First Annual Rutgers SWE GRAD Research Symposium
WE need ALL of the talent that we can muster to solve the myriad of issues that WE face!
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Keynote Speaker:

Dr. Serpil Guran
Director
EcoComplex

Dr. Serpil Guran is the Director of the Rutgers EcoComplex. Her responsibilities include management of the EcoComplex operations, programs, business incubator and facilities, as well as providing vision and leadership in establishing the EcoComplex as a nationally recognized center for the commercialization of environmental and alternative energy technologies. Additionally, Dr. Guran serves as liaison to the regional environmental and alternative energy business communities, government agencies, and related organizations. She was formerly a Research Scientist at the New Jersey Department of Environmental Protection, a Research Scientist at both Princeton University in the Mechanical-Aerospace Engineering Department, and at the National Renewable Energy Laboratory in Golden, CO.

Dr. Guran specializes in research, development and assessment of sustainable biofuel and recycling technologies, and life cycle analysis of alternative fuel production systems. She has authored more than 25 scientific articles and holds a U.S. patent and patent disclosure. Dr. Guran has a M.S. in Chemical Engineering from Anadolu University in Turkey and a PhD in Chemical Engineering, with a specialization in Fuel and Energy Technology, from the University of Leeds, UK.
Industrial Speaker:

Dr. Zhimei Du  
Senior Principal Scientist,  
Head of Cell Line Development  
Merck & Co., Inc.

Zhimei Du earned a Ph.D. from Cornell University Medical College, Immunology Program, studying the regulation of Jak/Stat signaling pathways during immune responses. After graduation, she joined Robert G. Roeder’s laboratory at Rockefeller University, studying transcriptional regulation mechanism and epigenetic effects during early B cell development. After three years, she was recruited by Regeneron’s antibody engineering group, focusing on bi-specific Antibody development. Later, she joined Amgen’s Cell Sciences & Technology department, focusing on cell line development and process development and then became the Upstream process lead at Teva Pharmaceuticals. She now works at Merck as the head of Cell Line Development team.
Networking Luncheon

Hosted by

Rutgers

SWE Graduate Branch

11:30 am to 1:00 pm
CoRE Atrium
Graduate Student Speaker:

Sally Stras
Ph.D. Student
Chemical and Biochemical Engineering

Sally is Ph.D. student in Chemical and Biochemical Engineering at Rutgers University under the direction of Dr. Stavroula Sofou. She is in her 4th year at Rutgers and is working on her thesis project which focuses on liposomes as drug delivery vehicles for cancer treatment. She received her bachelors in Chemical Engineering with a focus in Biochemical Engineering at the University of Massachusetts, Amherst in 2012.

Abstract:

Tunable Liposomal Cisplatin for Selective and Effective Treatment of Triple Negative Breast Cancer
Sally Stras1, Stavroula Sofou1,2
1Chemical and Biochemical Engineering, Rutgers University
2Biomedical Engineering, Rutgers University

Breast cancer is the 2nd leading cause of cancer related deaths in women. Triple negative breast cancer (TNBC) is a subgroup of breast cancer associated with poor prognosis and a higher chance of cancer reoccurrence outside the breast. To enable treatment of TNBC solid tumors, we study a pH-sensitive delivery carrier of cisplatin (CDDP) - a clinically accepted line of therapy for TNBC. These tunable liposomes are to be injected into the blood stream and enter the tumor. Within the tumor interstitium there could be an inherent drop in pH (~6.0-6.7), which causes the liposomes to become leaky and release their contents. We demonstrate the efficacy of the pH responsive liposomes with in vitro experiments, both 2-D monolayers and 3-D tumor analogues, using two TNBC cell lines.
Graduate Student Speaker:

Catrice Carter

Ph.D. Student
Material Science and Engineering

Catrice is a 4th year Ph.D. student in Materials Science and Engineering at Rutgers University under the direction of Dr. Deirdre O’Carroll. She is working on her thesis project which focuses on plasmonics for polymer based organic light emitting diodes. Catrice received her bachelor’s degree in Physics and Astronomy at Carleton College in 2011. She is a Teaching Assistant for Chemistry and Chemical Biology and a Rutgers Science Bus Fellow. Catrice works to introduce science to underrepresented groups through various Rutgers programs.

Abstract:

Polymer-based organic light-emitting diodes are of interest as a sustainable next-generation lighting and display application. Theoretical light-extraction efficiency (LEE) electromagnetic simulations are carried out for four P-OLED device architectures due to their potential to increase lifetime (inverted architecture) and LEE (top-emitting architecture). Preliminary data indicates that LEE is highest for bottom-emitting conventional (68%), and lowest (4%) for top-emitting inverted architectures. However, the thicknesses of the P-OLED device layers have not been optimized thus resulting in lower than literature expected values for the top-emitting inverted configuration. Next, optimization simulations are expected to yield insight into the dominant optical loss factors associated with various device architectures currently under consideration for P-OLED applications.
Graduate Student Speaker:

Jonathan Colón Ortiz
Ph.D. Student
Chemical and Biochemical Engineering

Jonathan is Ph.D. student in Chemical and Biochemical Engineering at Rutgers University under the direction of Dr. Alexander Neimark. He is in his 3rd year at Rutgers and is working on his thesis project which focuses on the in-situ growth of metal-oxide nanoparticles in polyelectrolyte membranes. Jonathan is active in outreach both within the Department of Chemical Engineering as well as within the Graduate School of New Brunswick. He received his bachelors in Chemical Engineering at the University of Puerto Rico, Mayaguez Campus in 2013.

Abstract:

Characterization of Polyelectrolyte Membranes with in-situ Metal-Oxide Nanoparticles
Jonathan Colon, John Landers, Sagar Patel, Aleksey Vishnyakov, Alexander V. Neimark
Department of Chemical and Biochemical Engineering, Rutgers University

The in-situ growth of metal-oxide nanoparticles (MONP) in polyelectrolyte membranes (PEM) has been investigated. Among several potential applications, such as fuel cells, water purification, and others, these PEM can serve as self-detoxifying composite PEM barriers against dangerous organic compounds, such as chemical warfare agents (CWA). These PEM have interconnected hydrophilic and hydrophobic sub-domains, which can allow for water permeation and block CWA. In addition, MONP are known to catalyze the decomposition of CWA. With the perm-selective properties of the PEM substrate with the catalytic activity of MONP this composite material can serve as a multi-functional barrier against dangerous organic compounds.
Poster Session

Biomedical Engineering

1. Maria Quadri
   Monitoring Cerebrovascular Systems After Traumatic Brain Injury
   Maria Qadri, Nam H Kim, Michael Wininger, Shabbar Danish, William Craelius
   Department of Biomedical Engineering

   Post-severe traumatic brain injury monitoring focuses on identifying elevated intracranial pressures (ICP) that indicate cerebrovascular-autoregulation failure and loss of tissue oxygenation. Our goal is to develop metrics that better capture current ICP behavior and predict future ICP hypertension thereby improving patient outcomes. Previous research shows phase domain analysis of cyclical waves increases discrimination that is imperceptible in the time domain. Therefore, we have developed a single measure of ICP cycle regularity using phase plane analysis - the phase area ratio (PAR). We will show the development and testing of PAR on clinical data and correlation to incidents of ICP hypertension.

Chemical and Biochemical Engineering

2. Vyshnavi Karra
   Self-Aggregation of Nanoparticles Functionalized with Homopolymers: A Simulation Study
   Vyshnavi Karra¹, Sarah Libring², Leebyn Chong¹, & Meenakshi Dutt¹
   ¹Department of Chemical and Biochemical Engineering
   ²Department of Biomedical Engineering

   We used coarse-grained molecular dynamics to model and simulate the aggregation of CPMV capsids decorated with PEG. Additional variations of
the system includes changing the polymer density on the capsids and the capsid volume fraction, to show how these changes affect the self-assembled structures. We analyzed the systems to find the overall shape of the clusters, via size, coordination number, radius of gyration, and the moments of inertia. Our observations suggest that (a) the excluded volume of the capsids and (b) the polymer density on the capsids play the largest role on the aggregation dynamics.

3. Amanda Okonmah

TiO$_2$ P25 Composition Analysis via Absolute Reflectance Derivative Peak Fitting

Amanda I. Okonmah, Ashley M. Pennington, Fuat E. Celik

Department of Chemical and Biochemical Engineering

Degussa (P25) is a very popular metal oxide, semi-conductor, photocatalyst used in industry. P25 is a fumed catalyst with a composition of anatase to rutile, three to one respectively. As a result of its ability to absorb energy from the ultraviolet region, P25 is of particular interest when discussing topics concerning photocatalysis. The diffuse reflectance of P25 and various altered P25 samples was measured by the use of UV-visible Spectroscopy. The resulting data was used to calculate the absolute reflectance and then the first derivative of the absolute reflectance, with a Spectralon® disk as the absolute reflectance. By analyzing the first derivative of the absolute reflectance, via the use of derivative peak fitting fityk software, the amount of rutile and anatase present in each representative TiO$_2$ P25 sample is quantified through the determination of the response factor of the two polymorphs. From this quantification it is possible to determine the effect that sieving, grinding, and calcination have on the composition of P25 with a relatively simple and available technique.
4. Rachel A. Yang  
Synthesis of Hydrogen Annealed TiO₂ for Photocatalytic Production of Sustainable Fuels  
Rachel A. Yang, Ashley M. Pennington, Fuat E. Celik  
Department of Chemical and Biochemical Engineering

Hydrogen gas is considered a source of green energy due to its clean emissions. However, about 95% is produced from unsustainable, exergonic processes like methane steam reforming or coal gasification. This project focuses on the synthesis, characterization, and photocatalytic activity of hydrogen-annealed anatase phase TiO₂ nanoparticles. TiO₂ is stable under catalytic conditions and due to its large bandgap of 3.2 eV, has high photocatalytic activity under irradiation. We reduce this large bandgap to incorporate the visible light range by inducing oxygen vacancy defects in the TiO₂ structure via annealing anatase under hydrogen in high temperature and pressure conditions. This contributes to the formation Ti³⁺ centers which can form donor levels in electronic structure and affect the charge recombination process, both of which influence the reactivity of TiO₂ in photocatalytic applications. By using sustainable feedstocks such as biomass or landfill derived methane, and increasing photocatalytic efficiency, we increase the sustainability of hydrogen gas production.

5. Katelyn A. Dagnall  
Characterization and Photocatalytic Activity of Low Pressure Flame Synthesized TiO₂ Nanoparticles for H₂ Production  
Katelyn A. Dagnall, Ashley M. Pennington, Fuat E. Celik  
Department of Chemical and Biochemical Engineering

Hydrogen gas has great potential for use in fuels and industrial applications, but it is currently produced from steam reforming of unrenewable natural gas. An alternative source of hydrogen could be accessed from the reforming of sustainably-grown biomass through photocatalysis. Titanium dioxide (TiO₂)
is a metal oxide semiconductor of particular interest in photocatalysis due to its activity under ultraviolet illumination and its stability under catalytic reaction conditions. Anatase and rutile phase TiO$_2$, with band gap energies (BGE) of 3.20 eV and 3.03 eV respectively, absorb energy in the UV region. Since a much larger fraction of solar irradiation is in the visible range, we aim to synthesize TiO$_2$-based photocatalysts with a BGE small enough to absorb energy from visible light. Through low pressure flame synthesis using a titanium (IV) isopropoxide precursor we have synthesized carbon doped TiO$_2$ nanoparticles with BGE smaller than 3.0 eV. XRD analysis indicated crystalline samples with a particle size of less than 10 nm. SEM imaging revealed elongated morphology. These characterizations indicate high surface area samples which we hypothesize to be photoactive under UV and visible light irradiation. The photoactivity of the flame synthesized TiO$_2$ was assessed for conversion of methanol under UV and visible light.

6. Nicole Zougheib

Theoretical investigation of the degradation pathway of phosphorus containing nerve agents on metal oxides
Nicole Zougheib, John Landers, Alec Hook, Alexandar V. Neimark, Fuat E. Celik

*Department of Chemical and Biochemical Engineering*

The mechanism for the decomposition of chemical warfare agents (CWA), particularly those classified as nerve agents, is investigated. It is experimentally known that metal oxides are capable of decomposing nerve agents. To date, however, a detailed mechanistic study revealing the path of degradation is lacking. The focus of this project is to investigate the different surface planes of zinc oxide as a catalyst for hydrolysis of phosphorus-containing agents and their simulants. In this study, the molecule POH$_3$, whose phosphorus containing functional group PO is incorporated in most nerve agents, is used as a starting point of interaction. In order to reveal the bonding nature with zinc oxide four different adsorption sites were chosen.
and include the top, bridge, hole-site, and off-site of zinc oxide. Binding energies were obtained by employing density functional theory (DFT), using the commercially available software VASP. It is predicted that the results obtained here will not only provide a mechanistic insight towards degradation, but aid in the future development of more efficient catalyst against CWA’s.

**Computational Biology and Molecular Biophysics**

7. Pamela J. Perez  
DNA Loops Mediated by Lac Repressor Protein Binding: Understanding the effects of sequence length, anisotropic bending and twist on DNA looping propensities.  
Pamela J. Perez, Wilma K. Olson  
*Department of Chemistry & Chemical Biology, Center for Quantitative Biology, Rutgers University*

DNA looping is often employed as method of regulating gene expression. Here we explore the influence of DNA sequence length, helical repeat and modes of deformation on the ease of loop formation by binding to the Lac repressor protein. We employ a novel approach to obtain minimum energy looped structures whereby the potential energy of elastic deformation is optimized. We examine the effects of preferential bending of the double helix into the grooves coupled with the local twist on the computed looping propensities. This approach allows us to identify the energetically preferred spatial pathways of varying length, protein-anchored DNA fragments.
8. Parneet Kaur  
From Photography to Microbiology: Eigenbiome Models for Skin Appearance  
Parneet Kaur, Kristin J. Dana, Gabriela Oana Cula  
Department of Electrical and Computer Engineering

Skin appearance modeling using high resolution photography has led to advances in recognition, rendering and analysis. Computational appearance provides an exciting new opportunity for integrating macroscopic imaging and microscopic biology. Recent studies indicate that skin appearance is dependent on the unseen distribution of microbes on the skin surface, i.e. the skin microbiome. While modern sequencing methods can be used to identify microbes, these methods are costly and time-consuming. We develop a computational skin texture model to characterize image-based patterns and link them to underlying microbiome clusters. The intersection of appearance and microbiome clusters reveals a pattern of microbiome that is predictable with high accuracy based on skin appearance.

9. Yanbiao Pan  
Organic Micro-Electro-Mechanical Relays for Ultralow-Power Flexible Transparent Large-Area Electronics.  
Yanbiao Pan, Jaeseok Jeon  
Department of Electrical and Computer Engineering

Organic thin film transistors (OTFTs) developed to date are subject to the following limitations: Low field-effect carrier mobility of the active layer requires rather large supply voltage (typically > 10 V) for reasonable on/off current ratio; Poor semiconductor/dielectric interface induces large off-state leakage current. Large Leakage and VDD lead to large static and dynamic power consumption. To overcome the limitations and enable ultralow-power
flexible large-area electronics, we propose organic micro-electro-mechanical (MEM) relay as alternative since its unique switching characteristics such as zero leakage and abrupt on/off switching can provide zero static power consumption and potentially very-low dynamic power consumption.

10. Mehrnaz Tavan

MobilityFirst: Ad hoc networking
Mehrnaz Tavan, Roy D. Yates, Dipankar Raychaudhuri

*Department of Electrical and Computer Engineering*

Growing popularity of smartphones and wide availability of vehicles with networking capabilities have increased the market demand for more reliable and disruption free access to Internet. In this work, we combine the urban Internet infrastructure with peer to peer transfer of data to provide a simple yet novel VANET protocol for improving Internet connectivity based on named object architectures. We form stable clusters of vehicles with similar movement patterns where stability and low-latency Internet connectivity are the main criteria for forming clusters. By implementing modifications to the transport protocol designed for named object architectures, we improve the data transfer reliability. This improvement are achieved by leveraging the storage capability of routers and adding delay tolerant network features to our clustering protocol.

11. Tianjiao Zeng

On the Relationship Between Trial-to-Trial Response Time Variability and fNIRS-Based Functional Connectivity
Tianjiao Zeng; Li Zhu; Yunqi Wang; Laleh Najafizadeh

*Department of Electrical and Computer Engineering*

This study explores the neuronal mechanisms underlying trial-to-trial variability (TTV) when performing a visual oddball task. TTV is measured here by response time (RT). We hypothesize that variability in the functional
connectivity (FC) is related to the variability in RT across trials. To test this hypothesis, we estimate FC map using wavelet transform coherence based on fNIRS data and perform a variety of statistical tests to identify the relationship between FC (across channels and across major brain regions) and variability in RT. A statistically significant correlation is observed between RT and FC across prefrontal and visual regions.

**Industrial and Systems Engineering**

**12. Ke Sun**

An Integrated Dynamic Flow Model for Supply Chain Risk Analysis
Ke Sun, James T. Luxhøj

*Department of Industrial Engineering*

A supply chain is an integrated system with dynamic flows of capital, goods, information and people. A Dynamic Bayesian Network (DBN) offers a solution that enables a time-dependent systemic risk analysis. However, the study is constrained by the separation of risk models and dynamic flows in a supply chain. System Dynamics (SD) is a simulation tool that specializes in modeling forward flows and feedbacks in a complex socio-technical system. By utilizing the essence of DBN and SD, my research proposes a Dynamic Flow Bayesian Network (DFBN) to offer a comprehensive methodology for supply chain risk analysis.
13. Jonathan Shi

Optimization of A Low Pressure Flame Synthesis Apparatus
Jonathan Shi¹, Mustafa M. Moazel², Ashley M. Pennington¹,
Stephen D. Tse²

¹Department of Chemical and Biochemical Engineering
²Department of Mechanical and Aerospace Engineering

Synthesizing various TiO₂ polymorphs using low pressure flame synthesis requires the apparatus to be set to specific parameters to synthesize quality, reproducible products. The pre-optimized set up produced sample, but the method used for this synthesis was limited by the subjectivity of human observation and skill. Further, the controls were too coarse for the sensitivity of the experiment. Therefore, we aim to reduce the amount of rough estimation and incorporate fine adjustments. This project optimizes the apparatus such that reproducible and high quality products can be produced, which in turn will provide a higher quantity of successful experiments. The optimization entails adding fine tuning controls, like needle valves, and designing a coupler for the ignition mechanism. With each new implementation, we find that the apparatus becomes less subjective to human error while providing more consistent results.
Thank you for supporting SWE GRAD at Rutgers University!

If you would like any further information, please contact Ashley Pennington (President) at Ashley.Pennington@Rutgers.edu or Ingrid Paredes (External Vice President) at ingpar93@gmail.com

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