engineering, University of California Santa Barbara

Polymer-colloid mixtures are widely used in many areas including foods, consumer products and, in particular, nanocomposites. It is well known that the properties of such nanocomposites depend strongly on the microstructure of the dispersed colloids. Since many nanocomposites are processed from solution, it is therefore critical to understand how polymer-colloid interactions affect fluid rheology and flow-induced microstructure. However, such knowledge has proven difficult due to a lack of model material systems where colloid-polymer and colloid-colloid interactions can be systematically tuned. To enable such a model system, we have developed nanoemulsions containing soluble polymers whose affinity for the droplet surface can be reversibly tuned with temperature. Specifically, the polymer forms a temperature-induced bridging network which imparts well-controlled viscoelasticity in the suspending medium and droplet-droplet attractions. The overall goal of this research is to understand how these temperature-sensitive properties can be used to understand and direct fluid microstructure and rheology.

In this presentation, I will focus on conditions of weak polymer bridging, which produce a transient network of interdroplet bridges without compromising colloidal stability. Such polymer-colloid transient networks are known to exhibit shear-induced particle clustering with associated strong shear thinning. To better elucidate the mechanism of clustering and shear thinning, we have performed 3D microstructural measurements under shear flow using flow-small angle neutron scattering in the flow-vorticity and flow-gradient planes. These fluids exhibit significant flow-induced anisotropy in the droplet microstructure consistent with cluster formation, which develops during strong shear thinning. Specifically, butterfly scattering appears in the flow-vorticity plane at shear rates corresponding to the shear thinning, with projected orientation in the vorticity direction, in agreement with previous studies. However, significant anisotropy also develops in the flow-gradient plane, with orientation along the compressional axis of shear, which is inconsistent with previous hypothesized mechanisms for shear-induced clustering. These results suggest vorticity-aligned aggregates possess anisotropic cross section, and that hydrodynamic interactions in the flow plane play an important role in the formation of shear-induced clusters. To demonstrate this, we show that collapse of the flow-induced alignment and shear thinning responses over a number of different viscoelastic parameters through a modified Peclet number for the suspended colloids. Overall, this structural information provides a basis to control the rheology and suspension microstructure of non-aggregating polymer-colloid mixtures.

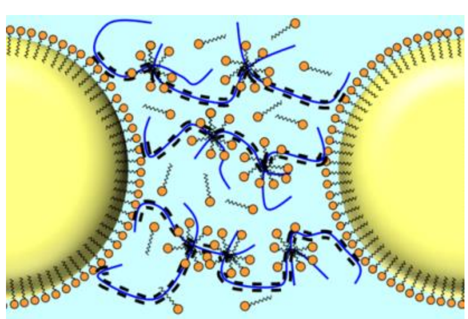

Figure 1: transient network between nanoemulsion droplets

Understanding the relation between polymer brush properties and antifouling

Edward Toumayan

University of California, Santa Barbara, Chemical Engineering, MRL

Reverse osmosis (RO) membrane filtration is the most common method of desalination and is a critical technology for water purification, particularly in water-stressed regions. However, a major concern for RO membranes is the accumulation of unwanted material (foulants) on the active surface, leading to increased transmembrane pressure, and subsequent decrease in the water flux. To combat the fouling process, filtration modules must undergo harsh cleaning cycles, ultimately decreasing the membrane lifespan. Creating fouling-resistant filtration membranes therefore could help decrease cleaning frequency and/or enable milder cleaning conditions. Fouling resistance is a direct consequence of surface properties, in particular, hydrophilicity, roughness, and surface charge are the most important determinants for fouling propensity. Consequently, careful control of surface coatings is vital to understanding the relation between foulants and surfaces.

The present study investigates the use of surface-tethered polymer brushes, as a way to manipulate surface properties. Polymers with a range of chemical compositions were synthesized using a grafting-from method for creating surface-tethered polymer brushes. The range of chemistries generated by this method enabled systematic investigation of different surface properties and their subsequent fouling propensity. Fouling propensity was evaluated using surfactants with anionic, nonionic, and cationic character. These experiments were conducted over a range of pH in order to elucidate the effect of ambient conditions on the fouling propensity.

Session IV: Biomedical Systems

Personalized MPC and PID strategies with an enhanced, dynamic IOB algorithm for automated glucose control

Joon Bok Lee, Eyal Dassau, Ravi Gondhalekar, Dale E. Seborg, Jordan E Pinsker, Francis J. Doyle III

Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

William Sansum Diabetes Center, Santa Barbara, CA

John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

Translating insulin sensitivity of individuals with type 1 diabetes mellitus into a dynamic control-relevant model is a challenging task. In this talk, a core model of insulin-blood glucose dynamics is expanded with a medically inspired personalization scheme based on each subject's insulin pump parameters. The proposed method yields a model tailored to each individual's insulin sensitivity. Additionally, an enhanced dynamic insulin-on-board (IOB) algorithm is proposed to minimize the likelihood of controller-induced hypoglycemia as a result of insulin suspension that is accompanied with rapid rise of blood glucose due to rescue carbohydrate load. The performance of Model Predictive Control and Proportional Integral Derivative controllers with the addition of this personalization is demonstrably improved for simulated clinical trials involving 100 *in silico* subjects. Statistically significant improvements were observed, with increases of the time in the 80-140 mg/dl glycemic range of 20% and the time in the 70-180 mg/dl safe glycemic range of 10%. Further, the controllers achieved statistically significant reductions in hyperglycemic incidents of 10% without increase in hypoglycemia. Robustness of this proposed method has been demonstrated for a wide range of uncertainties in subject clinical parameters for both *in silico* and clinical studies. The novel enhanced dynamic IOB algorithm has also been validated in advisory mode (simulated) testing of clinical data. The proposed approach can personalize controller action in an artificial pancreas without the need for individual model identification. It provides safe control action following large rebounds after a pump suspension, particularly when the suspension is accompanied by carbohydrate intake.

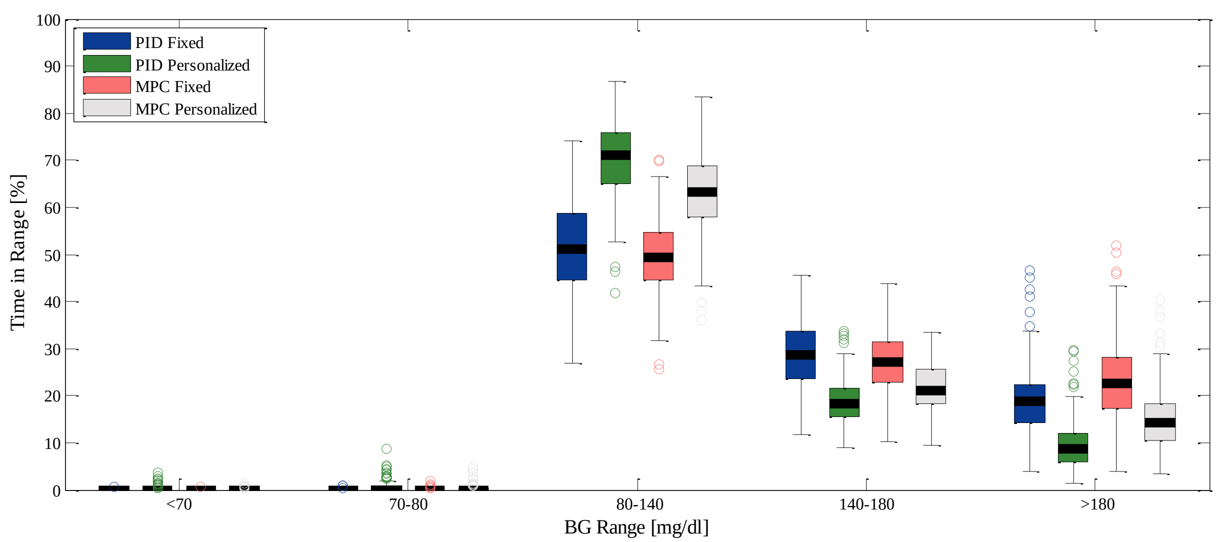

Figure 1: Blood glucose (BG) control performance characterized by boxplot representation of the overall times in different target ranges 100 *in silico* subjects controlled by PID and MPC controllers with personalized or fixed gains under the clinical protocol. Statistically significant differences occur between fixed and personalized controllers of each controller type for the 80-140, 140-180, and >180 mg/dl BG ranges.

Impact of sensing and actuation characteristics on artificial pancreas design

Lauren M. Huyett[1], Eyal Dassau[1,2], and Francis J. Doyle III[1,2]

[1]*Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA 93106-5080*

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Type 1 diabetes (T1D) is a chronic disease characterized by the body's inability to produce insulin, leading to chronically high blood glucose (BG) concentrations. T1D is treated by frequent self-administration of insulin based on BG measurements; however, there is a fine line between too little and too much insulin, and an overdose can lead to a dangerous drop in BG. The artificial pancreas (AP), consisting of a glucose sensor, an insulin pump, and a feedback control algorithm, will replace self-treatment by automatically calculating and delivering insulin dosages based on continuous glucose measurements. Many iterations of the AP utilize commercially available subcutaneous (SC) insulin pumps and glucose sensors, but these devices introduce physiological limitations that make control difficult. In this work, we investigate the intraperitoneal (IP) space as an alternative site for insulin delivery and glucose sensing to improve AP performance. Our results show that glucose sensors placed in the IP space have a lower time constant than SC sensors, allowing the controller to respond more quickly to BG disturbances. Similarly, insulin delivered through the IP space has faster pharmacokinetic and pharmacodynamic (PK/PD) characteristics than SC insulin. Based on models of the sensing and actuation dynamics, a proportional-integral-derivative control algorithm with anti-reset windup protection was designed for the IP-IP route and evaluated on 10 simulated T1D subjects. Using the IP-IP route lead to a more robust controller that provided excellent control during the simulation studies. Our results support the development of a fully implantable AP that will operate within the IP space to safely and effectively control BG levels.

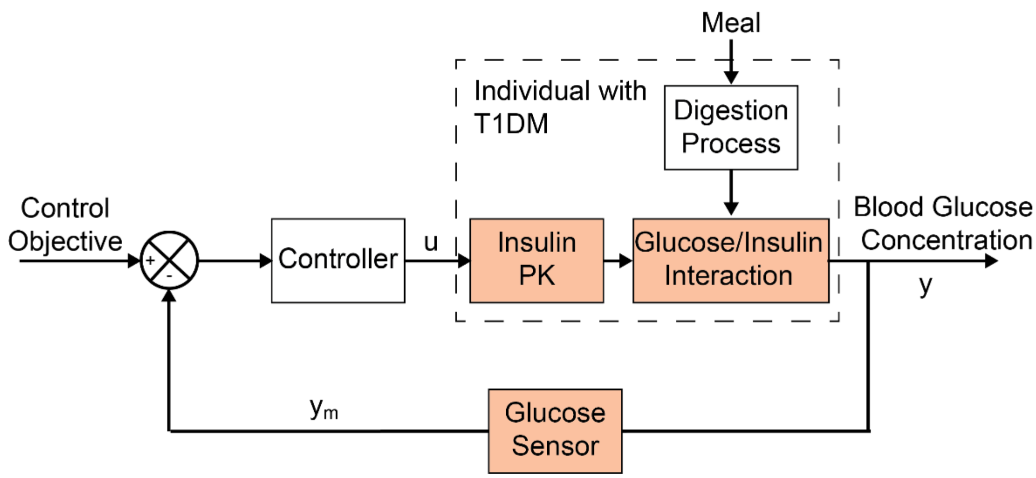

Figure 1: Block diagram demonstrating closed-loop control of blood glucose concentration for people with type 1 diabetes. The blocks highlighted in orange (Insulin Pharmacokinetics, Glucose/Insulin Interaction, and Glucose Sensor) indicate steps of the process that vary depending on choice of sensing and actuation site.

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Poster Presentation Abstracts

Complex Fluids, Colloids and Interfaces

Nicholas Cadirov	Influence of humidity on gecko-inspired adhesives
Howard Dobbs	Characterizing the enhanced dissolution and condensation of aluminosilicates in alkaline environments
Thomas Farmer & Katherine Brune	Understanding and controlling carbonate solubility, precipitation, and crystallization
Tanmoy Sanyal	Robust models of coarse-grained interactions using multi-body potentials with the relative entropy
Elizabeth Decolvenaere	Methods to extract interatomic interactions from experiment
Jimmy Liu	Phase field mapping of field-theoretic simulations
Mark Joswiak	The role of water in the growth of NaCl crystals

Materials and Catalysis

Scarlett Widgeon	Molecular compositions and structures of β-dicalcium silicates for greener cementitious materials
Niels Zussblatt	Fe,N-containing mesoporous carbon materials as non-precious metal electrocatalysts for alcohol and bio-hybrid fuel cells
Matthew Idso	Incorporation of photo-responsive membrane protein species into mesostructured silica for light-driven ion transport
Zachariah Berkson	Evidence for electron carriers in photoluminescent gallium nitride nanoparticles

Biophysics, Bioengineering and Controls

Abe Pressman	Estimating ribozyme kinetics from analysis of in vitro evaluation
Joel Bozekowski	Evaluating the sensitivity of unbiased serum antibody detection using bacterial display peptide libraries
John Henske	Regulation of biomass degrading enzymes in anaerobic gut fungi and their application in synthetic co-culture systems
Kelly Ibsen	Profiling the humoral immune response associated with type 1 diabetes mellitus via bacterial display libraries
David Smith	Nanoscale size and chemistry effects on passive transport
Sean Gilmore	Design of modular parts for synthetic systems inspired by anaerobic fungi

Complex Fluids, Colloids and Interfaces

Influence of humidity on gecko-inspired adhesives

Nicholas Cadirov[1], Jamie Booth[2], Saurabh Das[1], Sathya Chary[2], Kimberly L. Turner[2], and Jacob N. Israelachvili[1]

[1]*Department of Chemical Engineering, University of California Santa Barbara*

[2]*Department of Mechanical Engineering, University of California Santa Barbara*

Geckos have developed foot pads that allow them to maintain their supreme climbing ability despite vast differences in environment, from dry desert to humid rainforest. Successful gecko-inspired mimics should exhibit necessary adhesive and frictional performance across a similarly diverse range of climates. In this work we focus on the effect of relative humidity (RH) on the frictional adhesion behavior of gecko-inspired adhesive pads. A surface forces apparatus (SFA) was used to quantitatively measure adhesive and frictional forces of an anisotropic (tilted half-cylinder) microfibrillar polydimethylsiloxane (PDMS) surface against a smooth hemispherical glass disk at varying levels of relative humidity. Changes in the relative contributions of van der Waals and capillary forces with shearing direction and relative humidity have significant implications for frictional adhesion and 'reversibility'. These results can be extended to formulate design principles for reversible adhesive platforms in humid environments.

Characterizing the enhanced dissolution and condensation of aluminosilicates in alkaline environments

Howard Dobbs, Kai Kristiansen, Alex Schrader, Matthew Gebbie, Brad Chmelka, Jacob Israelachvili

Department of Chemical Engineering, University of California Santa Barbara

Alumina, silica, and aluminosilicate materials are prevalent in geological environments and complex materials used for catalysts, structural materials, and separation processes. In both systems, dissolution and subsequent condensation are complex processes integral to the development of aluminosilicate materials. Variations in reaction conditions, such as pH, ionic composition, and temperature, significantly influence these processes, resulting in a variety of materials with widespread applications. However, the difficulties in correlating molecular and macroscopic changes makes a general understanding of the impact of network formation on structural properties a significant challenge. In this work, we study the enhanced dissolution, observed when asymmetric materials are in proximity, and condensation of aluminosilicate networks to provide insight into the formation of aluminosilicate networks in alkaline environments. The surface forces apparatus (SFA) and nuclear magnetic resonance (NMR) spectroscopy are used to study the macroscopic and molecular changes that occur during dissolution and condensation of aluminosilicates. Specifically, enhanced dissolution of alumina and silica when in proximity to an electrochemically asymmetric surface was measured with the SFA. This suggests a previously unknown driving force that is drastically enhancing the dissolution of alumina and silica, even in low alkalinity solutions where bulk dissolution rates are low. Following dissolution, condensation of aluminosilicates was studied by comparing the change in ^{27}Al and ^{29}Si molecular environments, observed with NMR, with the development of network strength over time, measured by the SFA. Understanding the microscopic and macroscopic changes that occur during dissolution and condensation of aluminosilicate polymers in alkaline environments provides insights into a variety of systems, ranging from grain boundaries in geological systems to the development of reliable aluminosilicate based structural materials.

Understanding and controlling carbonate solubility, precipitation, and crystallization

Thomas Farmer, Katherine Brune, Rahul Sangodkar, Bradley Chmelka, and Michael Doherty

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The carbon dioxide/ bicarbonate/carbonate ($CO_2/HCO_3^-/CO_3^{2-}$) chemistry is ubiquitous in science and in nature. A variety of $CaCO_3$ polymorphs form in crustacean shells, coral reefs, and geologic formations. These solids are able to dissolve, precipitate, and crystalize to different polymorphs depending on the presence or absence of surface additives and proteins, the chemistry and pH of the immediate solution environment, and the temperature. The understanding of carbonate solubility, precipitation, and crystallization processes is expected to contribute significantly to the development of novel carbon capture technologies, as well as aid in understanding and modelling the $CO_2/HCO_3^-/CO_3^{2-}$ solution chemistries found throughout science and nature. Specifically, the synthesis of stabilized metastable calcium carbonate polymorphs such as amorphous calcium carbonate (ACC) from carbon dioxide may lead to the development of carbonate solids suitable for use in Portland cements. Biologically inspired saccharide surface additives have been successfully utilized to inhibit and control the progression of crystallization in amorphous calcium carbonate. Carbonate products have been characterized at a molecular level by solid-state nuclear magnetic resonance (NMR) spectroscopy to establish compositions, structures, and interactions with saccharide surface additives and by transmission electron microscopy (TEM) measurements to investigate the onset and progression of crystallization. These analyses have been correlated with the extents and types of long-range crystalline order present in the carbonate products, as assessed by wide-angle X-ray diffraction (XRD) measurements, and also with particle morphologies using scanning electron microscopy (SEM). Insights into the processes that lead to the formation of these carbonates and the design of new processes utilizing the $CO_2/HCO_3^-/CO_3^{2-}$ chemistry require high-fidelity transport models that are able to maintain applicability in concentrated, reacting ionic systems. Mass transport models capable of handling the difficulties and non-linearities present in such systems have been constructed based on the fundamental Maxwell-Stefan relations for multicomponent mass transport and used to determine the rates of CO_2 transport and chemical conversion to HCO_3^- and CO_3^{2-} in gas/liquid reactive absorption systems.

Robust models of coarse-grained interactions using multi-body potentials with the relative entropy

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Molecular simulation is an important tool for computational studies of a wide range of biomolecular phenomena. However, available computational resources limit simulation to small time and length scales, typically of the orders of sub micro-seconds and tens of nanometers, respectively. This has motivated the development of coarse graining methods. Detailed all-atom reference systems may be mapped to representative simpler coarse grained models with a lower number of sites and complexity, to enable simulations of larger length-scales and for longer times.

The conventional approach to coarse graining techniques involves the use of potentials that depend only on the distance between pairs of atoms, to describe interactions in the coarse grained model. Such potentials, while computationally simple, neglect the often complex contributions of the local environment of a particle to its energy, inherently due to the coarse graining procedure. Pair-wise potentials between two coarse grained sites often build in several correlations with neighboring particles, thus giving the coarse grained model an intrinsic dependence on the overall system density. This limits the transferability of the model i.e., its easy extension to states (densities and temperatures) other than the one at which it was parameterized.

The Shell group has developed a general method [1] using the relative entropy to produce CG models that best capture thermodynamic behaviors of all-atom systems and yet are simpler to simulate because of the lower level of detail. The basic theme of my research is to use this powerful framework to design more accurate coarse-graining algorithms and models. This report outlines our present work, which aims to mitigate the shortcoming of traditional pair-wise potentials by including additive corrections that depend on the local densities of the different atomic species in the system. The local density potentials capture the contribution of the local environment to the particles' energies to improve transferability of the coarse grained model. We validate our approach by using it to construct transferable implicit solvent coarse grained models of hydrophobic collapse of polymers. We also report briefly on a subsequent application of local density potentials to solutions of benzene and water, in constructing coarse grained models from dilute solutions, that affords transferability across different concentration regimes.

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Methods to extract interatomic interactions from experiment

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Generalized Ising models (e.g. cluster expansions) are an effective means for producing phase diagrams using *ab-initio* calculations to determine interatmoic interaction parameters. However, the most common *ab-initio* method, density functional theory, has been demonstrated to have systemic failures when applied to transition metal intermetallics. Here, we demonstrate a procedure to determine interaction parameters for atomistic models from experiment, rather than first-principles calculations. By using measurements made on a small number of high-temperature disordered alloys, a prediction of the alloy's entire phase diagram can be produced. We demonstrate a simple case of our method's application on simulated experimental data, and discuss the additional thermodynamic properties that can be calculated. Finally, we show that our method produces a unique set of interactions that correspond to the principal of maximum entropy, giving a thermodynamic basis for our results.

Phase field mapping of field-theoretic simulations

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Block copolymers are a versatile platform for nanoscale patterning. By selecting parameters such as confinement shape and size, wetting conditions, and polymer composition variables such as chain architecture, molecular weight and block fractions, polymer systems can be assembled into a variety of ordered structures [1, 2]. Exploring this expansive design space is key to a number of applications. In particular, in directed self-assembly (DSA), block copolymer melts are used to increase the resolution of features in semiconductor devices.

A wide range of models and simulation techniques have been applied to the study of polymers on these length scales. Of these, self-consistent field theory (SCFT) is among the most successful and shows strong agreement with experimental results [3, 4]. Although the speed of SCFT calculations is sufficient for some applications, a faster coarse-grained model is highly desirable for broadening parameter sweeps and extending the range of accessible length scales.

Phase field (PF) models are one such approach. Well-known PF models for diblock copolymers include the Landau-Brazovskii (LB) and Ohta-Kawasaki (OK) models [5-7]. These models express the system's free energy as a functional of the local species density through an asymptotic expansion. This expression is an approximation of SCFT; however, controlling the validity of the approximation is presently more of an art than a science.

We compared the performances of several PF models to SCFT (the benchmark) for a diblock copolymer melt and found that existing PF models exhibit quantitative and qualitative failures. To address these issues, we introduce an optimization procedure to systematically map an "exact" model (SCFT) onto an approximate (PF) model. The optimized models resolve important shortcomings in their predictions. Figure 1 shows that the domain spacing predicted by the optimized model is a marked improvement over the original model. Thanks to such improvements, PF models may become a more attractive replacement for SCFT.

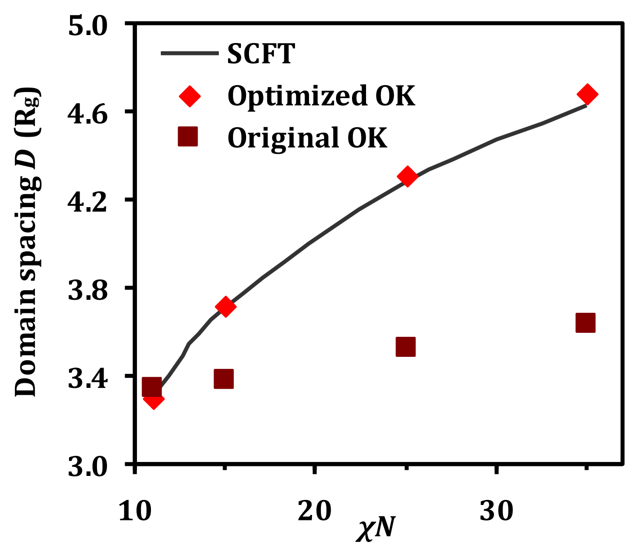

Figure 1: Domain sizes predicted by the original Ohta-Kawasaki model (squares), our optimized version (diamonds), and the benchmark, SCFT (line) as a function of the segregation strength χN.

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The role of water in the growth of NaCl crystals

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Crystal habits are influenced by characteristics of solutes and also by the solvent during crystallization [1]. Numerous studies explore how crystal shape depends on characteristics of the solute and interactions between the solvent and crystal facets [2]. However, several experiments and simulations have implicated desolvation barriers in the rate limiting steps for crystal growth [3-5]. Understanding these kinetic barriers is critical for accurate models of crystal growth. We employ simulation methods for rare events and mechanistic hypothesis testing [6] to understand the ion-desolvation process during attachment to a growing NaCl crystal. Additionally, we examine the ion-solvation process during dissolution, which is shown in Figure 1. We find that the solvation of kink sites is critical. We calculate the rate of ion attachment at kink sites to predict growth rates and crystal shapes. We also discuss possible extensions of our findings to other crystals, such as calcium carbonate.

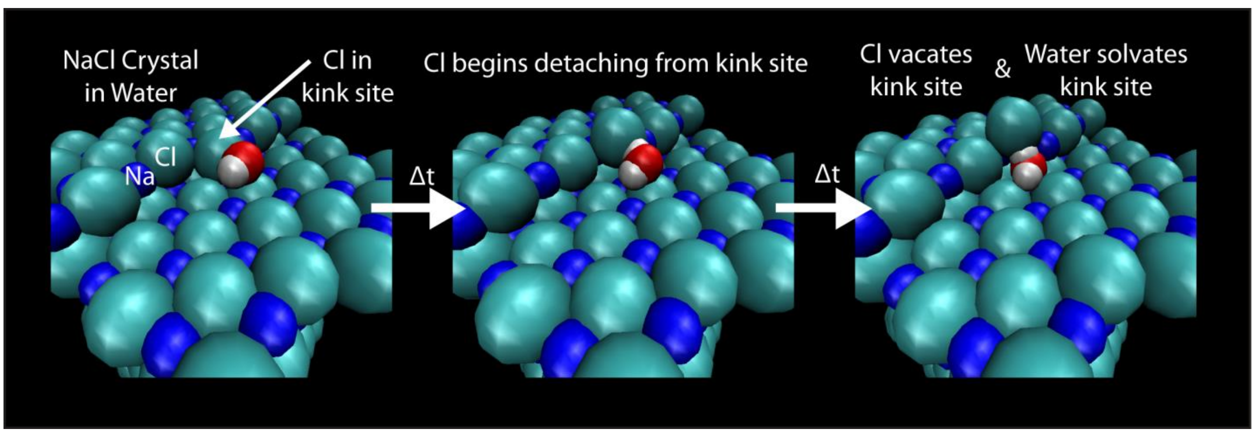

Figure 1: Snapshots from rare event simulations of a chloride ion detaching from a kink site. Only the water which solvates the kink site is shown for clarity. Sodium is dark blue, chloride is teal, oxygen is red, and hydrogen is white.

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Materials and Catalysis

Molecular compositions and structures of *β-di*calcium silicates for greener cementitious materials

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Cement manufacturing is responsible for approximately 8% of the world's carbon dioxide (CO_2) emissions, due to the release of CO_2 from limestone ($CaCO_3$) during high-temperature calcination to yield CaO. CaO is used as a source of calcium cations during the formation of anhydrous cement powders, which are comprised of calcium silicates and aluminates with typical particle sizes of several microns. The major components of anhydrous cement powders are *tri*calcium silicate (Ca_3SiO_5) and *di*calcium silicate (Ca_2SiO_4), which are responsible for the development of mechanical strength properties as cements hydrate. Though they are chemically similar, they hydrate at dramatically different rates: *tri*calcium silicate hydrates over days to weeks, compared to *di*calcium silicate which typically hydrates over months and years, due to its intrinsically slower hydration kinetics and large particle sizes. Increasing the overall hydration rate of *di*calcium silicate is an attractive option for replacing a portion of the *tri*calcium silicate to achieve similar mechanical strength properties with lower total calcium contents. Correspondingly, this could reduce the carbon foot print of the cement manufacturing process.

Recently, *β-di*calcium silicate was synthesized by three alternative synthesis methods rather than the conventional solid-state reaction to yield much smaller Ca_2SiO_4 particles, such that hydration is ~95% complete within 30 days. The conventionally prepared analogue, on the other hand, takes approximately 180 days to achieve the same degree of hydration. The increased rate of hydration in these materials is thought to be due principally to the smaller particle sizes. The molecular structures and compositions of *β-di*calcium silicate were monitored before and after hydration by solid-state ^{29}Si nuclear magnetic resonance (NMR) spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). The results provide new understanding of the influence of chemistry, surface area, and synthesis conditions on the rate of hydration. The analyses yield detailed molecular-level insights that can be correlated with macroscopic properties, such as the viscosities of hydrating slurries and the development of mechanical strength in cement materials.

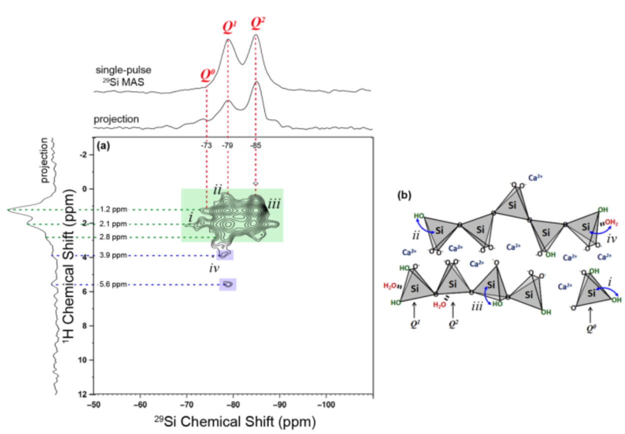

Figure 1. (a) 2D ^{29}Si{^{1}H} HETCOR NMR spectrum of sol-gel-derived *β*-dicalcium silicate that was hydrated for 180 days at 25 °C, and (b) cartoon representation of the intermolecular interactions that occur between various ^{29}Si silicate species and water molecules (blue shaded regions) and hydroxyl moieties (green shaded region).

Fe,N-containing mesoporous carbon materials as non-precious metal electrocatalysts for alcohol and bio-hybrid fuel cells

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Alcohol and bio-hybrid fuel cells, which generate electricity from alcohols, are promising energy conversion devices, due to their high energy density, and use of renewable and easily-managed liquid fuels [1]. However, it is necessary to overcome deficiencies in activated-carbon-supported platinum (Pt/C), the current standard cathode catalyst, which include poor tolerances to alcohols and certain side products [2]. We report oxygen reduction reaction (ORR) electrocatalysts based on iron- and nitrogen-containing mesoporous carbon that exhibit both high ORR activities and selectivities, making them suitable for use in alcohol-based fuel cells. The catalysts were synthesized by pyrolyzing an inexpensive organic precursor within the pores of mesoporous silica templates, in the presence of an iron salt. The resulting materials exhibit high surface areas and relatively high surface N contents, which enable promising catalytic properties. With optimization of surface N functionalities, Fe,N-containing mesoporous carbon catalysts exhibit ORR activities comparable to Pt/C catalysts. Ethanol tolerances were evaluated by measuring power density with increasing ethanol fuel concentration, and while Pt/C catalysts exhibited reduced ORR activity with greater concentrations of ethanol, Fe,N-containing mesoporous carbon catalysts exhibited increasing power densities [3]. This new non-precious-metal catalyst is promising as an alternative to Pt/C, because it enables comparable or superior device performances under a variety of conditions relevant to the commercial operation of fuel cells. Current efforts focus on evaluating the performance of Fe,N-containing mesoporous carbon catalysts in commercial-scale bio-hybrid fuel cell devices that have electrode areas of 200 cm^2.

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Incorporation of photo-responsive membrane protein species into mesostructured silica for light-driven ion transport

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Membrane proteins are versatile biomolecules with diverse functionalities that impart sensing, signaling, transport, or catalytic properties that support the viabilities of biological cells. Such functionalities are highly selective to particular ions or molecules and often occur at high rates, which would be attractive for technological applications, such as chemical or biological sensing, separations, bioanalytics, and energy conversion. To effectively exploit membrane proteins for technological purposes often requires their incorporation into synthetic host materials that enable the proteins to function stably and be integrated into macroscopic devices. One interesting example is the membrane protein proteorhodopsin, which functions as a light-driven H^+-ion-pump that might be harnessed for photochemical energy conversion. Synthetic host membranes that contain macroscopically aligned proteorhodopsin species are expected to generate bulk ion gradients across host materials under illumination. Here, we present a solution-based synthetic protocol that allows high concentrations (up to 15 wt%) of active proteorhodopsin species to be incorporated within mesostructured silica membrane hosts. Synthesis conditions and compositions were judiciously selected to stabilize proteorhodopsin molecules in the presence of the structure-directing surfactant and soluble network-forming silica species that co-assemble to form mesostructured silica host matrices, as established by small-angle X-ray diffraction analyses. Proteorhodopsin molecules incorporated within mesostructured silica hosts are shown to retain native-like structures, but with notable differences, based on multidimensional solid-state NMR spectra. The optical absorbance behaviors of proteorhodopsin within the synthetic hosts are analogous to those associated with the photochemical reaction cycle of proteorhodopsin in native-like environments. Macroscopic alignment of proteorhodopsin molecules within the silica mesochannels can be induced by imposing a strong (2.5 kV/cm) electric field during material synthesis. Resulting proteorhodopsin-containing mesostructured silica membranes are shown to yield transmembrane electrochemical potentials of up to ~1 mV under continuous illumination by green LED light, reflecting bulk transport of H^+ ions by the macroscopically aligned proteorhodopsin species. The synthesis protocol is expected to be general and has been adapted to incorporate other functionally active membrane proteins within mesostructured silica host membranes. This includes H^+-ion-pumping *Gloebacter violaceus* rhodopsin variants, which are activated by different wavelengths of light compared to proteorhodopsin and thus offer the potential to convert broader ranges of the solar spectrum. The versatile mesostructured silica-surfactant host materials presented here open new opportunities to harness the diverse functionalities of membrane proteins in engineered devices.

Evidence for electron carriers in photoluminescent gallium nitride nanoparticles

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Group III-V semiconductors, such as hexagonal gallium nitride (h-GaN), exhibit adjustable optoelectronic properties with applications in a wide variety of devices, including lasers, solid-state lighting, and light-emitting diodes. The structural origins of the light-emitting properties of h-GaN nanoparticles, notably the role of defects such as nitrogen vacancies, have been poorly understood, due to the inherent complexity of this heterogeneous multicomponent system. Detailed information on the long-range structural order and local atomic environments in h-GaN materials are provided by complementary transmission electron microscopy (TEM), X-ray diffraction (XRD), and nuclear magnetic resonance (NMR) spectroscopy analyses. TEM and XRD establish similar long-range crystal-like ordering in both bulk and nanoparticle h-GaN materials. In contrast, solid-state ^{69}Ga, ^{71}Ga, and ^{15}N NMR spectra reveal broad distributions of local atomic environments arising from electron-donating defect species. The results support the hypothesis that the light-emitting properties of h-GaN nanoparticles are directly related to the atomic-scale compositions and structures, particularly the influences of surfaces and of electron carriers at or near the conduction band. The atomic-level insights are correlated with the optoelectronic properties of h-GaN nanoparticles providing new understanding for the development and improvement of Group III-V semiconductor-based light-emitting devices.

Biophysics, Bioengineering and Controls

Estimating ribozyme kinetics from analysis of *in vitro* evolution

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Ribozymes and other biological reagents generated through *in vitro* selection have become important tools in medicine and the life sciences; but as selection methodology advances, our understanding of the evolutionary dynamics involved lags far behind. Selections often fail, require additional rounds to converge on a candidate sequence, or simply behave erratically. Existing theory does little to predict such difficulties or offer solutions, relying on distribution parameters and assumptions never tested in a selection environment. By combining selection theory with observations of real-world evolving molecular populations, we seek to find a mathematical description of the actual dynamics involved in a ribozyme selection. Using multiple rounds of High-Throughput Sequencing (HTS), we analyze a triphosphorylation ribozyme selection, using specifically-weighted regression to estimate the activity and kinetics of a large number of unique sequences present during selection. Estimated fitness values correlate with measured ribozyme activity, aiding in the selection of high-activity ribozymes and providing a viable alternative to the heuristic methods typically used to interpret HTS-selection data. Population genetic relations derived from Fisher's Fundamental theorem suggest that we have obtained an accurate picture of sequence fitness distribution. By analyzing changes in ribozyme abundance and fitness distribution over all rounds of selection, we provide the first measurement and estimate of non-ideality in *in vitro* selection, suggesting mathematical causes for current challenges in the field of artificial selection. In addition, we demonstrate a new method for constructing selection fitness landscapes, suggesting further applications of these analytical methods.

Evaluating the sensitivity of unbiased serum antibody detection using bacterial display peptide libraries

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Many autoimmune disorders are characterized by a production of antibodies that can facilitate an attack on the body's own tissues. Because antibodies are highly specific for their targets, identifying these antibodies using their binding partners, or antigens, can indicate disease risk, onset, or progression. Diagnostic assays utilizing serum antibodies have proven effective for multiple autoimmune disorders including rheumatoid arthritis [1] and celiac disease [2], but these technologies are predicated on understanding antigens implicated in the disease. Unfortunately, antigens involved in the majority of diseases are still unknown. This presents the need for an unbiased, high-throughput technology to screen patient serum for antibodies specific to diseases.

Random peptide libraries can be used to screen for peptides that specifically bind to serum antibodies, mimicking the native antigens [3]. By screening billions of unique peptides, peptides that react only in patients with disease may be identified and used as diagnostic reagents. Furthermore, identifying the sequences of reactive peptides could lead to biological connections providing insights into disease pathology. However, achieving sensitivities capable of unbiased antibody detection using random peptide libraries can be difficult. Here, we examine two methods for detecting serum antibodies using randomized bacterial display peptide libraries and next-generation sequencing. The sensitivity of each method is evaluated using a model system comprised of known monoclonal antibodies spiked into human serum at various concentrations. Initial results indicate improved sensitivity can be achieved by depleting patient serum of abundant antibody species prior to screening, while preserving antibody repertoire coverage. We aim to apply these methods to various autoimmune, inflammatory, and infectious diseases to discover novel diagnostic reagents and identify disease-associated antigens.

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Regulation of biomass degrading enzymes in anaerobic gut fungi and their application in synthetic co-culture systems

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To support renewable technologies, it is necessary to develop more efficient methods to extract sugars from crude plant biomass. Plants contain cellulose that depolymerizes into fermentable sugars for microbial biofuel production. However, in crude biomass, cellulose is trapped within lignin, hemicellulose and other biopolymers that complicate its hydrolysis. To address this issue, one can turn to nature, particularly to microbes that routinely degrade plant biomass. Many large herbivores, such as cows and horses, harbor a consortium of microbes in their digestive tracts that convert recalcitrant biomass into sugars. Within this consortium, anaerobic gut fungi are the primary colonizers of plant material, and represent a rich source of biomass degrading enzymes. We have isolated several novel strains of gut fungi from animals at the Santa Barbara Zoo to characterize their ability to release sugars from crude biomass. We have used transcriptomic analysis to identify specific enzymes required for the breakdown of plant material including cellullases (GH5, GH9, GH48), hemicellulases (GH10, GH11, GH43), and accessory enzymes (Polysaccharide deacetylases). Through examining the regulatory pattern of these enzymes during growth on a variety of carbon sources, those that are most important for degradation of crude plant material can be identified. We have also used transcriptomics to identify regulatory proteins that may be responsible for the regulation of these enzymes. Through examination of these putative regulatory proteins and the stimuli that trigger their response, we can develop methods for the control of gut fungal metabolism and the production of biomass degrading enzymes. While tools to engineer gut fungi directly are severely underdeveloped, another way to incorporate them into industrial processes is to create co-culture systems. Natively, gut fungi maintain a syntrophic relationship with archaeal methanogens by which the fungi produce CO_2 and H_2 that the methanogens convert into methane. This relationship results in enhanced biomass breakdown by the fungus. In a synthetic system gut fungi are used for their degrading power to release sugars from biomass (~5 g/L released from cellulosic substrates). This excess sugar is then used to fuel production of a value-added chemical in a model microbe, such as *S.* cerevisiae or *E.* coli. We have used the production of Flavin-based fluorescent proteins (FbFPs) to quantify growth in both systems and production of n-butanol in *E. coli* to assess the ability to produce a fuel molecule in this system. If methanogens are incorporated into this synthetic system, it is expected that the amount of sugar released, and therefore the amount of product made by the model microbe, will be increased. By coupling the capabilities of the gut fungi and model microbes, many different products may be generated directly from biomass. By harnessing the power of these organisms, through creation of new enzyme cocktails or synthetic consortia, we can create a more sustainable industry with production directly from biomass.

Profiling the humoral immune response associated with Type 1 Diabetes Mellitus via bacterial display libraries

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Type 1 Diabetes Mellitus (T1DM) is characterized by an aberrant immune response that results in the production of autoantibodies that target islet cell molecules. While their exact role in the pathology is unclear, the number and type of autoantibodies present correlates with risk of T1DM, which is valuable in screening genetically at-risk populations. Since antibodies bind with high specificity, they can be screened using peptides that mimic their epitopes, providing information about their target molecules, or antigens. Bacterial cells displaying peptides can be used to represent a large, unbiased library of epitope mimics. The physical and chemical properties of ligands can be used to develop markers for disease and search for antigens that may play a role in disease genesis.

Using random peptide libraries coupled with fluorescent and magnetic-based cell sorting techniques (Figure 1), we performed an initial screening of 10 T1DM and 10 non-T1DM (control) plasma samples to uncover disease-specific peptide patterns, or motifs. 60% of the T1DM samples contained several motifs that were not prevalent in the control samples. However, these discovered motifs, when screened against a validation set of 78 additional T1DM and control samples, reacted with only a few additional disease samples (Figure 2).

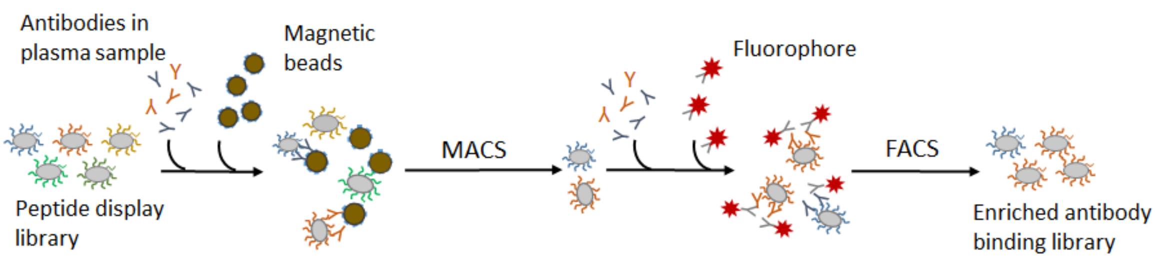

Figure 1: Screening bacterial display libraries with patient sera using magnetic-activated (MACS) and fluorescence-activated (FACS) cell sorting. Antibodies in plasma bind to peptides expressed by bacterial cells, allowing preferential collection using either magnetic beads or flow cytometry. Multiple rounds of sorting result in a library enriched in cells displaying peptides that bind to antibodies in the patient plasma.

Based on these initial findings and the knowledge that T1DM has a highly heterogeneous pathology, we expanded the screening strategy, organizing the samples into well-characterized subgroups, such as those patients positive for a specific T1DM-associated autoantibody. Peptides isolated from subgroups may have properties that confer T1DM specificity. For example, we screened an additional 11 T1DM samples predominately positive for the insulin autoantibody (IAA) to facilitate comparison with sequences from patients testing negative for IAA, with the aim of identifying candidate antigens with similarities to peptides isolated from these distinct T1DM patient subgroups.

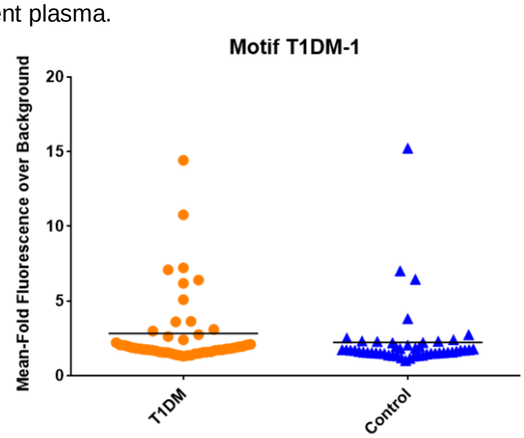

Figure 2: Flow cytometry screening of a motif. The discovered motifs were not cross-reactive with most of the validation samples, demonstrated by fluorescence similar to the background signal.

Nanoscale size and chemistry effects on passive transport

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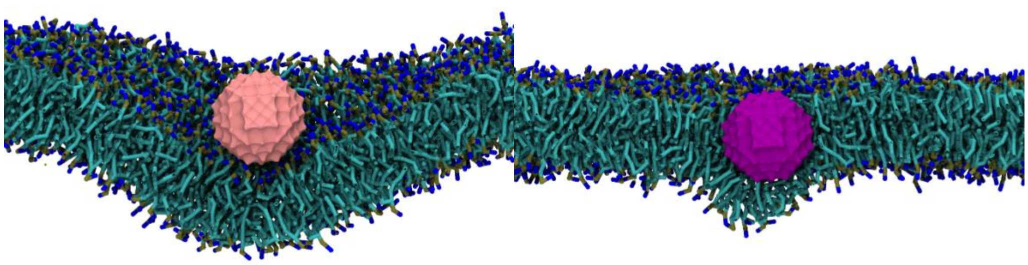
Department of Chemical Engineering, University of California, Santa Barbara

Controlling passive solute transport across semipermeable membranes is an essential component of therapeutic design, yet a fundamental physical understanding of the process is incomplete. Overton's rule states that the membrane permeability of a solute is directly related to its membrane-solvent partition coefficient, and despite passive transport advancements with inhomogeneous membrane and multilayered kinetic theories, the rule remains theoretically consistent [1,2,3]. By extension of the partitioning argument, the translocation kinetics are dominated by the thermodynamic barrier (or well) in the solute's free energy profile across the membrane. We explore the free energy landscape of generic hydrophilic and hydrophobic nanoparticles across a lipid bilayer membrane through both continuum-level theory and classical coarse-grained molecular dynamics (CG MD) simulation. Particularly, we elucidate the nanoscale interdependence of solute size and chemistry in the determination of equilibrium solute-membrane configurations, where various chemical, steric, pre-pore, pore, and wrapping mechanisms are all possible and both molecular and continuum theories appear to break down [4,5,6,7]. We evaluate previous work on the relevance of thermodynamic metastability to the kinetics, and conclude with design principles for solute size and chemistry to inform future investigations of shape and elasticity[8].



(a) (b)

Figure 1. Interaction of a (a) hydrophilic and (b) hydrophobic nanoparticle with a lipid bilayer membrane.

References:

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[4] Finkelstein, A. *J. Gen. Physiol.* **1976**, *68* (2), 127.
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Design of modular parts for synthetic systems inspired by anaerobic fungi

Sean P. Gilmore[1], Charles H. Haitjema[1], Kevin V. Solomon[1], John K. Henske[1], Jessica Sexton[1], Mike K. Theodorou[2], Dave Valentine[3], Michelle A. O'Malley[1]

[1] Department of Chemical Engineering, University of California Santa Barbara

[2] Harper Adams University, Shropshire, United Kingdom

[3] Department of Earth Sciences, University of California Santa Barbara

Anaerobic fungi in the hindgut of large herbivores are among the most robust organisms at degrading crude lignocellulose. They achieve this efficiency through the production of large, multi-enzyme complexes called fungal cellulosomes. The fungi also act synergistically with other microorganisms in the microbiome, such as archaea, bacteria, and protozoa. By elucidating the parts responsible for efficient biomass degradation at both the protein and cellular level, we seek to replicate this efficiency in synthetic systems.

At the protein level, fungal cellulosomes are similar to bacterial cellulosomes in that the protein-protein interactions are mediated through parts termed the dockerin and cohesin. However, many differences exist. The dockerin domains exist in tandem repeats and bear no species specificity like those in the bacterial systems. Furthermore, the exact sequence for the cohesin module has yet to be established. Through analysis of transcriptomic data for three fungal isolates, patterns governing the native placement of dockerin domains on fungal cellulases were characterized. By recombinantly grafting these dockerin domains onto similar enzymes from other organisms, the original activity of the enzymes were retained while allowing for incorporation of these exogenous enzymes into fungal cellulosomes. This was demonstrated for the TmCel5A, TmXynA, and TmBglB from Thermotoga maritima. These incorporated enzymes demonstrated a greater level of synergy with the native cellulosomes when compared to the catalytic domain without the grafted dockerins. The eventual goal is to create entirely synthetic cellulosomes, which could be applied to any biocatalytic process.

At the cellular level, the anaerobic fungi have also been shown to interact closely with methane producing archaea (methanogens). The methanogens siphon hydrogen and other metabolites from the fungi, allowing the fungi to more efficiently produce energy by increasing the flux through their hydrogenosomes. This increased energy is hypothesized to increase production of cellulases, accelerating the degradation of lignocellulose in co-culture. To further investigate this mechanism, native fungal/methanogen co-cultures were isolated from herbivore fecal materials. These co-cultures were maintained together and also separated into monocultures, effectively creating parts for synthetic co-cultures. The native co-cultures showed greatly enhanced growth on a variety of biomass substrates. By introducing the methanogens into cultures of other well-characterized anaerobic fungi, stable synthetic co-cultures were established. With this proof of concept, other parts to the consortia can be introduced, such as non-native methanogens capable of funneling other accumulating metabolites like acetate. These stable synthetic consortia should increase the efficiency of conversion of crude biomass, allowing for the production of sustainable chemicals.

Curriculum Vitae

NIKOLAI D. PETSEV

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EDUCATION

University of California, Santa Barbara **2011 - Present**
Ph. D. Candidate, Chemical Engineering

University of New Mexico **2006 - 2011**
B.S., Chemical Engineering
Concentration: Materials Processing
Minors: Mathematics, Chemistry
Honors: *magna cum laude*, *summa cum laude* in chemical engineering

RESEARCH EXPERIENCE

Graduate Research Assistant **2012 – Present**
Advisors: M. Scott Shell, L. Gary Leal, University of California, Santa Barbara

- Developed analytical transport model for the stability of interfacial nanobubbles that explains experimental observations in the literature
- Performed numerical simulation of nanobubbles along hydrophobic surfaces using COMSOL package to demonstrate feasibility gas recirculation model for nanobubble stability
- Studied dynamics of gas enrichment at hydrophobic interfaces via molecular dynamics simulation
- Developed new hybrid techniques for multiscale simulation that allow stable bridging between atomistic scales and mesoscale continuum solutions
- Developed novel particle-based techniques for multicomponent mesoscale hydrodynamic problems
- Generalized multiscale SDPD techniques to multicomponent problems

Chemical and Nuclear Engineering Departmental Honors Program **2010**
Advisor: Frank van Swol, Sandia National Laboratories, University of New Mexico

- Worked on molecular dynamics simulations of ferromagnetic particles subjected to an oscillating uniform magnetic field

Undergraduate Research Assistant **2008 – 2010**
Advisor: Frank van Swol, Sandia National Laboratories, University of New Mexico

- Performed computational/statistical mechanical analysis of anisotropic particle distributions in nanochannels to characterize experimental efforts at the University of New Mexico

SKILLS

Simulation techniques: Molecular dynamics, Brownian dynamics, Monte Carlo, smoothed particle hydrodynamics, smoothed dissipative particle dynamics
Programming languages: FORTRAN, Python, MATLAB, Mathematica

HONORS AND AWARDS

- DOW Discovery Fellowship 2013 – present
- Member of Tau Beta Pi Engineering Honor Society 2010 – present
- UNM Scholars Scholarship 2006 – 2010
- School of Engineering Dean's List Award 2006 – 2008

TEACHING

Teaching Assistant, University of California, Santa Barbara **2014**
Transport processes (ChE120A)
Teaching Assistant, University of California, Santa Barbara **2012**
Transport processes (ChE120A)
Tutor, University of New Mexico **2011**
Physics/math/chemistry tutor, Center for Academic Program Support (CAPS)
Private Tutor (Physics) **2011**
Private Tutor (French) **2003 – 2006**

ACTIVITIES

- UCSB MRL "It's a Material World!" outreach 2012
- University of New Mexico AIChE chapter officer 2009 – 2010
- Organizer for 2010 AIChE regional conference 2010
- MCTP summer math workshop participant 2009

CONFERENCES

1. N. D. Petsev, L. G. Leal, M. S. Shell. "*Hybrid Molecular-Continuum and Multicomponent Simulations Using Smoothed Dissipative Particle Dynamics*". UCSB Graduate Student Symposium 2014 (poster).
2. N. D. Petsev, L. G. Leal, M. S. Shell. "*Hybrid Molecular-Continuum and Multicomponent Simulations Using Smoothed Dissipative Particle Dynamics*". American Institute of Chemical Engineers (AIChE) National Conference 2014 (talk).

PUBLICATIONS

1. N. D. Petsev, M. S. Shell, L. G. Leal. "*Dynamic equilibrium explanation for nanobubbles' unusual temperature and saturation dependence*". Phys. Rev. E **88**, 010402 (2013).
2. N. D. Petsev, L. G. Leal, and M. S. Shell. "*Hybrid molecular-continuum simulations using smoothed dissipative particle dynamics*". The Journal of Chemical Physics **142**, 044101 (2015).

PENG CHENG

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Department of Chemical Engineering
University of California
Santa Barbara, CA 93106-5080

EDUCATION

Ph.D. Chemical Engineering, University of California, Santa Barbara, CA 12/2016 (expected)
Advisors: M.E. Helgeson and L.G. Leal
GPA: 3.82

B.S. Chemical Engineering, Texas A&M University, College Station, TX 8/2010
Summa Cum Laude GPA: 3.93

WORKING EXPERIENCE

Graduate Research Assistant, Department of Chemical Engineering, UCSB 7/2012-now
Advisors: M.E. Helgeson and L.G. Leal
Research project: Multi-scale investigation of viscoelastic polymeric fluids in complex flows

Graduate Teaching Assistant, Department of Chemical Engineering, UCSB 2012 - 2013
CHE 120A *Transport Processes: Fluid Dynamics*
CHE 141 *The Science and Engineering of Energy Conversion*
CHE 180 *Chemical Engineering Laboratory*

Graduate Research Assistant, Department of Chemical Engineering, UCSB 2/2011 - 6/2012
Advisors: S.L. Scott and M.F. Doherty
Research projects: Alkane metathesis and conversion of carbohydrates to terephthalic acid

Undergraduate Research Assistant, Department of Chemical Engineering, TAMU 5/2008 - 8/2009
Advisor: A. Jayaraman
Research project: Dynamics of Jak-STAT and Erk-C/EBPβ pathways in response to cytokine stimulation in HepG2 cells

SERVICE AND LEADERSHIP

Outreach Activities, *Society of Rheology* 10/2014
Co-chairman, Organization Committee of 6th Amgen-Clorox Graduate Student Symposium
Department of Chemical Engineering, UCSB 4/2013 – 10/2013

PROFESSIAONAL MEMBERSHIP

America Chemical Society
Society of Rheology

AWARDS

Student-Member Travel Grant Recipient, *Society of Rheology* 2014
Outstanding Undergraduate Research Award, *Department of Chemical Engineering, TAMU* 2009
Undergraduate Research Scholar, *TAMU* 2009
Undergraduate Summer Research Grant Recipient, *College of Engineering, TAMU* 2008
Ruth and William J. Neely ’52 Scholarship, *Department of Chemical Engineering, TAMU* 2007

SKILLS

Computation: Windows, Microsoft Office, MATLAB, Mathematica, Python, Fortran, R Programming
Experiments: Rheometry, Particle Tracking/Imaging Velocimetry (PTV/PIV), Small-angle Light Scattering (SALS), Rheo-NMR, NMR spectroscopy
Language: Fluent in English and Mandarin Chinese

PUBLICATIONS

1. C. Moya, Z. Huang, **P. Cheng**, A. Jayaraman, and J. Hahn. Investigation of IL-6 and IL-10 Signaling via Mathematical Modeling. *IET Systems Biology* **5**, 15-26 (2011).
2. Z. Huang, C. Moya, **P. Cheng**, A. Jayaraman, and J. Hahn. In Silico Investigation of IL-6 and IL-10 Signaling in Steatosis. Proceedings Foundations of Systems Biology in Engineering 2009, Denver, Colorado, 28-31 (2009).

PRESENTATIONS

1. **P. Cheng**, L.G. Leal, and M.E. Helgeson. Testing Shear-induced Breakage as the Mechanism of Shear Banding for Linear Wormlike Micelles. 87th Annual Meeting of the Society of Rheology, Baltimore, MD (2015).
2. **P. Cheng**, L.G. Leal, and M.E. Helgeson. Effect of Curvature on Shear Banding of Wormlike Micelles in Taylor-Couette Flow. 86th Annual Meeting of the Society of Rheology, Philadelphia, PA (2014).
3. **P. Cheng**, S.L. Scott, and M.F. Doherty. Alkane Metathesis: Kinetic Analysis and a Preliminary Design of Reactive Distillation. Center for Enabling New Technologies through Catalysis (CENTC) Annual Meeting, Seattle, WA (2011).
4. Z. Huang, C. Moya, **P. Cheng**, A. Jayaraman, and J. Hahn. Mathematical Modeling of IL-6 and IL-10 Signal Transduction in Steatosis. AIChE Annual Meeting, Nashville, TN (2009).
5. C. Moya, Z. Huang, **P. Cheng**, J. Hahn, and A. Jayaraman. Investigation of the Jak-STAT and Erk-C/EBPβ Signaling Pathways in Response to Cytokine Stimulation in HepG2 Cells. AIChE National Student Conference, Nashville, TN (2009).
6. C. Moya, Z. Huang, **P. Cheng**, J. Hahn, and A. Jayaraman. Investigation of the Jak-STAT and Erk-C/EBPβ Signaling Pathways in Response to Cytokine Stimulation in HepG2 Cells. Houston Society for Engineering in Medicine and Biology (HSEMB) 26th Annual Meeting, Houston, TX (2009).

Nicole Schonenbach
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Santa Barbara, CA 93106
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Objective

It is my goal to build my career in advancement of biomedical research. I currently focus on biophysical characterization of the adenosine A2a G-protein coupled receptor, which plays a major role in mediating circulatory function, inflammation, and interacts with other receptors integral to the central nervous system. I am developing methods to structurally and functionally characterize A2a oligomers for the advancement of structure-based drug design.

Education

Candidate for Doctor of Philosophy 2011-2016 (Projected)
Chemical Engineering
University of California Santa Barbara

Bachelor of Science in Chemical Engineering 2006-2011
Montana State University, Bozeman, MT GPA: 3.79

Work Experience/ Skills

Position: Graduate Student Researcher **2011-Present**
Employer: University of California Santa Barbara Santa Barbara, CA
Advisor: Michelle O'Malley (805)-893-4769
Songi Han (805)-893-4858

Description: I am developing the tools to express and biophysically characterize the oligomers formed by pharmacologically relevant GPCRs for application in structure-based drug design. Throughout the course of this project I have become skilled in fluorescence microscopy, spin-label magnetic resonance techniques (EPR), affinity chromatography, size exclusion chromatography coupled with multi-angle light scattering (SEC-MALS) and biochemical techniques such as molecular cloning, SDS-PAGE, and membrane protein purification.

Position: Undergraduate Research Intern **2010**
Employer: Massachusetts Institute of Technology Cambridge, MA
Supervisor: Dr. Michael Strano Phone (617) 324-4323

Description: As part of NSF's Research Experience for Undergraduates program I worked with Dr. Michael Strano and a graduate student, Joel Abrahamson to study the reaction mechanism of thermopower waves, high thermoelectric pulses of electrons, over carbon nanotubes. The nature of this work was highly computational utilizing COMSOL and MATLAB.

Position: Lab Research Assistant **2008-2011**
Employer: MSU Undergraduate Scholars Program MSU Bozeman, MT
Supervisor: Dr. Brent Peyton Phone: (406) 994-7419
Mentor: Rob Gardner, Ph.D. student

Description: I worked with a team to characterize optimal growth conditions for various strains of algae to identify candidates for large scale algae to biodiesel production. With this work, I became practiced in spectrophotometry to monitor nitrate depletion, bright field microscopy, monitoring lipid accumulation via Nil Red fluorescence, as well as practical biological lab techniques.

Position: Summer Intern **Summer 2009**
Employer: Idaho National Laboratory/ Battel Energy Alliance Idaho Falls, ID
Mentor: Dr. Robert Bean Phone: (208) 526-9609

Description: At INL, I worked in the nuclear nonproliferation division on part of the Safeguards Envelope project which strived to improve process monitoring systems currently utilized to monitor nuclear material.

Publications

Schonenbach, N. S.; Hussain, S.; O'Malley, M. A., "Structure and function of G protein-coupled receptor oligomers: Implications for drug design", *Wires Interdisciplinary Reviews for Nanomedicine and Nanobiotechnology*, 2015 7(3): 408-27.

Hussain, S.; Kinnebrew, M.; Schonenbach, N. S.; Aye, E.; Han, S., "Functional consequences of the oligomeric assembly of Proteorhodopsin", *Journal of Molecular Biology*, 2015, 427(6 pt B): 1278-90.

Abrahamson, J. T.; Choi, W.; Schonenbach, N. S.; Park, J.; Han, J.-H.; Walsh, M. P.; Kalantar-zadeh, K.; Strano, M. S. Wave Front Velocity Oscillations of Carbon Nanotube-Guided Thermopower Waves: Nanoscale Alternating Current Sources. *ACS Nano*, December, 2010.

Presentations

Biophysical Society 59th Annual Meeting in Baltimore, MD, Poster Presentation	2015
FASEB Molecular Biophysics of Membranes in Big Sky, MT, Poster Presentation	2014
American Chemical Society 247th National Meeting in Dallas, TX, Oral Presentation	2014
Biophysical Society 58th Annual Meeting in San Francisco, CA, Poster Presentation	2014
UC Santa Barbara Chemical Engineering Graduate Student Symposium, Poster Session	2013
Massachusetts Institute of Technology Research Experience for Undergraduates, Poster Fair	2010
AIChE Pacific Northwest Regional Conference Paper Competition	2010
Undergraduate Scholars Program Research Celebration	2009-'11

Awards/Honors

WCC/Eli Lilly Travel Grant	2014
National Science Foundation Graduate Research Fellowship Program (NSF GRFP)	2011-'14
Heslin Fellowship	2011-'12
Undergraduate Scholars Program	2008-'11
Austin C. Olson Scholarship	2010-'11
Montana University System Honor Scholarship	2006-'10

Professional Memberships

Biophysical Society	2014-Present
American Chemical Society	2014-Present
Tau Beta Pi	2009-Present
AIChE	2008-Present

Outreach

Activity: Graduate Student Mentor to Undergraduate Researchers — 2012-Present
Location: UC Santa Barbara, CA

Activity: Science Saturdays Tau Beta Pi outreach — 2010
Location: MSU Bozeman, MT

Activity: AICHE Engineer-a-thon — 2009
Location: MSU Bozeman, MT

References

Dr. Michelle O'Malley	Assistant Professor	UCSB Chemical Engineering	(805)-893-4769
Dr. Songi Han	Professor	UCSB Chemistry/ChemEng	(805)-893-4858
Dr. Brent Peyton	Professor	MSU Chemical Engineering	(406) 994-7419

MICHAEL ZAKREWSKY, PH.D.

CHEMICAL & BIOTECHNICAL ENGINEER

Visionary ~ Pharmaceutical Research ~ Process Development ~ Complex Project Management

Innovative, detailed research scientist and engineer with extensive experimental and developmental training and experience within pharmaceutics and academia. Analytical strategist skilled in successfully collecting, interpreting, and formulating conclusions from data and identifying practical applications. Collaborative communicator focused on building and managing effective research and development project teams to generate pharmaceutical advancements and comprehensive biotech solutions. Strong science-to-business acumen. *Areas of Expertise include:*

- ✓ Pharmaceutical Formulation
- ✓ Product Development & Patents
- ✓ Chemical Manufacturing Processes
- ✓ Characterization Methodology
- ✓ Drug Delivery Technologies
- ✓ Cell Culture & Purification
- ✓ Intellectual Property
- ✓ Project Management
- ✓ Nanotechnology

EXPERIENCE & NOTABLE CONTRIBUTIONS

SELF-EMPLOYED • Santa Barbara, CA • 2014 to Present

TECHNOLOGY & INNOVATION CONSULTANT

Developed and implemented improved solutions for delivery of existing pharmaceuticals, capitalizing on new technological advances.

KEY PROJECTS:

- **Ferring Pharmaceuticals**: Developed oral formulations with increased GI tract residence times and created oral formulations for extended/delayed release liquids of high-dosage drugs.
- **International Vitamin Company**: Designed formulations of orphan drugs utilizing soft gelatin capsule carrier.
- **Teva Pharmaceuticals**: Catalyzed development of implantable stimuli-responsive drug delivery device.

GENENTECH • South San Francisco, CA • 2011

TECHNICAL DEVELOPMENT INTERN

Designed and evaluated second-generation alkali-resistant, high-capacity Protein A chromatography resins.

CONTRIBUTIONS:

- Independently packed chromatography columns, ran affinity separation experiments with HCCF and purified antibody, and analyzed results.
- Effectively tailored prototypes to meet strict Genentech productivity, safety, and environmental standards in collaboration with EMD Millipore.
- Provided results, recommendations, and project direction to Genentech and EMD Millipore leadership through teleconference and departmental presentations.

BRISTOL-MYERS SQUIBB • East Syracuse, NY • 2010

TECHNICAL OPERATIONS INTERN

Studied culture and fermentation additive influencing significant biopharmaceutical characteristic.

ACHIEVEMENTS:

- Initiated 1-L and 7-L bioreactors, prepared media, and successfully cultured CHO cells from cryopreservation to protein production.
- Developed and presented research plan based on experimental data and comprehensive literature review to explore underlying mechanism behind observed phenomenon.
- Effectively solicited departmental leadership for allocation of resources to efficiently perform experiments.
- Enhanced departmental teamwork and communication through participation in Bristol-Myers Squibb Positively Pink community service program.

CONTINUED

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EDUCATION

Doctor of Philosophy, Chemical Engineering
UNIVERSITY OF CALIFORNIA | Santa Barbara, CA | 3.80 GPA
***Thesis**: Formulation development for enhanced drug delivery; expertise includes ionic liquids as solvents, antimicrobials, and prodrugs; skin penetrating peptides; cell penetrating peptides; and nanoparticulate systems.*

Certificate, Technology Management Practices
UNIVERSITY OF CALIFORNIA | Santa Barbara, CA | 3.83 GPA

Bachelor of Science, Chemical Engineering (Summa Cum Laude)
RENSSELAER POLYTECHNIC INSTITUTE | Troy, NY | 3.99 GPA

SELECT PUBLICATIONS & PATENTS

Zakrewsky M, Lovejoy KS, Kern TL, Miller TE, Le V, Nagy A, et al. Ionic liquids as a class of materials for transdermal delivery and pathogen neutralization. Proceedings of the National Academy of Sciences USA. 2014.

Zakrewsky M, Kumar S, Mitragotri S. Nucleic acid delivery into skin for the treatment of skin disease: Proofs-of-concept, potential impact, and remaining challenges. Journal of Controlled Release. 2015.

Kumar S, **Zakrewsky M,** Chen M, Menegatti S, et al. Peptides as skin penetration enhancers: mechanisms of action. Journal of Controlled Release. 2015.

Chen M, **Zakrewsky M,** Gupta V, Anselmo AC, Slee DH, Muraski JA, et al. Topical delivery of siRNA into skin using SPACE-peptide carriers. Journal of Controlled Release. 2014.

Menegatti S, Ruocco N, Kumar S, **Zakrewsky M**, et al. Synthesis and characterization of a self-fluorescent hyaluronic acid-based gel for dermal applications. Advanced Healthcare Materials. 2015.

Anselmo AC, Gupta V, Zern BJ, Pan D, **Zakrewsky M**, Muzykantov V, et al. Delivering nanoparticles to lungs while avoiding liver and spleen through adsorption on red blood cells. ACS Nano. 2013.

Aoyagi K, **Zakrewsky M**, and Mitragotri S. Formulating propranolol as an ionic liquid for transdermal delivery with reduced skin irritation. Technology. *In Review*.

Menegatti S, **Zakrewsky M**, et al. De-novo design of skin-penetrating peptides for enhanced transdermal delivery of macromolecules. Advanced Healthcare Materials. *In Review*.

Kumar S, Anselmo AC, Banerjee A, **Zakrewsky M**, and Mitragotri S. Shape- and size-dependent immune response to antigen-carrying nanoparticles. Journal of Controlled Release. *In Review*.

Zakrewsky M, et al. Ionic liquids as prodrugs for minimizing skin irritation of small molecules and enhancing delivery of nucleic acids into skin. Gordon Research Conference. Barrier Properties of Mammalian Skin. 2015.

Zakrewsky M, Mitragotri S, Fox DT. "Ionic Liquids for Transdermal Drug Delivery." USSN 61/899,294. 2013.

AWARDS & AFFILIATIONS

Mellichamp Systems Biology and Bioengineering Graduate Fellowship (2015)
UC Bioengineering Symposium Fellowship (2015) • Mellichamp Travel Award (2015) • Grand Slam Finalist (2014)
Harold Frank Scholar (2014) • Graduate Symposium Best Poster (2013) • Rensselaer Leadership Award (2011)
Ricketts' Prize (2011) • Honors Convocation 4.0 Award (2010) • Amgen Scholar (2010) • Rutgers NSF-REU (2010)
Malcom Davry Springer Scholarship (2007) • Fred C. and Mary Koch Scholarship (2007)

Tau Beta Pi • American Institute of Chemical Engineers • Society of Biological Sciences • Society for Biomaterials

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Building 570
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michael.v.rapp@gmail.com

EDUCATION

University of California-Santa Barbara (UCSB), Santa Barbara, California
Ph. D. in Chemical Engineering, 2011-present (Expected Graduation: March 2016)
Specialization: Interfacial Phenomena, Biomolecular Adhesion, Surface Forces

Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, Virginia
B.S. in Chemical Engineering, Magna Cum Laude, 2006-2011

RESEARCH EXPERIENCE

Doctoral Research: Dept. of Chemical Engineering, UCSB, 2011-2016
Thesis: Polymer and bio-inspired adhesive interactions at hydrophobic and hydrophilic surfaces
Advisor: Prof. Jacob N. Israelachvili

- Understanding the fundamentals of protein, peptide, and biomolecular interactions at organic and inorganic surfaces
- Translating the fundamentals of wet bioadhesion into synthetic adhesives across multiple length scales, for marine and physiological applications
- Managed (6-member team) a 2-yr collaboration with Procter & Gamble to study solvation (hydrophobic and hydrophilic), electrostatic, and non-equilibrium forces within complex polymer, surfactant, and polyelectrolyte systems.

Undergraduate Research: Department of Chemical Engineering, Virginia Tech, 2008-2011
Advisor: Prof. William A. Ducker

- Complex wetting phenomena at thin organic films
- Development of electroresponsive peptide films capable of selective antibody binding

FELLOWSHIPS & AWARDS

NSF Graduate Student Fellowship Program (3-yr self-obtained funding), 2012-2015
UC-Santa Barbara Doctoral Student Travel Grant, 2015
Dow-Materials Research Lab Travel Fellowship, 2014
Chlorox-Amgen Graduate Student Symposium Best Poster Award, 2014
Denmark Technical University Scholarship (Kgs. Lyngby, Denmark), 2010

PUBLICATIONS (Lead Author)

(1) *Adaptive Synergy between Catechol and Lysine Promotes Wet Adhesion by Surface Salt Displacement*. Maier, GP*; **Rapp, MV* (co-1st author)**; Waite, JH; Israelachvili, JN; Butler, A. (2015) ***Science***, 349 (6248):628-632

(2) *Surface Force Measurements and Atomistic Simulations of Mussel-Derived Peptide Adhesives at Wet Organic Surfaces.* Levine, ZA*; **Rapp, MV* (co-1st author)**; Wei, W; Mullen, RG; Wu, C; Mittal, J; Israelachvili, JN; Waite, JH; Shea, JE. ***In Submission***

(3) *Effects of Surfactants and Polyelectrolytes on the Interaction between a Negatively Charged Surface and a Hydrophobic Polymer Surface*. **Rapp, MV**; Donaldson, SH; Gebbie, MA; Y; Gizaw, Y; Koenig, P; Roiter, Y; Israelachvili, JN (2015) ***Langmuir***, 31 (29):8013-8021

(4) *Hydrophobic, Electrostatic, and Dynamic Polymer Forces at Silicone Surfaces Modified with Long-Chain Bolaform Surfactants.* **Rapp, MV**; Donaldson, SH; Gebbie, MA; Das, S; Kaufman, Y; Gizaw, Y; Koenig, P; Roiter, Y; Israelachvili, JN (2015) ***Small***, 11 (17):2058-2068

(5) *Enantiospecific Wetting.* **Rapp, M**; Ducker, WA (2010) ***J. Am. Chem. Soc.***, 132 (51):18051-18053

PUBLICATIONS (Co-Author)

(1) *Measuring Concentration Fields in Microfluidic Channels In Situ with a Fabry-Perot Interferometer.* Vogus, DR; Mansard, V; **Rapp, MV**; Squires, TM (2015) ***Lab on a Chip***, 15 (7):1689-1696

(2) *Developing a General Interaction Potential for Hydrophobic and Hydrophilic Interactions.* Donaldson, SH; Royne, A; Kristiansen, K; **Rapp, MV**; Das, S; Gebbie, MA; Lee, DW; Chmelka, B; Valtiner, M; Israelachvili, JN (2014) ***Langmuir (Feature Article)***, 31, (7):2051-2064

(3) *The Intersection of Interfacial Forces and Electrochemical Reactions.* Israelachvili, JN; Kristiansen, K; Gebbie, MA; Lee, DW; Donaldson, SH; Das, S; **Rapp, MV**; Banquy, X; Valtiner, M; Yu, J (2013) ***J. Phys. Chem. B (Feature Article)***, 117 (51):16369-16387

(4) *Adaptive Hydrophobic and Hydrophilic Interactions of Mussel Foot Proteins with Organic Thin Films.* Yu, J; Kan, Y; **Rapp, M**; Danner, E; Wei, W; Das, S; Miller, DR; Chen, Y; Waite, JH; Israelachvili, J.N. (2013) ***Proc. Natl. Acad. Sci. USA***, 110 (39):15680-15685

(5) *Asymmetric Electrostatic and Hydrophobic-Hydrophilic Interaction Forces Between Mica Surfaces and Silicone Polymer Thin Films.* Donaldson, SH; Das, S; Gebbie, M; **Rapp, M**; Jones L; Roiter, Y; Koenig, P; Gizaw, Y; Israelachvili JN (2013) ***ACS Nano***, 7 (11):10094-10104

(6) *The Formation of Hydrophobic Films on Silica with Alcohols.* Dion, M; **Rapp, M**; Rorrer, N; Shin, DH; Martin, S; Ducker, WA (2010) ***Colloids and Surfaces A***, 362 (1-3):65-70

NEWS & PRESS

(1) *Positive Charges and Underwater Adhesion*. Wilker, JJ. (2015) ***Science***, 349 (6248):582-583

(2) *One Mystery of How Mussels Stick to Rocks, Boats Solved*. Everts, S (Aug 6, 2015) ***Chemical & Engineering News***. (http://cen.acs.org/articles/93/web/2015/08/One-Mystery-Mussels-Stick-Rocks.html)

(3) *A Sticky Situation*. Cohen, J (Aug 6, 2015) ***The UC-Santa Barbara Current***. (http://www.news.ucsb.edu/2015/015797/sticky-situation). Republished by: (Aug 10, 2015) ***Materialsgate***, ***Futurity, Lab Manager***, & ***Chem Europe***

(4) *UCSB Researchers Create Underwater Super Glue.* (Aug 6, 2015) ***Pacific Coast Business Times***. (http://www.pacbiztimes.com/2015/08/06/ucsb-researchers-create-underwater-super-glue/)

(5) *Improved CTC Molecule Shows Excellent Adhesive Strength in Aqueous Environments*. Ellison, B (Aug 10, 2015). ***AZO Materials***. (http://www.azom.com/news.aspx?newsID=44288)

INDUSTRIAL EXPERIENCE

Process Engineering Co-op: ExxonMobil, Beaumont, Texas, 2008-2009

- Two-term summer co-op working in the Process Safety and Technical divisions of the Beaumont chemical plant and oil refinery

Rahul P. Sangodkar

Ph.D. Candidate in Chemical Engineering

530W Anapamu St Apt. A, Santa Barbara CA 93101.
Tel: +1-(805)-570-8022. E-mail: rahulsangodkar@umail.ucsb.edu

Education

- **Ph.D. in Chemical Engineering**
  University of California, Santa Barbara (UCSB), CA
  September 2011 - present. *GPA: 3.92/4.00*
  - *Advisors*: Prof. Bradley F. Chmelka & Prof. Michael F. Doherty
  - *Research*: Understanding & controlling hydration & crystallization of heterogeneous inorganic materials, including in cementitious solids, biominerals, semiconductors, and for carbon capture.

- **Bachelor of Chemical Engineering**
  Institute of Chemical Technology, Mumbai, India
  (formerly Mumbai University Institute of Chemical Technology)
  July 2007 - June 2011. *Absolute percentage: 79.5%*. Among top 5% of graduating class.
  - *Advisors*: Prof. Ashwin W. Patwardhan & Prof. Bhaskar N. Thorat

Work Experience

- **Department of Chemical Engineering. University of California, Santa Barbara, CA.**
  Teaching Assistant. April-June 2015, January-March 2014, January-March 2013.
  Course: Design of Chemical Processes. Typical class sizes of approximately 60 students.
  - Assisted and supervised instructors in teaching classes of 60 senior-year undergraduates during their 10-week long techno-economic Design Project.

- **Rashtriya Chemicals and Fertilizers Ltd., Mumbai, India**
  Summer Intern. May-June 2010
  - Designed a product acid heat exchanger for a medium pressure Nitric Acid plant with production capacity of 750 tons per day.
  - Techno-economic analysis of the new design suggested approximately an order-of-magnitude improvement in operating efficiency, compared to that of the existing heat exchanger.

Publications

- **Sangodkar, R. P.**; Smith, B. J.; Gajan, D; Rossini, A. J.; Roberts, L. R.; Funkhouser, G. P.; Lesage, A.; Emsley, L.; B. F. Chmelka, "*Influences of dilute organic adsorbates on the hydration of low-surface-area silicates*," *Journal of the American Chemical Society* **2015,** *137*, 8096-8112.
- Pustovgar, E.; **Sangodkar, R. P.**; Andreev, A. S.; Palacois, M.; Chmelka, B. F.; Flatt, R.; d'Espinose, J-. B. "*Transient Hydration of Silicate Surfaces*," *Nature Communications*, submitted and under peer-review.

Selected Presentations

- 8th Alpine Conference on Solid-State NMR, Chamonix-Mont Blanc, France.
  13-17 September 2015. Poster presentation.
- 56th Experimental NMR Conference, Pacific Grove, CA.
  19-24 April 2015. Poster presentation.
- Materials Research Outreach Program (MROP), University of California, Santa Barbara, CA.
  4 February 2015. Poster presentation.

- American Institute of Chemical Engineers (AIChE) Annual Meeting, Atlanta, GA.
  19 November 2014. Oral presentation.
- National Institute of Standards and Technology (NIST), Gaithersburg, MA.
  2 September 2014. Oral presentation.
- Nanocem Cement Hydration Workshop, Villars, Switzerland.
  26-28 June 2014.
- Institute of Terahertz Science and Technology, University of California, Santa Barbara, CA.
  22 May 2014. Oral presentation.
- 55th Experimental NMR Conference, Boston, MA.
  23-28 March 2014. Poster presentation.
- American Institute of Chemical Engineers (AIChE) Annual Meeting, San Francisco, CA.
  6 November 2013. Oral presentation.
- 8th Alpine Conference on Solid-State NMR, Chamonix-Mont Blanc, France.
  8-12 September 2013. Poster presentation.
- Process Systems Engineering Consortium, Massachusetts Institute of Technology, Cambridge, MA.
  27 June 2013. Oral presentation.
- 54th Experimental NMR Conference, Asilomar, CA.
  14-19 April 2013. Poster presentation.
- 6th Amgen Clorox Graduate Student Symposium, Department of Chemical Engineering, UCSB, CA.
  5 October 2012. Poster presentation.

Teamwork and Leadership Experiences

- **Research collaborations with external academic and industrial teams**
  - ***Halliburton Inc.***, Houston, TX. January 2012-present.
  - ***Centre de RMN à Très Hauts Champs*** (European Centre for High-Field NMR), Université de Lyon, France. Research visits in September 2013, July 2014, and September 2015.
  - ***École Polytechnique Fédérale de Lausanne*** (Swiss Federal Institute of Technology), Switzerland. Research visit in September 2015.
- **Organizing Committee** for the Graduate Student Symposium, Department of Chemical Engineering, UCSB, October 2015.
- **Organizing Core Committee** of Exergy, Institute of Chemical Technology, Mumbai, India, 2011. Identified and coordinated sponsorship from industrial partners, supervised organization and scheduling of festival events. Exergy was the annual four-day technical college festival with participation of over 1000 undergraduates from over 100 institutions from across 60 Indian cities.
- **Community Outreach Programs**, 2008-2010. Volunteered and facilitated programs to develop educational databases, practical training workshops, and community building opportunities (e.g., field trips, holiday festivities) for at-risk youth from low resource communities in Mumbai, India.

Skills

Applications: Microsoft Office, Adobe Creative Suite, Mathematica

Laboratory: NMR spectroscopy, dynamic nuclear polarization NMR spectroscopy, X-ray diffraction, electron microscopy, ICP mass spectroscopy

Edward P. Toumayan

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<u>CURRENT RESEARCH:</u> Exploring new approaches to increase the anti-fouling properties of water filtration membranes using surface-tethered polymer brush structures. Experience includes surface modification and characterization of polymers, polymer synthesis and characterization, quartz crystal microbalance (QCM), ellipsometry, x-ray reflectivity, x-ray photoelectron spectroscopy, dynamic light scattering, gel permeation chromatography, and nuclear magnetic resonance.

EXPERIENCE

Fall 2011-Current

Graduate Student Researcher for Professors Glenn Fredrickson, Craig Hawker, and Ed Kramer

- Exploring the fouling resistant nature of block copolymer-modified surfaces.
- Active member of three research groups, with collaborations in the Materials Science and Chemistry Departments, as well as industry partners at Dow Chemicals.

Spring 2010-Spring 2011

Research Assistant for Prof. Raymond Adomaitis in Chemical Engineering

- Operated a chemical vapor deposition (CVD) reactor to deposit thin films of copper oxides.
- **Publication**: D. Arana-Chavez, E. Toumayan, F. Lora, C. McCaslin, R. A. Adomaitis, *Chemical Vapor Deposition*, **2010**, 16, 336-345.

Summer 2009

Research Assistant for Prof. James Duncan in Mechanical Engineering

- Designed and constructed an experimental wave tank, including methods and materials selection.

Fall 2007-Spring 2011

Team Liaison and Group Leader – Gemstone Team WAVES

- Conducted original, multi-disciplinary research with a team of 7 undergraduates studying the viability of Wave Energy Converters (WECs) as a cost-efficient, alternative energy technology.
- Built a prototype rotary-WEC and tested our design using a programmable wave tank.
- **Thesis**: Analysis of Ocean Power Extraction Capabilities of a Rotary Wave Energy Conversion System <http://hdl.handle.net/1903/11390>

EDUCATION

University of California Santa Barbara, CA

Ph.D., Chemical Engineering, expected Summer 2016; Cumulative GPA: 3.75.
Advisors: Professors Glenn Fredrickson, Craig Hawker, and Ed Kramer.

University of Maryland College Park, MD

B.S., Chemical Engineering, May 2011; Cumulative GPA: 3.836.

Awards and Achievements:

- Active member in the Gemstone and Honors Programs (Fall 2007-Spring 2011).
- Banneker-Key Full Scholarship Award (Fall 2007-Spring 2011).
- Center for Minorities in Science and Engineering (CMSE): Certificate of Academic Excellence; (Fall 2007-Spring 2011).
- Studied at Imperial College, London (Summer 2010); worked in the university laboratories.

NOTABLE SEMINARS

- Q-Sense QCM-D Workshop – UCSB – "Protein Adsorption on Polymer Brushes: A QCM Study"
  - June 26, 2013, Invited by Dr. Elizabeth Schneider, Territory Manager at Biolin Scientific
- Complex Fluid Design Consortium – UCSB – "Antifouling for Filtration Membranes"
  - Feb. 4, 2013, Invited by Prof. Glenn Fredrickson, UCSB Chemical Engineering Professor

- Dow Materials Institute (DowMI) Workshop – UCSB – “Antifouling for Filtration Membranes “
    - February 4, 2013; November 5, 2013; March 19, 2015
- Amgen-Clorox Annual Graduate Student Symposium – “Understanding the Relation Between Polymer Brush Properties and Antifouling”
    - October 2, 2015

ACADEMIC-RELATED EXPERIENCE

Engineering Graduate Student Lab Safety Committee Member – UCSB (Fall 2012 – Current)
Section Leader – Freshman Honors Colloquium: Intro to Gemstone – GEMS100 (Fall 2008, 2009, 2010)
Student Coordinator – Freshman Honors Colloquium: Introduction to Gemstone (Spring 2009 – Fall 2009)
Section Leader – Research Topic Exploration – GEMS102 (Spring 2009, 2010)
Resident Assistant (RA) – Department of Resident Life (Fall 2009-Spring 2011)

ACTIVITIES and SKILLS

- Fluent, native speaker of Spanish and French.
- Experience with Python, Mathematica, MATLAB, CHEMCAD, AutoCAD, and COMSOL.
- Multiple sailing and scuba diving certifications; experienced sailing instructor.

SERVICE and MENTORSHIP

- Teaching Assistant – Chemical Engineering Laboratory Course (Spring 2013, Winter 2014)
- Mentor to undergraduate researchers – polymer synthesis and characterization (Summer 2013, 2014)
- FUSE Outreach Program – Santa Barbara Junior High School (October 2013)

Joon Bok Lee

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Santa Barbara, CA 93106
(805) 618-8289
joonbok@engineering.ucsb.edu

EDUCATION

University of California, Santa Barbara — Santa Barbara, CA
Ph.D. student in Chemical Engineering, expected completion in June 2016 — 2011-Present

Harvard University — Boston, MA
Ph.D. Fellow in the School of Engineering and Applied Sciences — 2015-Present

Sansum Diabetes Research Institute — Santa Barbara, CA
Adjunct Research Associate — 2011-Present

University of California, Riverside — Riverside, CA
B.S. in Chemical Engineering (GPA 3.88/4.0, Magna Cum Laude, Honors Program) — 2008-2011

RESEARCH EXPERIENCE

PhD Candidate, Chemical Engineering, University of California, Santa Barbara — Santa Barbara, CA, 2011-Present
Advancement of Control Algorithms for Artificial Pancreas Applications in People with Type 1 Diabetes Mellitus
Advisor: Professor Francis J. Doyle III

Research Assistant, Korea Institute of Materials Science — Changwon City, Gyeongnam, South Korea, Summer 2011
Participated in two projects.
CZTS Nanofilm production via Layer-by-Layer Electrodeposition of Sulfurized Metal Precursors
Electrodeposition of Cu_2O on FTO as an Alternative to Standard Cu Metal Oxidation

Undergraduate Research Assistant, CCRAA Summer Research Program — Riverside, CA, 2009-2011
Peptide Guided CdS and Cu_2S Nanostructure Assembly
University of California, Riverside

EPA P3 (People, Planet, Prosperity) Competition — Riverside, CA, 2009-2011
Grid-independent Electricity Generation for Remote Areas Based on a Unitized Hydroxide Exchange Membrane Fuel Cell System.
University of California, Riverside

SUNRISE Research Experience for Undergraduates Program — Riverside, CA, Summer 2008
Solar Cell Applications of Quantum Confinement Effects in Sub-10nm Diameter CdS and CdSe Nanowires
University of California, Riverside

BRITE Research Experience for Undergraduates Program — Riverside, CA, Summer 2007
Production of Nanowires with Nano-Twin Substructures
University of California, Riverside

INDUSTRIAL EXPERIENCE

Summer PhD Intern, Chief Engineer's Office, Air Products and Chemicals — Allentown, PA, Summer 2015
Advanced Development of the Steam Methane Reformation Model

Summer Assistant Researcher, Quantiative Systems Pharmacology, Genentech — San Francisco, CA, Summer 2013
Computational Model of Cancer Cell Signaling Pathways

Nissan Motor Company, Ltd. — Carson, CA, Summer 2005
Quality Control Division

SELECTED PUBLICATIONS

Lee J, Dassau E, Gondhalekar R, Seborg D, Doyle III FJ. Medically Inspired Personalization of MPC and PID Strategies for Closed-Loop Control of an Artificial Pancreas. *IEEE Transactions of Biomedical Engineering (In Review)* — 2015

Lee J, Dassau E, Doyle III FJ, Personalized, Enhanced CGM Calibration Algorithm Based on Continuous Wear. *Proceedings of the IFAC Symposium on Biological and Medical Systems* (2015) — 2015

Dassau E, Brown S, Basu A, Pinsker J, Kudva Y, Gondhalekar R, Patek S, Lv D, Schiavon M, Lee J, et al. Multicenter Outpatient Randomized Crossover Trial of Closed-Loop Control in Type 1 Diabetes: Effects of Initialization Strategies, *Industrial and Engineering Chemistry Research* — 2015

Srinivasan A, Lee J, Dassau E, Doyle, FJ III. Novel Insulin Delivery Profiles for Mixed Meals in Basal-Bolus and Closed-Loop Artificial Pancreas Therapy for Type 1 Diabetes Mellitus, *Journal of Diabetes Science and Technology* 8:957-68, 2014 — 2014

Doyle III FJ, Huyett L, Lee J, Zisser H, Dassau E. Engineering the Algorithms for the Closed-Loop Artificial Pancreas, *Diabetes Care* 37:1191-1197, 2014 — 2014

Lee J, Dassau E, Seborg D, Doyle III FJ. Model-Based Personalization Scheme of an Artificial Pancreas for Type 1 Diabetes Applications, (Patent) US WO 2014110538 A1 — 2014

Lee J, Dassau E, Seborg D, Doyle III FJ. Model-Based Personalization Scheme of an Artificial Pancreas for Type 1 Diabetes Applications, *Proceedings of the American Controls Conference 2013* — 2013

Lee J, Skovgard, S, Contreras, C, Chiu, M, Tam, K, Yan, Y. Residential Fueling With Hydrogen. Student proposal featured in *International Journal of Hydrogen Energy* — 2011

Lee J, Haberer, E. Discovery of CuS and Cu_2S Binding Peptides. *University of California, Riverside Upper Division Honors Program Thesis 2011* — 2011

SELECTED CONFERENCE PRESENTATIONS

Lee J, Dassau E, Doyle III FJ. A Run-to-Run Approach to Enhance Continuous Glucose Monitor Accuracy Based on Continuous Wear. (Oral Presentation) *International Federation of Automatic Control Symposium on Biological and Medical Systems 2015* — 2015

Lee J, Skovgard, S, Contreras, C, Chiu, M, Tam, K, Yan, Y. Residential Fueling With Hydrogen. (Oral Presentation) *Fuel Cell and Hydrogen Energy Association Annual Conference 2011* — 2011

HONORS

University of California, Santa Barbara Air Products Graduate Fellowship	2014-2015
Juvenile Diabetes Research Foundation (JDRF) Training Travel Award	2013
UCSB Chemical Engineering Teaching Assistant of the Year Award	2013
University of California, Riverside Top Senior Design Team Scholarship	2011
University of California, Riverside Top Individual Senior Design Student Scholarship	2011
Hydrogen Education Foundation's Hydrogen Student Design Contest Second Place Winner, Top US Team	2011
American Public Power Association Demonstration of Energy Efficient Developments Program Student Grant Winner	2011
University of California, Riverside Upper Division Honors Fellowship	2011
EPA P3 Competition First Phase Winner (Grant ID#SU834726)	2010
National Science Foundation S-STEM Scholarship	2009
National Merit Scholarship	2005

MENTORING AND COMMUNITY OUTREACH

Mentorship: Brigid Ehrlich (Undergraduate Student); Outcome: 1 Conference Abstract	2014-2015
Mentorship: Jordan Bittner and Genevieve (Middle School Students); Science Fair	2014
Mentorship: Asavari Srinivasan (Master's Student); Outcome: 1 Journal Publication	2013-2014
Presenter and University Student Panel Member for the CE-CERT Student Local Outreach Program	2011
Leading presenter of renewable energy outreach programs in local high schools – presented in 3 local high schools	2011

Lauren Maria Huyett

Contact Information	784 Laurel Walk Apt. D Goleta, CA 93117	*Phone:* (610) 223-9592 *E-mail:* huyettL@gmail.com

Education

University of California Santa Barbara, Santa Barbara, CA — **Expected 2016**
PhD in Chemical Engineering

Advisor: Francis J. Doyle III
GPA: 3.98/4.00

Lafayette College, Easton, PA — **May 2011**
BS in Chemical Engineering, Minor in Bioengineering and Biotechnology

Summa Cum Laude, Thesis Honors
GPA: 4.00/4.00

Honors and Awards

Schlinger Fellowship for Excellence in Chemical Engineering Research	**2015**
JDRF Training Travel Award	**2013**
National Science Foundation Graduate Research Fellowship	**2011**
Barry M. Goldwater Scholarship	**2010**
American Institute of Chemical Engineers Donald F. Othmer Award	**2010**

Journal Publications

Huyett, L.M., Dassau, E., Zisser, H.C., Doyle, F.J. III, Design and evaluation of a robust PID controller for a fully implantable artificial pancreas, *Industrial Engineering & Chemistry Research*, 2015.

Burnett, D.R., **Huyett, L.M.**, Zisser, H.C., Doyle, F.J. III, Mensh, B.D., Glucose sensing in the peritoneal space offers faster kinetics than sensing in the subcutaneous space, *Diabetes*, 63 pp. 2498-2505, 2014.

Doyle, F.J. III, **Huyett, L.M.**, Lee, J.B., Zisser, H.C., Dassau, E., Closed-loop artificial pancreas systems: engineering the algorithms, *Diabetes Care*, 37 pp. 1191-1197, 2014.

Nguyen, T.H., Easter, N., Gutierrez, L., **Huyett, L.M.**, Defnet, E., Mylon, S.E., Ferri, J.K., and Viet, N.A., The RNA core weakly influences the interactions of the bacteriophage MS2 at key environmental interfaces, *Soft Matter*, 7 pp. 10449-10456, 2011.

Conference Proceedings

Huyett, L.M., Dassau, E., Zisser, H.C., Doyle, F.J. III, The impact of glucose sensing dynamics on the closed-loop artificial pancreas, *Proc. of American Control Conference*, Chicago, IL, June 2015.

Platform Presentations

Huyett, L.M., Dassau, E., and Doyle, F.J. III. Trends in the clinical development of an artificial pancreas: guidance for the future. Presented at the *8th International Conference on Advanced Technologies and Treatments for Diabetes*, Paris, France, February 2015.

Huyett, L.M., Seborg, D.E., and Doyle, F.J. III. Design of a digital controller for a fully implantable closed-loop artificial pancreas. Presented at the *American Institute of Chemical Engineers Annual Meeting*, Atlanta, GA, November 2014.

Dassau, E. and **Huyett, L.M.**. Controversies in artificial pancreas development. Presented at the *Diabetes Technology Meeting*, Bethesda, MD, November 2014.

Huyett, L.M., Harvey, R.A., Bevier, W., Zisser, H., Jovanovič, L., Dassau, E., and Doyle, F.J. III. Closed-loop control and quality of continuous glucose monitor data based on prospective closed-loop clinical trial. Presented at the *6th International Conference on Advanced Technologies and Treatments for Diabetes*, Paris, France, February 2013.

Selected Poster Presentations

Huyett, L.M., Dassau, E., and Doyle, F.J. III. Application of fuzzy anti-reset windup for PID control in an implantable artificial pancreas. Presented at the *Diabetes Technology Meeting*, Bethesda, MD, 2014.

Larson, G.M., **Huyett, L.M.***, Lee, J.B., Dassau, E., and Doyle, F.J. III. Artificial pancreas clinical trial publication database. Presented at the *Diabetes Technology Meeting*, Bethesda, MD, 2014.

Huyett, L.M., Tao, A., Pinzon-Arango, P., and Camesano, T.A. Observing the effects of cranberry juice on biofilm formation of E. coli in urine. Presented at the *Biomedical Engineering Society National Conference*, Pittsburgh, PA, 2009.

Research Experience

University of California Santa Barbara, Santa Barbara, CA — **January 2012 - present**
Graduate Researcher
- Develop closed-loop control algorithms to automate insulin delivery for type 1 diabetes treatment using novel implanted medical devices
- Identify models from physiological datasets to inform and evaluate controller design
- Compiled a publicly available searchable database of protocol details from >74 published clinical trials of closed-loop control for type 1 diabetes: www.thedoylegroup.org/apdatabase

William Sansum Diabetes Research Center, Santa Barbara, CA — **January 2012 - present**
Adjunct Research Associate
- Provide technical expertise and supervision during clinical trials evaluating closed-loop control for type 1 diabetes, including 5 unique studies

Lafayette College, Easton, PA — **May 2010 - May 2011**
Research Assistant
- Completed honors thesis: "Adsorption of bacteriophage MS2 at the air-water interface as a model for soft nanoparticle behavior"

Worcester Polytechnic Institute, Worcester, MA — **June - August 2009**
Research Assistant
- Investigated the effects of cranberry juice on biofilm formation of uropathogenic bacteria

Professional Development

National Institutes of Health Clinical Center, Bethesda, MD — **July 2013**
Clinical and Translational Research Course for PhD Students
- Selected to participate in summer course for 28 PhD students in the basic sciences
- Gained experience with protocol design, biostatistics, bioethics, and FDA regulations

Teaching Experience

University of California Santa Barbara, Santa Barbara, CA — **January - March, 2013 - 2015**
Teaching Assistant, Advanced Process Control

Lafayette College, Easton, PA — **August 2010 - May 2011**
Supplemental Instructor, General Chemistry I and II

Johns Hopkins University, Baltimore, MD — **June - August, 2008, 2010, 2011**
Teaching Assistant, Center for Talented Youth Summer Program

Skills

Software: Mathematica, Microsoft Office, EndNote, Adobe Creative Suite, Aspen
Programming: Matlab, Python, Visual Basic for Applications, LaTeX, some MySQL and PHP
Laboratory: NMR, IR, UV-Vis spectroscopy, pendant drop tensiometry, bacteria culture
Language: Proficient in Spanish

NICHOLAS A. CADIROV

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University of California Santa Barbara
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EDUCATION

University of California Santa Barbara (UCSB), Santa Barbara, California
Ph.D. in Chemical Engineering **2012 - present**
Specialization in Intermolecular and Surface Forces and Interactions
Advisor: Professor Jacob N. Israelachvili

University of Massachusetts Amherst (UMass), Amherst, Massachusetts
B.S. in Chemical Engineering **2008-2012**
Summa Cum Laude, Departmental Honors

RESEARCH EXPERIENCE

Doctoral Research: Chemical Engineering, UCSB
Advisor: Professor Jacob N. Israelachvili **2012 – present**

- Study biolubrication and wear properties of synovial fluid and its constituents between model surfaces
- Investigate surface interactions between gecko-mimetic structured adhesives and diversified substrates and environments
- Development of integrated device capable of simultaneous surface force measurements and fluorescence imaging

Undergraduate Research: Chemical Engineering, UMass
Advisor: Professor Susan Roberts **2010 – 2012**

- Utilized sterile technique and hemocytometry to characterize the growth of single cell suspensions of Taxus cells
- Established a method for reculturing protoplasts in plant cell culture to study heterogeneity in production of the anti-cancer agent paclitaxel

Research Internships in Science and Engineering: Chemical Engineering, UCSB
Advisor: Professor Jacob Israelachvili **Summer 2011**

- Developed a method for imaging modeled myelin sheaths utilizing Langmuir-Blodgett technique and fluorescence microscopy
- Discovered differences in lipid domains between models of healthy and diseased myelin

Research Experience for Undergraduates: Chemical Engineering, USC
Advisor: Professor Branko Popov **Summer 2010**

- Synthesized and characterized titanium dioxide-supported catalysts for the oxygen reduction reaction in polymer electrolyte membrane fuel cells

- 1st place prize in Research Symposium oral presentation competition

FELLOWSHIPS & AWARDS

Heslin Fellowship (UCSB)	**2012**
Commonwealth Honors College Recognition Award (UMass)	**2011**
Chemical Engineering Endowment Scholarship (UMass)	**2011 – 2012**
John and Abigail Adams Scholarship (UMass)	**2008 – 2012**

TEACHING EXPERIENCE

Teaching Assistant: Chemical Engineering Undergraduate Laboratory, UCSB
- Instructed and supervised students during lab experiments **2014**

Teaching Assistant: Colloids, Biomolecules, and Biosurfaces, UCSB
- Held office hours and assisted students on homework assignments **2014**

OUTREACH

ScienceLine "Ask a Scientist": Materials Research Lab, UCSB **2014 - present**
- Answer weekly questions from local K-12 students and teachers about science and engineering related topics

PUBLICATIONS AND PAPERS

1. Lee, DW; Kristiansen, K; Donaldson, SH; **Cadirov, N**; Banquy, X; Israelachvili, J; (2015) Real time intermembrane force measurements and imaging of lipid domain morphology during hemifusion ***Nature Communications***

2. Das, S; **Cadirov, N**; Chary, S; Kaufman, Y; Hogan, J; Turner, K; Israelachvili, J; (2015) Stick-slip friction of gecko-mimetic flaps on smooth and rough substrates. ***Journal of The Royal Society Interface***

3. Lee, DW; Banquy, X; Das, S; **Cadirov, N**; Jay, G; Israelachvili, J; (2014) Effects of molecular weight of grafted hyaluronic acid on wear initiation. ***Acta Biomaterialia***

4. Huang, SY; Ganesan, P; Jung, WS; **Cadirov, N**; Popov, B; (2010) Development of supported bifunctional oxygen electrocatalysts with high performance for unitized regenerative fuel cell applications. ***ECS Transactions***

PRESENTATIONS

1. Poster presentation 2015 Gordon Conference Science of Adhesion, Mount Holyoke College, MA, Influence of humidity on gecko inspired adhesives

2. Poster presentation 2014 Chemical Engineering Graduate Student Symposium, UCSB, Stick-slip friction of gecko-mimetic structured surfaces on smooth and rough substrates

3. Poster presentation 2014 Surface Forces Apparatus Conference Cancun, Mexico, Stick-slip friction of gecko-mimetic structured surfaces on smooth and rough substrates

Tanmoy Sanyal

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Department of Chemical Engineering
University of California Santa Barbara
Santa Barbara, CA 93106-5080

Education

2013 — 2^{nd} year Ph.D candidate, Chemical Engineering, University of California Santa Barbara, Santa Barbara CA
currently working on: Robust models of coarse-gained interactions using multi-body potentials with the relative entropy
advisor: M. Scott Shell

2012-2013 Master of Technology, integrated dual degree, Chemical Engineering, Indian Institute of Technology, Kharagpur, Kharagpur, WB, India
masters' thesis: Stability analysis of patterned states in homogeneous autocatalytic reactions
advisor: Saikat Chakraborty

2008-2012 Bachelor of Technology, Chemical Engineering, Indian Institute of Technology, Kharagpur, Kharagpur, WB, India
bachelors' thesis: Multiscale analysis of hypoxemia in methemoglobin anemia
advisor: Saikat Chakraborty

Honors and Awards

- Department of Chemical Engineering, Indian Institute of Technology Kharagpur: Best bachelors thesis, 2012
- Technopreneur Promotion Programe (TePP), Ministry of Science and Technology, Govt. of India : Seed money for prototype scale-up of novel bio-reactors for algal-biodiesel generation, 2009
- Jagdis Bose National Science Talent Search (JBNSTS) foundation, WB, India : Fellowship, 2008

Outreach activities

- 2014 Co-organized the first ChE Graduate Simulation Seminar Series, University of California Santa Barbara
- 2014 — President of the non-profit organization *India Association of Santa Barbara*
- 2010-2013 Served as executive editor of the Technology Literary Society, Indian Institute of Technology, Kharagpur

Teaching Assistance

University of California, Santa Barbara
- ChE 10, Introduction to Chemical Engineering, Fall 2014

Indian Institute of Technology Kharagpur
- Biochemical Engineering, Fall 2012
- Physiological Transport Phenomena, Spring 2013

Research Interests

Multiscale modeling and simulation, coarse-graining algorithms, numerical analysis,

Publications

1) T. Sanyal and S. Chakraborty, "Micro- and Meso- Scale analyses for quantifying hypoxemia in Methemoglobinemia", *Lecture Notes in Engineering and Computer Science* 2192(1), 2640-45 (2011) - also presented at World Congress of Engineering (WCE- 2011)

2) T. Sanyal and S. Chakraborty, "Multiscale analysis of hypoxemia in methemoglobin anemia", *Mathematical Biosciences* 241, 167-180 (2013)

3) T. Sanyal and S. Chakraborty, "Multiscale analysis of simultaneous uptake of two interacting gases in the human lungs and its application to methemoglobin anemia", *Computers & Chemical Engineering* 59, 226-242 (2013) - selected paper from ESCAPE-22(European Symposium on Computer Aided Process Engineering-22)

Contributed Conference Presentations

1) **International Workshop on Mathematics in Chemical Kinetics and Engineering**; Chennai, India; 2013
Poster: "Multiscale modeling of methemoglobin anemia induced by reactive uptake of NO in the human lungs"

2) **American Institute of Chemical Engineers Annual Meeting**; San Francisco, CA, November 2013
Poster: "Stability of mixing limited patterns in isothermal homogenous autocatalytic reactions"

Internships

May-July 2012 — Department of Biotechnology, Indian Institute of Technology, Madras, Chennai, India
project: Variable structure control algorithm development for fed-batch fermenters
advisor: K.B. Ramachandran

May-July 2011 — Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX
project: Fundamentals based low dimensional mathematical modeling of compression ignition engines
advisor: Vemuri Balakotaiah

May 2010 — Condensed Matter Physics Division, Saha Institute of Nuclear Physics, Kolkata, India
project: Phase transitions in Classical Heisenberg and related models
advisor: Pradip K. Mohanty

Skills

- Python, Fortran, C++, bash scripting, TCL
- MatLab, Mathematica, COMSOL
- Creative writing and cooking

Niels P. Zussblatt

Ph.D. candidate, UCSB Department of Chemical Engineering

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Goleta, CA 93117

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Education

Doctor of Philosophy in Chemical Engineering Sep. 2012 – Dec. 2017
University of California, Santa Barbara, CA
Dissertation title: "Synthesis and Characterization of Functionalized Mesoporous Carbons for Electrochemical Device Applications"
Advisors: Prof. Bradley F. Chmelka and Prof. Todd M. Squires

Bachelor of Science in Chemical Engineering Sep. 2008 – Jun. 2012
Massachusetts Institute of Technology, Cambridge, MA

Research Experience

Graduate Research Assistant Jan. 2013 – Present
Department of Chemical Engineering, University of California, Santa Barbara
Mentors: Prof. Bradley F. Chemlka and Prof. Todd M. Squires

- Synthesized transition metal and nitrogen-containing mesoporous carbon materials and characterized their physical and chemical properties
- Evaluated resultant materials as low-cost replacements for precious metal-based functional and/or catalytically-active electrodes for fuel cells, batteries, and supercapacitors
- Contributed to efforts to integrate carbon-based electrode materials with biological technologies (e.g., functional protein-containing membrane materials) which could result in novel renewable energy sources

Undergraduate Research Assistant Sep. 2010 – Jun. 2011
Department of Chemical Engineering, Massachusetts Institute of Technology
Mentors: Prof. Clark K. Colton, Dr. William Dalzell, and Prof. Paula Hammond

- Synthesized films of functionalized polymers and characterized their responses to chemical species in order to develop new low-concentration organic contaminant detection devices
- Developed alternative high-throughput nanoparticle sizing technique based on pulsed ultrasound of particle solutions

Professional Experience

Risk and Decision Analyst May 2012 – Jan. 2013
U.S. Army Corps of Engineers, Concord, MA
Mentors: Matthew Bates and Dr. Igor Linkov

- Conducted value of information and portfolio optimization analyses to prioritize research regarding the environmental and human health hazards of emerging nanotechnologies
- Performed database analysis to identify primary cost-drivers for US Army Corps of Engineers projects (e.g., waterway dredging)

Engineering Intern May 2011 – Jul. 2011

U.S. Army Corps of Engineers, Champaign, IL

Mentors: Prof. Charles Marsh and Dr. Meredith Sellers

- Developed high-performance supercapacitor components, including electrodes, based on metal-oxide-doped carbon nanotubes and a solid-state electrolyte
- Evaluated supercapacitor devices based on these electrode and electrolytes using a high-sensitivity self-designed testing assembly

Publications

Fechler, N.; **Zussblatt, N. P.**; Rothe, R.; Schlögl, R.; Willinger, M.-G.; Chmelka, B. F.; Antonietti, M., "Eutectic Syntheses of Graphitic Carbon with High Pyrazinic Nitrogen Content," *Advanced Materials*, **2015**, DOI: 10.1002/adma.201501503

Sellers, M. C. K.; **Zussblatt, N. P.**; Marsh, C. P., "Potassium perruthenate-treated carbon nanotube sheets for flexible supercapacitors," *Electrochemistry Communications*, **2012**, *18*, 58-61.

Presentations

"Understanding Synthesis, Molecular Compositions, and Conductivity of Nitrogen-Doped Carbon Materials with Solid-State ^{13}C and ^{15}N NMR," Poster presentation, *Experimental Nuclear Magnetic Resonance Conference*, Pacific Grove, CA (Apr. 2015)

"Fe,N-doped mesoporous carbon materials as non-precious metal electrocatalysts for alcohol and bio-hybrid fuel cells," Poster presentation, *Institute for Energy Efficiency Research Review*, Santa Barbara, CA (Apr. 2015)

"Understanding heteroatom-doped carbon electrodes in energy storage and conversion devices," Oral presentation, *Total Sponsored Students Meeting*, Santa Clara, CA (Feb. 2015)

"Understanding heteroatom-doped carbon electrodes in energy storage and conversion devices," Oral presentation, *Total Sponsored Students Meeting*, Cambridge, MA (Mar. 2014)

"Fe,N-doped mesoporous carbon materials as non-precious metal electrocatalysts for bio-hybrid fuel cells," Poster presentation, *Materials Research Outreach Program*, Santa Barbara, CA (Feb. 2014)

"Understanding and controlling geometry and functionality in porous electrochemical materials," Oral presentation, *Total Sponsored Students Meeting*, Berkeley, CA (Jun. 2013)

Skills

Software/Coding: MATLAB, Mathematica, Microsoft Office, Visual Basic

Experimental Methods: Nanostructured material synthesis, NMR spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, atomic force microscopy, electrochemistry and potentiostat operation

Professional Memberships

American Chemical Society 2011 – Present

American Institute of Chemical Engineers 2010 – Present

Matthew Idso

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EDUCATION

Doctorate of Philosophy, Chemical Engineering — September 2012 – June 2017 (expected graduation)
University of California, Santa Barbara

Bachelor of Science, Chemical Engineering — August 2008 – June 2012
University of Washington, Seattle
Departmental honors, Magna Cum Laude

RESEARCH HISTORY

Graduate Research Assistant — January 2013 – current
University of California – Santa Barbara, Dept. of Chemical Engineering
P.I. Dr. Bradley Chmelka

- Proteorhodopsin-incorporated Inorganic-organic Hybrid Materials for Electrochemical Energy Generation and Storage
- Investigation into Organic Photovoltaic Polymer-fullerene Blends using Solid-state Nuclear Magnetic Resonance Spectroscopy
- Development of Mesoporous Silica Proton Exchange Membranes for Hydrogen Fuel Cell
- Understanding the affinity of drug guest species to various functional groups of mesoporous silica nanochannels using Nuclear Magnetic Resonance Spectroscopy

Undergraduate Research Assistant — June 2009 – June 2012
University of Washington, Department of Chemical Engineering
P.I. Dr. Qiuming Yu

- Investigated the fundamental aspects of Quasi-3D plasmonic nanohole structures with the goal of improving surface enhanced Raman scattering signal enhancement
- Conducted a feasibility study of Quasi-3D plasmonic nanostructure materials as biosensors for harmful bacteria and trace pesticides in solution

EMPLOYMENT HISTORY

Process Engineering intern – Coker unit — June – September 2011
British Petroleum
Mentor: Kieth Zinc, Process Engineer

- Developed protocols to test the efficiency of three coker antifoams
- Collaborated with operators and engineers to implement experiments in the field
- Assessed experimental data to determine the optimally performing and economic antifoam

SERVICE ACTIVITIES

Faculty Executive committee: Graduate student representative — September 2014 – June 2015
University of California – Santa Barbara, College of Engineering

Fundraising Director February 2010 – February 2012

Engineers Without Borders: University of Washington Seattle chapter

Grant Writing Co-lead September September 2009 – February 2010

Engineers Without Borders: University of Washington Seattle chapter

Awards:

- Outstanding Teaching Assistant Award UCSB 2014
- National Science Foundation Graduate Research Fellowship Honorable Mention awardee UCSB 2012-13
- Heslin Fellowship UCSB 2012
- University of Washington Emerging Leader in Engineering Scholarship UW 2011-12
- University of Washington Tau Beta Pi member UW 2011
- University of Washington Chemical Engineering departmental scholarship UW, 2010-11, 2011-12
- Bert Johnson Memorial Scholarship 2008-12
- Frank Robinson Scholarship 2008-09, 2010-11
- University of Washington Dean's List UW, each quarter, 2008-2012

PUBLICATIONS

Deng, Y.; Idso, M. N.; *et al.* "Optofluidic microsystem with quasi-r dimensional gold plasmonic nanostructure arrays for online sensitive and reproducible SERS detection," Analytical Chimica Acta, **2015**, 863, 41-48.

Graham , K. R.; Cabanetos, C.; Jahnke, J.; Idso, M. N.; et al. "Importance of Donor:Fullerene Intermolecular Arrangement for High-Efficiency Organic Photovoltaics," *JACS*, **2015**, 136, 9608-9618.

Xu J.; Turner J.; Idso, M. N.; *et al*. "Quasi-3D Plasmonic Nanostructures for Strain Specific Identification of Marine Bacteria Vibrio Parahaemolyticus Using SERS," *Analytical Chemistry*, **2013**, 85, 2630-2637.

Xu, J.; Kvasnička, P.; Idso, M. N.; *et al*. "Understanding the effects of dielectric medium, substrate, and depth on electric fields and SERS of quasi-3D plasmonic nanostructures", *Optics Express*, **2011**, 19, 20493-20505.

PRESENTATIONS

M. N. Idso; J.P. Jahnke; K.R. Graham; A. Amassian; P.M. Beaujuge; M. D. McGehee; B.F. Chmelka. 46th annual Experimental NMR Conference, *Assessing fullerene proximities to donor and acceptor moieties in bulk heterojunction materials using solid-state NMR spectroscopy*. April 20, 2015. Asilomar, CA. Poster presentation.

M. N. Idso; S. Hussain; J. P. Jahnke; S. Han; B. F. Chmelka. 4th bilateral UCSB-Chalmers workshop on Materials Science and Engineering, *Incorporation of the membrane protein proteorhodopsin in inorganic-organic nanocomposites for light activated ion-transport*. June 30, 2014. Chalmers University, Gothenburg, Sweden. Invited workshop talk.

Jahnke J.P.; Idso M. N.; K. R. Graham; A. Amassian; P. M. Beajuge; M. D. McGehee; B. F. Chmelka. 2014 Materials Research Outreach Program, *Assessing fullerene proximities to donor and acceptor moieties in bulk heterojunction materials*. February 4, 2014. University of California - Santa Barbara, Santa Barbara, CA. Poster presentation.

Jahnke J.P.; Idso M. N.; K. R. Graham; A. Amassian; P. M. Beajuge; M. D. McGehee; B. F. Chmelka. 2013 Annual Center for Advanced Molecular Photovoltaics, *Assessing fullerene proximities to donor and acceptor moieties in bulk heterojunction materials*. August 23, 2013. Stanford University, Stanford, CA. Poster presentation.

Idso, M.**;** Yu, Q. (2012). 15th University of Washington Undergraduate Research Symposium, *Rapid and Sensitive Detection of Pesticides in Aqueous Solution Using Surface-enhanced Raman Spectroscopy (SERS)*. June, 2012. University of Washington, Seattle, WA. Oral presentation.

Joel Bozekowski

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EDUCATION

University of California, Santa Barbara **2013 – Present**
Ph.D. Chemical Engineering
Advisor: Patrick S. Daugherty

University of Colorado, Boulder **2009 – 2013**
B.S. Chemical and Biological Engineering
Summa cum laude

RESEARCH EXPERIENCE

Department of Chemical Engineering **Jan 2014 – Present**
University of California, Santa Barbara
Doctoral Candidate – Daugherty Group

- Evaluated sensitivity of unbiased serum antibody detection methods using a model system comprised of human serum spiked with known monoclonal antibodies
- Analyzed antibody repertoire of schizophrenia patients using bacterial display peptide libraries and next-generation sequencing
- Applied magnetic- and fluorescence-activated cell sorting techniques for peptide library screening
- Constructed and transformed large (~10^{10}) randomized *Escherichia coli* display peptide library for screening applications

Department of Chemical and Biological Engineering **Aug 2012 – May 2013**
University of Colorado, Boulder
Undergraduate Research Assistant – Yin Lab

- Screened short peptide libraries for inhibition of transmembrane proteins
- Transfected mammalian cells with reporter genes for *in vitro* signaling assays
- Analyzed transmembrane protein expression and activity in mammalian cells using fluorescence-activated cell sorting

Duke University Biomedical Engineering **May 2012 – July 2012**
Undergraduate Research Intern – Chilkoti Group

- Developed enzymatic protein conjugation method for drug delivery applications
- Purified recombinant chimeric proteins using inverse transition cycling
- Quantified purified fusion-protein activity *in vitro*

OUTREACH & MENTORING

Research Mentor **Spring 2014**

- Mentored visiting Jagiellonian University graduate student Kasia Falkowski with protease substrate screening using fluorescence-activated cell sorting and peptide display systems

Undergraduate Research Mentor **Fall & Spring 2014**

- Mentored UCSB chemical engineering undergraduate student Austin Graham with antibody repertoire analysis research

Family Ultimate Science Exploration (FUSE) **Fall 2014**

- Demonstrated physics and chemistry related experiments to local junior high school students and their families

CU Chemical Engineering Alumni Student Mentoring Program **2014 – Present**

- Mentored chemical engineering undergraduate students in academic and professional development

HONORS & AWARDS

- Klaus D. and Jean L. Timmerhaus Scholarship Fund **2012**
- Oscar L. Robertson Scholarship Endowment Fund **2011**
- CU College of Engineering Dean's List **2009 – 2013**

John K. Henske

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Education

B.S. in Chemical Engineering, Northeastern University (May 2012)

Omega Chi Epsilon (Chemical Engineering Honor Society), Tau Beta Pi, Honors Program
Minor in Biochemical Engineering
Summa cum laude

Academic Employment

University of California, Santa Barbara, Santa Barbara, CA **2012-Present**

Advisor: Michelle O'Malley

- Isolation and culture of anaerobic fungi for lignocellulosic biofuel applications
- Analysis of transcriptomic data for identification of regulatory proteins

Northeastern University, Boston, MA **2010 – 2012**

Advisor: Shashi Murthy

- Ran experiments using microfluidics devices to capture desired cell types
- Performed surface modifications on devices to be tested
- Prepared cell culture from rat tissue for use in experiments

Massachusetts Institute of Technology, Cambridge, MA **Jan 2010 – Jun 2010**

Novartis-MIT Center for Continuous Manufacturing, Charles Cooney Lab

- Conducted experiments to explore applications of wet extrusion of pharmaceutical drug substance
- Collaborated with Novartis experts and mechanical engineers to develop novel wet extrudate forming mechanism
- Examined samples using analytical techniques, i.e. X-Ray Diffraction, HPLC, and Tablet Dissolution
- Aided in melt extrusion research and conducted several melt extrusion experiments
- Performed preliminary tablet coating experiments to improve stability of melt extrusion product

Industrial Employment

GVD Corporation, Cambridge, MA **Jan 2011 – Jul 2011**

Research and Development Engineering Co-op

- Assisted in reaction chamber installation and qualification
- Improved reproducibility of existing coating deposition process
- Performed quantitative measurements on coatings, including profilometry and electrical testing
- Produced coated samples and identified best conditions to meet customer requirements

Genzyme Corporation, Allston, MA **Jan 2009 – Jun 2009**

Process Engineer Co-op: Purification Manufacturing Technical Support

- Managed project to re-design a process storage container, tested prototype, and created standard operating procedures for new equipment in cGMP facility
- Analyzed data to review historical process performance to support product quality investigations
- Designed studies to test equipment capabilities and model mixing to ensure product consistency
- Executed a study to develop filter integrity testing procedures for downstream purification filters
- Performed statistical analysis and made recommendations to update In-Process Controls

Awards

Mellichamp Sustainability Fellow, University of California, Santa Barbara (January 2015 – Present)
Sears B. Condit Award, given to top 100 students (top 3%) in Northeastern graduating class (2012)
Dean's Scholarship, Northeastern University (2007-2012)

Publications

Journal Articles

1. Haitjema, C.H., Solomon, K.V., **Henske, J.K.** Theodorou, M.K., O'Malley, M.A. Anaerobic Gut Fungi: Advances in Isolation, Culture, and Cellulolytic Enzyme Discovery for Biofuel Production. *Biotechnology and Bioengineering* (2014).
2. Gilmore, S.P., **Henske, J.K.**, O'Malley, M.A. Driving biomass breakdown through engineered cellulosomes. *Bioengineered*. (2015).
3. **Submitted:** Solomon, K.V., **Henske, J.K.**, Theodorou, M.K., O'Malley, M.A. Robust and effective methodologies for cryopreservation and DNA extraction . from anaerobic gut fungi. *Scientific Reports*.
4. **In Process:** Solomon, K.V., Haitjema, C.H., **Henske, J.K.**, Borges-Rivera, D., Thompson, D.A., O'Malley, M.A. Integrated analysis of a primitive gut fungus reveals extraordinary degradation capabilities.

Oral Presentations

1. **Henske, J.K.***, Solomon, K.V., O'Malley, M.A. A novel co-culture approach to compartmentalize biomass deconstruction and biofuel production. 2015 ACS BIOT, Denver, CO, March 2015.

Poster Presentations *(*denotes speaker)*

1. KV Solomon*, **JK Henske***, CH Haitjema, D. Borges-Rivera, D Thompson, A Regev, MA O'Malley. Engineering Anaerobic Gut Fungi for Lignocellulose Breakdown. 2014 Southern California Systems Biology, Irvine, CA, 2014.
2. KV Solomon*, **JK Henske***, CH Haitjema, D. Borges-Rivera, D Thompson, A Regev, MA O'Malley. Identification and Regulation of Novel Cellulases within Anaerobic Gut Fungi. 2014 JGI User Meeting, Walnut Creek, CA, 2014.
3. **JK Henske***, KV Solomon, SA Maxel, MA O'Malley. Engineering Regulation in Anaerobic Fungi During Lignocellulose Breakdown. 2014 Synthetic Biology: Engineering, Evolution, and Design, Manhattan Beach, CA, 2014.
4. **JK Henske*,** KV Solomon, CH Haitjema**,** SP Gilmore, MA O'Malley. Engineering Synthetic Anaerobic Consortia for Sustainable Chemical Production from Crude Biomass. DOE Grantee Meeting, Washington D.C., 2015

5. **JK Henske*,** KV Solomon, SP Gilmore, J Sexton, MK Theodorou, MA O'Malley. Regulation of biomass degrading enzymes in anaerobic gut fungi and their application in synthetic co-culture systems. 2015 Synthetic Biology: Engineering, Evolution, and Design, Boston, MA, 2015.

Kelly N. Ibsen, PE

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Goleta, CA 93117
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PROFESSIONAL SUMMARY

Professional Chemical Engineer with more than 25 years' experience in research, development and deployment for a variety of industries. Distinguished 15-year career at NREL, DOE's premier renewable energy laboratory, where a diverse career path culminated with a lead role managing multi-disciplinary R&D programs to develop technically sound and financially robust processes. Directed the scale-up of chemical and biological systems for Myriant Corporation. Started a consulting business in 2009 to provide project management, engineering expertise and proposal development for the renewable energy sector. Transitioned to biochemical research for medical applications in 2013; currently pursuing a doctoral degree in Chemical Engineering at UC Santa Barbara with a research emphasis on *de novo* investigation of the antibody repertoires in autoimmune disease using bacterial display peptide libraries.

KEY SKILLS

Research and Development
Skilled in developing and completing robust, multi-year R&D projects to achieve technology goals. Expert in conducting research at bench, pilot, demonstration and commercial scales.

Project/Program Management
Successfully directed multi-million dollar R&D advanced technology programs and projects for biofuels with directed, economics-driven targets.

Engineering & Design
Lead complete systems' design and build activities including process simulation, equipment and facilities specifications, and life cycle/environmental assessments for targeted processes. Completed design reports for cellulose to ethanol and full design packages (FEL2) for biomass to chemicals.

Proposal Development and Review
Expert in leading teams in development of winning proposals for funding opportunities. Regular participant in review committees for DOE's Energy Efficiency and Renewable Energy Program including R&D, pilot and demonstration scale proposals for grants, financial assistance, small business and loan guarantees.

Partnership Development
Expertise in identifying partnership and funding opportunities. Able to key develop relationships with industry and government organizations necessary to successfully negotiate lasting partnerships.

CERTIFICATIONS

Licensed Professional Engineer in Colorado
Served on the Board of Directors of the Transport & Energy Processes Division of the American Institute of Chemical Engineers 2010 – 2013.

CAREER HISTORY

University of California, Santa Barbara — August 2013 – present

Graduate Student Researcher
Advisor: Professor Patrick Daugherty
Antibody Repertoire Analysis Research Group

Using bacterial display peptide libraries, investigate the humoral response in patients with Type 1 Diabetes Mellitus (T1DM) and other autoimmune diseases. Develop experimental protocols and screening assays to evaluate mimotope binding to T1DM patient antibodies, identify disease specific motifs and use them to identify candidate antigens involved in T1DM pathology. Served as a teaching assistant for undergraduate Biochemical Engineering courses.

Lynx Engineering LLC — July 2009 – September 2013

Owner/Principal Engineer

Provided project management, process engineering and consulting services to the renewable fuels industry including the National Advanced Biofuels Consortium. Skilled at team and individual proposal development and critical review for state/federal funding opportunities. Expert engineering and analysis support including process design, cost estimation and data analysis. Independent engineering services for development, piloting and construction projects. Performed technology reviews and audits for DOE.

Myriant Corporation — 2007 – June 2009

Director of Technology Transfer & Scale-up

Responsible for the scale-up of fuels and chemicals developed in the lab. Collaborated with and advised Central R&D teams to develop robust processes with advanced biochemical methods. Managed engineering firm teams in the development of basic and detailed design packages. Oversaw construction and operations teams including EPC contractors, operations and maintenance personnel to successfully build, shakedown and operate biorefineries using green feedstocks in the US and South America. Conducted due diligence for partnership opportunities.

National Renewable Energy Laboratory

Biochemical Platform Lead — 2004 – 2007

Developed and directed a multi-million dollar R&D portfolio for DOE's Biomass Program that provided the highest quality research to achieve targeted results. Using diverse engineering and research teams including pilot plant operations developed cost effective conversion processes for biomass to fuels and chemicals. Wrote multi-year plans to attract and maintain funding sources. Managed annual budgets including capital equipment, facilities, contracts and personnel.

Analysis and Partnership Development Group Manager — 2002 – 2004

Managed the teams charged with engineering and partnering roles to the Biomass Program. Implemented an economics-driven approach to R&D for DOE's Biomass program which resulted in projects moving more directly to commercially viable processes.

Process Engineering and Analysis Team Lead — 1997 – 2002

Lead engineer for several DOE and industry projects including enzyme development contracts and Biochemical Conversion Platform. Developed designs, cost analysis, and directed cost-driven experimentation. Supervised 8 staff and annual budgets of $2 million. Led the use of innovative tools for mass/energy balances and cost analyses.

Pilot Plant Team Lead & Process Engineer — 1992 – 1997

Responsible for the full-time operation of a $16 million pilot facility to convert biomass to ethanol. Assembled annual capital and operating budget of $5 million and managed a staff of 15 operators. Recommended and supervised plant upgrades through design, procurement and installation. Interfaced with subcontractors and in-house personnel during shake-down, maintenance and upgrades.

Nestle Foods — 1985 - 1990

Senior Project Engineer & Plant Operations Engineer

Developed production lines for new food products including safe ingredient handling. Established quality control standards for ingredients, packaging and products. Responsible for obtaining approval by USDA and FDA. Led startup teams for several processing lines. Supervised a $50 million plant renovation including utilities, equipment and instrumentation. Developed layout and installed new equipment for 20,000 square foot pilot plant.

EDUCATION & TRAINING

University of California, Santa Barbara **2013 - present**
Ph.D. Candidate in Chemical Engineering
Expected Graduation: Fall, 2018

Colorado State University
B.Sc. in Chemical Engineering **1985**

Additional professional and college level courses in
- Process Simulation & Design (Aspen Plus)
- Computer programming (Visual Basic, VB for Applications, XML)
- Database development (MS Access, SQL)
- Monte Carlo analysis (Crystal Ball)

PUBLICATIONS

1. Dutta A, Dowe N, **Ibsen K**, Schell D, Aden A. "An economic comparison of different fermentation configurations to convert corn stover to ethanol using *Z. mobilis* and *Saccharomyces*". Published online in Biocatalysts and Bioreactor Design, September 2009. DOI: 10.1002btpr.311.
2. Foust TD, **Ibsen KN**, Dayton DC, Hess JR, Kenney KE. <u>Biomass Recalcitrance: Deconstructing the Plant Cell Wall for Bioenergy, Chapter 2 - The Biorefinery</u>. Michael E. Himmel, Editor. Blackwell Publishing, Oxford, 2008.
3. Schell DJ, Dowe N, **Ibsen KN**, Riley CJ, Ruth MF, Lumpkin RE. "Contaminant occurrence, identification and control in a pilot-scale corn fiber to ethanol conversion process". Bioresource Technology 98(15):2942-8, November 2007.
4. **Ibsen, Kelly**. "Match the Effort to the R&D Investment", Chemical Engineering Progress, 102(1):47-51, January 2006.
5. Schell DJ, Riley CJ, Dowe N, Farmer J, **Ibsen KN**, Ruth MF, Toon ST, Lumpkin RE. "A Bioethanol process development unit: initial operating experiences and results with a corn fiber feedstock". Bioresource Technology 91(2): 179-88, January 2004.
6. Tucker MP, Nagle NJ, Jennings EV, **Ibsen KN**, Aden A, Nguyen QA, Kim KH, Noll SL. "Conversion of distiller's grain into fuel alcohol and a higher-value animal feed by dilute–acid pretreatment". Applied Biochemistry and Biotechnology 113-116:1139-59, January 2004.
7. Aden A, Ruth MF, **Ibsen KN**, Jechura J et al. "Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover". NREL/TP-510-32438, June 2002.
8. **Ibsen KN**, McAloon A, Taylor F, Wooley R, Yee W. "Determining the Cost of Production Ethanol from Corn Starch and Lignocellulosic Feedstocks", Joint technical paper with USDA-ARS. NREL/TP-580-28893, October 2000.
9. Wooley R, Ruth MF, Sheehan J, **Ibsen KN** et al. "Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis Current and Futuristic Scenarios". NREL/TP-580-26157, July 1999.
10. Nguyen QA, Dickow JH, Duff BW, Farmer JD, Glassner DA, **Ibsen KN**, Ruth MF et al. "NREL/DOE Ethanol Pilot Plant: Current Status and Capabilities". Bioresource Technology 58(2): 189-196, 1996.

PRESENTATIONS

Chaired and presented at various national and international meetings including the 24th and 25th Biotechnology Symposium for Fuels and Chemicals, the spring 2004 National American Chemical Society meeting, the 2002 American Institute of Chemicals Engineers National meeting and several Pacific Rim Biofuels conferences in Singapore, Thailand and Australia.

Contact Information

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Students

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