Poster Presentations
(Listed by presenting author.)

1. **Arneja, Abhinav**, Yaakov Nahmias, David J. Odde
   *Cell Spraying Techniques for Directed Capillary Formation and Applications in 3-D Tissue Engineering*
   Summer Sponsor: Biomedical Engineering
   Abstract: The successful incorporation of capillaries in engineered tissue is a major challenge in the field of Tissue Engineering. We found that the culture of Endothelial Cells on soft collagen gels (0.75mg/ml) resulted in the formation of capillary like structures, which were absent on the culture of HUVECs on hard collagen gels (3.0mg/ml). Suspension of HUVECs sprayed onto a collagen gel (2.0mg/ml) resulted in viable cells, which were maintained in culture for at least 3 days. We are attempting to spray HUVECs through masks containing 10-100 micrometer wide slits to obtain a specific pattern. The development of direct writing approaches such as Cell Spraying and Laser Guidance offer novel and promising methods to make successful 3-D tissue engineering a feasible goal in the near future.

2. **Anderson, Amelia**, Brian Holmes, Michael Ward
   *The Design and Synthesis of Oligothiophene Substituted Semiconductors*
   Summer Sponsor: Clemson REU/MRSEC
   Abstract: The objective of this research project is the synthesis of organic molecules that will crystallize into packing motifs considered optimal for high performance in thin film field effect transistors (FETs). The primary synthetic targets will be oligothiophenes equipped with phenyl substituents at the termini that serve as "molecular clamps" capable of optimizing π–π overlap of oligothiophene cores in the crystalline state. Single crystals of these targets will be characterized by X-ray diffraction to elucidate the role of the molecular clamps in crystal packing. Materials for mobility measurements will be identified based on important crystal attributes, including small interplanar separations between the oligothiophene cores and a propensity to form plate-like crystal habits that will naturally form thin film morphologies in the FET platform.
3. **Arrechea, Pedro, Dr. Johnson, Marc Hillmyer**  
*Water Compatible Ordered Nanoporous Polymers from Block Copolymer Blending*  
Summer Sponsor: MRSEC  
Abstract: Nanoporous polystyrene monoliths have been prepared from polystyrene-polylactide (PS-b-PLA) block copolymers that form hexagonally packed nanocylinders of PLA in a PS matrix. The ability to uptake methanol into these pores has been demonstrated in previous publication. Due to the hydrophobic nature of PS, the pores are not accessible to many aqueous solutions. In this work, hydrophilic polyethylene oxide (PEO) has been incorporated onto the pore walls of the nanocylinders via blending of PS-b-PLA with PS-b-PEO. Removal of the PLA via hydrolysis of the polyester bonds gives pores with the ability to uptake pure water.

4. **Awde, Matt, L. E. Scriven**  
*Are Mismatches Unavoidable in Laminating?*  
Summer Sponsor: CEMS  
Abstract: Lamination, a common post-coating operation, in which two continuous flexible webs, at least one bearing an adherend layer, are pressed together while passing though the nip of two counter-rotating rolls. They become a multilayer composite once the adhesive cures or dries. Curling and cupping are unwanted after-effects due to the non-uniform in-plane stress that would exist across the thickness of the composite if it were flat. Basic elements of the elasticity of thin plates lead to the hypothesis that perfect matching to avoid variation of in-plane stress across a laminate’s thickness is impossible except in circumstances that the two webs are identical, under the same tension, and wrap their rolls equally at the nipentry.

5. **Bailey, Jaclyn, Dr. Timothy M. LaPara, Dr. R. Lee Penn**  
*Reduction of Synthetic Iron (III) Oxides by Shewanella oneidensis MR-1*  
Summer Sponsor: Chemistry - Lando  
Abstract: Microbial reduction of synthetic iron (III) oxides was studied using the dissimilatory metal reducing bacterium *Shewanella oneidensis*, strain MR-1 (ATCC 700550). Experiments investigated whether application phase (solid vs. liquid suspension) or particle size affected the susceptibility of goethite ([FeOOH]) to biotransformation. The influence of crystallite order, particle morphology, and substitution with the aluminum (III) metal cation on goethite reduction was also studied. Incubations were performed anaerobically with lactate supplied as the electron donor. The rate of goethite reduction was measured as a function of lactate consumption over time by high performance liquid chromatography (HPLC). Analysis revealed that liquid suspensions of the goethite particles, rather than applications of dried, solid-state particles, were more susceptible to biological reduction.
6. **Bovum, James, Michael T. Bowser**  
*Capillary Electrophoresis-Laser Induced Fluorescence Assay for Zinc Using a Fluorogenic Indicator*  
Summer Sponsor: Chemistry - Lando  
Abstract: Recent work in neurochemistry suggests that zinc plays a key role in brain function. It has been hypothesized that zinc is co-released with glutamate in the forebrain, acting as a neuromessenger. In this study, zinc was labeled with the high affinity fluorogenic dye Fluozin-3, which fluoresces when bound to zinc. Zinc that formed a complex with Fluozin-3 was separated from excess indicator by capillary electrophoresis. Separating the zinc complex reduces background fluorescence contributed by excess Fluozin-3, which should yield lower limits of detection. A fluorescence calibration based on varying zinc concentrations in HEPES buffer was generated. In the future, this assay will be used to monitor extracellular zinc dynamics in neuronal samples.

7. **Breid, Derek, Matt Panzer, C. Daniel Frisbie**  
*Poly(3-hexylthiophene) as an Organic Semiconductor in Thin-film FETs*  
Summer Sponsor: MRSEC  
Abstract: Poly(3-hexylthiophene) (P3HT) is currently a leading candidate for use in organic field-effect transistors (FETs), due to its relatively high charge mobility and flexibility. It can be easily applied by spin-coating a solution onto the substrate. Our research focused on creating a suitable thin film of P3HT, building a FET with P3HT as the semiconducting layer, and attempting to incorporate gold nanoparticles into this layer.

8. **Bulfer, Stacie, Carmen Silvers, Karin Musier-Forsyth**  
*Characteristics of Deinococcus radiodurans Proline-tRNA Synthetase in Amino Acid Editing*  
Summer Sponsor: Chemistry – Lando  
Abstract: Aminoacyl-tRNA synthetases ensure accurate translation of the genetic code by catalyzing a two-step reaction where a specific amino acid is attached to its cognate tRNA. To maintain high accuracy during translation, some aminoacyl-tRNA synthetases have developed editing mechanisms where errors resulting in misactivated amino acids or misaminoacylated tRNAs are corrected. In this work, we begin to investigate the editing ability of Deinococcus radiodurans proline-tRNA synthetase (ProRS). This enzyme was overexpressed in bacteria, purified using affinity chromatography, and shown to be active in amino acid activation. The results of pre and post transfer editing assays will be presented.

9. **Chellappan, Annapoorani, Mauris DeSilva, Dr. David Odde, Dr. Peter Steinmetz**  
*The effect of varying the size and surface coatings of magnetic beads during neurite initiation using Magnetic Bead Force Application (MBFA)*  
Summer Sponsor:  
Abstract: The technique of magnetic bead force application is used to investigate the role of force during force-induced neurite initiation. Force-induced neurite initiation from embryonic chick forebrain neurons seems to be affected not only by the amount of force
applied, but by the size of the magnetic beads and the surface coatings of the beads as well. Previous work has shown that 4.5 µm magnetic beads coated with anti-integrin could initiate and elongate neurons. The goal of this project is to reduce the size of the magnetic beads, and vary the surface coatings of the beads to observe the effect on initiation. Results have shown that fewer neurites initiated when the bead size was reduced to 2.8 µm and the surface coating was changed to laminin. Thus, it can be concluded that the 4.5 µm magnetic beads coated with anti-integrin are the optimal conditions investigated so far for neurite initiation.

10. Clark, Christopher, Wayland E. Noland

Synthesis of 7-Methylbenzofurazan 1-Oxide (5)

Summer Sponsor: Chemistry - Wayland E. Noland Research Fellowship Fund

Abstract: For purposes of X-ray crystallographic studies, a synthesis of 7-methylbenzofurazan 1-oxide (5) was undertaken. Commercially available 3-methyl-2-nitrobenzoic acid (1) is first converted to the ammonium salt (2) by evaporation with NH₄OH followed by evaporation to dryness. Thermal elimination of water formed 3-methyl-2-nitro-benzamide (3). A Hofmann rearrangement on the amide (3) with calcium hypochlorite gave the amine, 3-methyl-2-nitroaniline (4). A heterocyclic ring closure is then accomplished with a sodium hypochlorite oxidation of the amine to form 5.
11. **Copp, Laura, Kwanho Chang, Chris Macosko**  
*Effect of the Addition of Poly(isoprene-b-dimethylsiloxane) on the Interfacial Tension of Polyisoprene/Poly(dimethylsiloxane) Blends*  
Summer Sponsor: MRSEC  
Abstract: The effect of poly(isoprene-b-dimethylsiloxane) on the interfacial tension of an immiscible polymer blend of polyisoprene and poly(dimethylsiloxane) homopolymers was investigated. A PI drop will be added to a PDMS matrix containing P(I-b-DMS), in an attempt to simulate equilibrium between the PI and PDMS polymers. A spinning drop tensiometer will be used to calculate the interfacial tension as the concentration of block copolymer in the tertiary system is varied. It is expected that the interfacial tension will approach zero when the proper concentration of P(I-b-DMS) is added if the system is in pseudo-equilibrium state, assuming that the concentration of block copolymer is less than the critical micelle concentration.

*Kinetic Analysis and Comparison of Single-Site Aluminum Alkoxide Catalysts*  
Summer Sponsor: Chemistry – Lando  
Abstract: The goal of this project is to determine whether electron withdrawing groups, electron donating groups or both would increase the rate of polymerization of ε-caprolactone on single site aluminum catalysts. The other aspect of this project is to determine whether each catalyst reacts by the same mechanism to support that a comparison between electrophilicity of substituents and rates of polymerizations is logical. Aluminum complexes were made using the bis(phenolato)-bis(amine) (R1,R2BPBA) ligand framework and an isopropoxide initiator keeping the R1 group constant and substituting different groups in for R2. Substituents used included hydrogen, bromine, methoxy, and t-butyl groups.

13. **Ellis, Afton, Victor Barocas**  
*Generation and Evaluation of Collagen Fiber Network Models*  
Summer Sponsor: MRSEC  
Abstract: The basis of many different types of tissues is formed by collagen fiber networks. Specific examples include tendons, skin, ligaments, cartilage, and fetal membranes. Artificial collagen networks are important as potential tissue replacements. In order to repair a damaged network or create an artificial network, we must first understand the structure. We will develop a computer program to evaluate the properties of the fiber networks and compare them to actual collagen gel networks. We will generate collagen fiber network models by various algorithms and determine which models best match the actual networks. The selected model can then be used as a standard for studying the properties of tissue equivalents.
14. **Embry, Bethaney, Angela DeGreeff, Kristopher McNeill**  
*Synthesis of chlorovinyl cobalt compounds*  
Summer Sponsor: Chemistry – Lando  
Abstract: Perchloroethylene (PCE) and trichloroethylene (TCE), which are used as dry cleaning and industrial degreasing solvents, respectively, are commonly found environmental water pollutants. Vitamin B12 has been found to break down this class of chlorinated ethylenes, although the mechanism of decomposition is not fully understood. This research has utilized cobalt porphyrins as model compounds in which to study this process. Specifically, cobalt tetraphenylporphyrin was used to synthesize chlorovinyl cobalt compounds, which have been proposed as intermediates in the reaction pathway. These compounds will be used to examine the role of organometallic intermediates in the vitamin B12 dechlorination of chlorinated ethylenes.

15. **Ertel, Ethan, Eric Cochran, Frank Bates**  
*Mechanical Testing of Shear Aligned PC-PE\textsubscript{E}-PE Block Copolymer in the O\textsuperscript{52} Morphology*  
Summer Sponsor: MRSEC  
Abstract: This research investigates the mechanical properties of a PC-PE\textsubscript{E}-PE block copolymer that microphase separates into the O\textsuperscript{52} network morphology. Copolymers are known to combine the mechanical properties of their homopolymers in a number of different ways. We combine glassy PC, semi-crystalline PE and PE\textsubscript{E} rubbery blocks. Anionic synthesis and subsequent hydrogenation produced PC-PE\textsubscript{E}-PE with composition of 0.25-0.5-0.25, respectively, as confirmed by light scattering and NMR. Dynamic mechanical analysis determined order-order and order-disorder transition temperatures. Samples were formed by hot pressing. These samples were shear-aligned under varying shear conditions, resulting in long-range order. Small angle x-ray scattering confirmed sample crystal structure and alignment. Tensile bars were cut and tested for each axis of the crystal unit cell.

16. **Field, Christopher, J. Ilja Siepmann**  
*A Computational study of the Absorption of a Variety of Alkanes and Alcohols onto an Amorphous Silica Surface*  
Summer Sponsor: Chemistry – Lando  
Abstract: Gibbs Ensemble Monte-Carlo simulations were conducted for the absorption of a variety of alkanes and alcohols onto an amorphous silica surface. To establish an appropriate silica surface the potential proposed by van Beest et al. (BKS) was used. Once the silica surface was equilibrated, the absorption energy for a variety of alkanes and alcohols was calculated using the transferable potentials for phase equilibria-united atom (TRAPPE-UA) force field and compared to experimental results. It was found that the Monte Carlo (MC) simulations compared relatively well with the experimental data for simple alkanes and alcohols. Based on the relative accuracy of the Monte Carlo simulations for simple molecules it is then possible to calculate the absorption energy for more complex compounds.
17. **Glawe, Brett**, Aimee R. Erickson, T. Andrew Taton  
*Developing Crosslinked Gold Nanoparticles for DNA Sequence Detection*  
Summer Sponsor: Chemistry – Lando  
Abstract: DNA-modified gold nanoparticles have been used to detect specific DNA sequences, and could be applied to diagnosing genetic and pathogenic diseases. However, nanoparticle-bound oligonucleotides dissociate from nanoparticle surfaces under commonly encountered biological conditions like high temperature and disulfide-containing reagents. We have investigated the hypothesis that chemically crosslinking these oligonucleotides binds them more permanently to nanoparticle surfaces. One method is to synthetically incorporate a crosslinkable functionality into the oligonucleotides. Another route involves functionalizing nanoparticles with a pre-modified crosslinkable polymer, which is subsequently connected to oligonucleotides. We report data of new gold surface chemistry with potential for increasing nanoparticle stability by creating a crosslinkable shell around the nanoparticle.

18. **Hang, Ta-Chun**, Koby Nahmias, David Odde  
*Developing Assays for Visualization of Capillary Tube Formations in Endothelial Cells*  
Summer Sponsor: Biomedical Engineering  
Abstract: During angiogenesis, cells undergo a drastic change in their shape. The cytoskeleton plays an important role in this process. A study was planned to examine the microtubule dynamics during capillary network formation in endothelial cells. Using human umbilical vein endothelial cells (HUVECs) and microvascular endothelial cells (MVECs), different visualization techniques were tested to optimize the goal of imaging the cytoskeleton during angiogenesis. To aid in this process, phorbol ester is applied to accelerate and induce capillary formation within 10 hours of introduction to the cells. We hope to understand the mechanism of endothelial cell tubulogenesis in terms of its cytoskeleton rearrangements, as well as when it is artificially stimulated. These results will hopefully contribute to creating more complex bioartificial organs in tissue engineering.

19. **Hiller, Alex**, Chris Leighton  
*Dependence of Exchange Bias on Annealing Time in Ni$_{50}$Mn$_{50}$/Ni$_{80}$Fe$_{20}$ Thin Film Bilayers*  
Summer Sponsor: MRSEC  
Abstract: Our research entailed investigating the hysteresis loop, exchange bias and coercivity as a function of annealing time and temperature in NiMn/NiFe, antiferromagnetic (AF)/ferromagnetic (F) bilayers. Bilayers such as these are used in the magnetic recording industry in “state-of-the-art” read heads. Annealing is required to transform the NiMn from the as-deposited non-magnetic face centered cubic (fcc) phase to the AF face centered tetragonal (fct) phase. We have discovered that a balance exists between annealing aggressively (to completely transform the fcc phase to fct) and restricting the growth of an interdiffused layer at the interface.
20. **Hosokawa, Ayako, Ben Duckworth, Mark Distefano**  
*Synthesis of a cysteine reactive selenium containing reagent for the construction of a protein-based epoxidation catalyst*  
Summer Sponsor: Chemistry  
Abstract: Preparation of enantioselective catalysts is a very challenging topic in modern synthetic chemistry. Here, we have developed the strategy of designing selective reaction catalysts by synthesizing various cysteine reactive conjugation reagents. These catalytic molecules position specifically inside the protein cavity made up of two orthogonal â-sheets and link to the protein via a disulfide bond. The preparation of artificial epoxidation catalyst from 4-amino-DL-phenylalanine and its conjugation to the previously purified two possible proteins, IFABP (Intestinal Fatty Acid Binding Protein) V60C and Helixless, is done by taking advantage of the catalyst's resioselective characteristic that will be described. Further, these experiments will enable us to control the reaction catalysts by position as well as stereochemistry.

21. **Husby, Daniel, Nagalingam Balakrishnan, David Norris**  
*Synthesis of Planar Synthetic Opals*  
Summer Sponsor: MRSEC  
Abstract: Currently semi conductors are used in computer and communication networks. As this technology begins to reach its useful limit, photons are one possible future. This future technology will require a photonic material much the same way electronics sought the semi conductor. One possible solution is the photonic crystal, a synthetic crystal where the “atoms” are nearly one thousand times larger than in conventional crystals. Also of interest is the fact these solids are nanostructured on an optical length scale. Diffraction can cause the propagation of light to be modified within the material. Thus, photonic crystals hold great promise for revolutionizing the current electronics industry, possibly enabling optical integrated circuits. To fabricate photonic crystals we will follow a two step procedure. The first step involves formation of synthetic opals, which will be used as the template from which silicon inverse opals (photonic crystals) will be formed. We will prepare the template from silica spheres, these spheres are formed by reacting ethanol, water, ammonium hydroxide and tetraethylorthosilicate. The amount of each chemical controls the size of spheres obtained. We will explore these chemical combinations to improve the quality of the silica spheres. Through particle analysis the size of the spheres will be determined. The second step involves the actual formation of photonic crystals. A substrate is placed into the suspension of silica spheres. Under the proper conditions evaporation leads to deposition of an opal of uniform thickness. This material is the eventual goal of the project. The anticipated results from our methodology quite simply are a large quantity of high quality planar opals. These planar opals can then be used to create high quality inverse opals (photonic crystals). Our fellow researchers will then have enough raw materials to further their own experiments. Thus furthering the cause of photonics in future technology.
22. **Johnson, Brandon, Dr. Eric Brown, Prof. Bill Tolman**  
*Modeling the Catalytic Site of Nitrous Oxide Reductase*  
Summer Sponsor: Chemistry  
Abstract: Nitrous oxide reductase (N2OR), an important metalloprotein involved in the global nitrogen cycle, is responsible for catalyzing the two-electron reduction of nitrous oxide to dinitrogen. The catalytic site of N2OR consists of four copper atoms bound to a tetrahedral $\mu$-sulfide; a structure unique in Nature. Our progress towards the synthesis of synthetic model complexes, which mimic the structural arrangement, spectroscopic properties and reactivity of the active site, will be presented. Specifically, we will describe the design and synthesis of various N-donor ligands capable of forming tetranuclear copper-sulfide clusters similar to the active site in N2OR.

23. **Lange, Brandon, Jizhou Wang, Chris Jeffrey, Thomas R. Hoye**  
*An Introduction to the Hoye Lab: The Epoxidation of Geraniol*  
Summer Sponsor: Chemistry – Lando  
Abstract: New researchers entering the Hoye laboratory are encouraged to perform the epoxidation of geraniol on a small scale (1.0 mg), using less than two equivalents of m-chloroperoxybenzoic acid (MCPBA), to separate the epoxide products, and to characterize them by GC/MS and 1H NMR spectroscopy. My experiences with this initiation will be presented.

**Synthesis of Relay Ring Closing Metathesis Precursors**  
Abstract: Relay ring closing metathesis (RRCM) is being explored in the Hoye laboratory in order to create cyclic alkenes that are difficult to synthesize using standard olefin metathesis strategies. Various relay precursors have been synthesized (~three steps) and different reaction conditions have been evaluated in the course of comparing the RCM of relay vs. non-relay substrates.

24. **Leas, Jill, Ahren Jasper, Shikha Nangia, Donald Truhlar**  
*A Comparative Study of the Photodissociation of LiFH and NaFH van der Waals Complexes*  
Summer Sponsor: Chemistry – Lando  
Abstract: We have used semiclassical methods to model the photodissociation of M$\text{H}$$\text{F}$, where M is either Li or Na, and "$\text{H}$$\text{H}$" indicates a weak van der Waals interaction. The system is vertically excited from the ground state van der Waals well, which forms MF$\text{H}$* (termed the exciplex). The "$\text{H}$" indicates that the complex is electronically excited. The exciplex can decay by one of two pathways: a "harpooning" process, which results in the formation of MF and H; and a quenching process, which results in the formation of M and HF. In this second process, the vibrational and rotational modes of HF have been excited. It is hoped that experimental results will soon be available for comparison.
25. Lynch, Jenny, Mark Nicosia
   Mechanical Properties of Isolated Porcine Esophageal Tissue
   Summer Sponsor: MRSEC
   Abstract: Fundamental understanding of the behavior of the muscle tissue in the esophagus can be a valuable and useful tool to determine better cures for such diseases as gastroesophageal reflux, i.e. heartburn. The goal of the research is to develop insight into the esophageal muscle mechanics. The esophagus is composed of two distinct types of muscle: circular and longitudinal. These types of muscle tissue will be tested both separately and together using uniaxial and biaxial testing. The stretch of the muscle tissue on each axis will be closely monitored along with the load and displacement to determine the mechanical properties.

26. Maciejewski, John, Mamoun Bader, C. Daniel Frisbie, Michael Ward
   Synthesis, Purification, and Characterization of New Crystalline Organic Semiconducting Materials
   Summer Sponsor: MRSEC
   Abstract: Functionalized derivatives of triphenodithiazine (TPDT), n-thiophene, and n-ethylenedioxythiophene (EDOT) will be synthesized, characterized, and tested in Thin Film Transistor (TFT) applications. Electronic applications involving TPDT are severely limited due to its insolubility in common organic solvents. To remedy this problem, a procedure to functionalize TPDT has been developed. It is believed that these functional groups will not only improve solubility, but increase uniformity in π-π stacking in the solid state. End substituted (and un-substituted) thiophene/EDOT oligomers will be more deeply investigated for their electronic properties. Oligo-thiophenes are especially versatile since the number of repeat units (n) can be modified through multi-step syntheses. By working with the Suzuki, Stille, Heck, and Grignard reactions, new novel thiophene compounds incorporating the EDOT molecule are anticipated to be produced.

27. Massich, Matthew, Thomas Marsh, C. Dan Frisbie
   Development of a Nanometer Scale Wire Using G-DNA
   Summer Sponsor: MRSEC
   Abstract: G-DNA is a quadruple helix composed of guanine tetrads called G-quartets, and is stabilized by metal cation coordination. The purpose of this study is to create a nanometer scale wire using G-DNA as a scaffold element. Tet1.5 [GGGGTTGGGG] and amino and thiol modified sequences will be allowed to self-assemble into long strands of G-DNA called G-wires. The G-wires will be doped with gold particles via biotin streptavidin interactions. The gold particles tethered to the G-wire scaffold will nucleate the deposition of silver particles, forming a nanometer scale wire. Atomic force microscopy, AFM, will provide images of the self-assembled nanoscale structures.

28. McKusky, Gregory, Ambrose Wolf, E. Dan Dahlberg
   Study of Fe/ FeO bi-layers on MgO
   Summer Sponsor: MRSEC
   Abstract: Ferromagnetic (F) Fe and anti-ferromagnetic (AF) FeO layers were sputtered onto a magnesium oxide substrate to observe exchange bias in the Fe layer (F) caused by
the FeO layer (AF). Different argon and oxygen pressures were used to produce various grades of FeO. Fe$_2$O$_3$ and Fe$_3$O$_4$ do not display the necessary AF behavior. Measurements with the VSM proved to be in conclusive due to limitations in temperature control and field strength. However, the magnitude of the magnetic moment given by the VSM combined with thickness calibration results do indicate the successful growth of the Fe/FeO bi-layer. Measurements are underway using the SQUID in an attempt to observe exchange bias in the bi-layer system.

29. Milbridge, Nigel, Timothy Lodge  
*DSC of Glassy Mixtures*  
Summer Sponsor: MRSEC  
Abstract: The purpose of my research was to make polymer blends of various sorts and analyze them using a Differential Scanning Calorimeter (DSC). Several blends were made that ranged from solvent/solvent mixtures to high molecular weight polymer mixtures. These mixtures were made to help try and understand the relationship between two characteristics of the glass transition phase and the variation of molecular weight in these mixtures. The two aspects of the glass transition phase that we were looking at were the point of $T_g$ and the width of the transition phase itself. The point of $T_g$ is where the substance starts breaking apart, and loses its cohesive properties due to increase in kinetic energy.

30. Mohamad, Ahmad Kamal, Randy Mrozerk, T. Andrew Taton  
*Synthesis of a Liquid-Crystalline Poly(oxazoline) Monomer*  
Summer Sponsor: Chemistry  
Abstract: The purpose of the research was to investigate the effect of modifying the synthesis steps of dialkyloxazoline monomer which was reported in literature. This oxazoline monomer was synthesized with the intention of producing a liquid crystalline polymer (LCP) and composite materials with carbon nanotubes. The synthesis of 2-[3,4-bis(n-decan-1-yloxy)phenyl]-2-oxazoline began with a single-step synthesis of atrialkylated ester, with alkyl = C$_{10}$H$_{21}$, rather than via a multistep synthesis of a dialkylated ester. Macroscale synthesis was performed from about 20 g of trialkylated ester. A major problem was encountered in the macroscale while synthesizing $N$-[3,4-bis(n-decan-1-yloxy)benzoyl]-2-aminoethanol, and the obtained monomer yield was less than 50%. However, the purity of the monomer synthesized was comparable to that reported in the literature by comparing the $^1$H NMR of each product for each synthesis step. Reference: (1) Percec, V., Holerca, M. N., Magonov, S. N., et al, *Biomacromolecules* 2001, 2, 722-726.

31. Moore, Chris, Richard Thomas, David Caven, Jim Eckert, E. Dan Dahlberg  
*An Investigation of Exchange Interactions in AgMn Spin Glasses Using AC Susceptibility*  
Summer Sponsor: MRSEC  
Abstract: We measure the vertical AC susceptibility of AgMn samples in the spinglass state and compare our results to those obtained by similar experiments on AFM-FM bilayers. The samples are cooled to 4.2 K in a vertical magnetic field. This field is turned off, and the vertical AC susceptibility is measured as a function of horizontal applied
field. The observed behavior is similar to that seen in exchange-coupled AFM-FM bilayers.

32. Nash, William, Frank Hunte, E. Dan Dahlberg
*Determination of Exchange Anisotropy by ac-AMR and Planar Hall Effect*
Summer Sponsor: MRSEC
Abstract: Exchange anisotropy is an interfacial phenomenon resulting from the direct exchange coupling of a ferromagnet and an antiferromagnet. A basic understanding is lacking even though this exchange anisotropy has aided technological advancements in controlling magnetization in particular devices. We use Ta/Co samples grown on single crystal CoO orientated substrates by dc magnetron sputtering. We are attempting to use an alternative to the hysteresis loop technique while expecting to help lead to the enhancements of this phenomenon’s use in science.

33. Oehlke, Stephanie, Jeff Haley, Timothy Lodge
*Viscosity of Miscible Polymer Blends*
Summer Sponsor: MRSEC
Abstract: A central issue in polymer blend dynamics is determining how to predict the viscosity of blends given the viscosity of the individual polymers. Contrary to intuition, the blend viscosity is not simply the weighted average of the two components' viscosities. This research seeks to confirm or alter a recent model that makes blend viscosity predictions possible. For this research, a model miscible blend system of polystyrene (PS) and poly(vinyl methyl ether) (PVME) will be used, because viscosity predictions show unusual behavior. Several PS/PVME blend systems should provide a wide range of viscosity values, measured over a range of temperatures and compositions. Results are pending.

34. Orilall, Mahendra Chris, Dr. Ken Leopold
*A Study of Hydrogen-Bonded Systems*
Summer Sponsor: Chemistry – Lando
Abstract: Our research is based on the study of hydrogen-bonded systems. Three topics have been investigated recently. One, the observation of the microwave spectrum of DNO$_3$$^-$$^\text{H}_2$$O$$^-$$^\text{H}_2$$O$, is needed for the overall solution of the structure and internal dynamics of the HNO$_3$$^-$H$_2$O $^-$$^\text{H}_2$$O$ complex (currently an ongoing project). We have also used ab initio calculations to determine the theoretical structures of the isomeric forms of the NH$_3$$^-$HF $^-$$^\text{HCl}$ complex. These structures have indicated that NH$_3$$^-$HCl$^-$$^\text{HF}$ appears to be really NH$_4$$^+$-Cl $^-$$^\text{HF}$ (indicating proton transfer) while NH$_3$$^-$HF $^-$$^\text{HCl}$ appears to be a hydrogen-bonded complex. Currently, we are beginning an investigation of the dipole moments of NH$_3$$^-$HX complexes (where X= halide) via the Stark effect.

35. Rollings, Tedrick, C. Dan Frisbie
*Construction and Characterization of Organic Thin-Film Transistors*
Summer Sponsor: MRSEC
Abstract: The possibilities of the creation of new products have led to significant interest in the use of organic materials as semiconductors. With this in mind, a high mobility (approximately 1 cm$^2$/Vs) Thin Film Transistor will be constructed using an organic
material (Pentacene) of exceptional electrical properties. The process will be completed using various methods of deposition, including thermal evaporation for the metal electrodes and organic semiconductor, as well as chemical vapor deposition for the dielectric. Also, these films will be structurally characterized using Atomic Force Microscopy & X-Ray Diffractometry and the semiconductor itself will be electrically characterized by taking current voltage measurements.

36. Scroggins, Steven, Son Nguyen, Craig Forsyth
Synthesis of the second enantiomer of the C27-C40 fragment of azaspiracid
Summer Sponsor: Chemistry – Lando
Abstract: A synthesis of one enantiomer of the C27-C40 fragment of the marine toxin azaspiracid has already been reported. Researchers have determined that the structure containing the opposite enantiomer is the more likely form of the natural product. This summer's project included the synthesis of a precursor to the C27-C40 fragment using a procedure developed for the synthesis of the opposite enantiomer. S 1-OPMB 3,4 bisbenzooyl butanone was synthesized in a nine-step process from diethyl tartrate with a >20% yield. R 3-methyl 5-hexynal was synthesized in an eight-step process from methylglutaric anhydride with a >40% yield. The fragment synthesis was completed with a boron-mediated reverse aldol reaction joining these two molecules.

37. Sibbald, Paul, Dr. Paul Ewbanks, Dr. Kent Mann
Design, Synthesis, and Characterization of new materials for potential use as organic semiconductors
Summer Sponsor: Chemistry
Abstract: Recent years have seen a substantial increase in n-type organic semiconductor research. These organic semiconductors have certain advantages over their inorganic counterparts. One likely starting material for the syntheses of novel n-type semiconductors is 1-p-tolyl-2,5-di(2-thienyl)pyrrole (TTP), due to its extended \[\pi\]-conjugation. For example, tricyanovinyl-capped TTP may exhibit n-type properties. To this end, we have explored various routes of TTP synthesis and functionalization. The synthesis of 1,4-di(2-thienyl)-1,4-butanedione (DTB) was the first step in the production of TTP. Various routes for the synthesis of DTB were also explored. Several methods of characterization were employed, including NMR and mass spectrometry.

38. Sizova, E. P., R.P. Hsung
An intramolecular formal aza \([3+3]\) cycloaddition approach for synthesis of immunosuppressant FR901483
Summer Sponsor: Chemistry – Lando
Abstract: The unique intramolecular formal \([3+3]\) cycloaddition reaction developed by our research group uses vinylogous amides tethered with enal functional group to give complex piperidinyl heterocycles. We were drawn to the possibility that the azaspiro[4,5]decane nucleus of the powerful immunosuppressant FR901483 (1) may form during the course of this significant method (Scheme 1). To demonstrate the feasibility of this approach, a previously unknown vinylogous amide 2 and some of its derivatives were prepared through 11-linear steps pathway including Sonagashira
coupling as a key step. The construction of desired heterocycle was accomplished via an intramolecular formal aza [3+3] cycloaddition the iminium salt of 2.

Scheme 1

39. Sjulson, Justin, Joel Bell, Christopher W. Macosko
Mapping Chaotic Mixing Flows Using Computational Fluid Dynamics
Summer Sponsor: Supercomputing Institute for Digital Simulation and Advanced Computation
Abstract: Chaotic mixing of a polymer mixture is a requirement for the formation of a cocontinuous polymer morphology. Computational fluid dynamics provide a method to observe chaotic behavior in fluid systems. Simulations were performed in Fluent which is based upon solving the continuity and conservation of momentum equations with a CFDA (centered finite difference approximation) to many discrete control volumes in a complex geometry. Two systems were analyzed: a double-cylinder couette and a screw-type mixer. We mapped regions of chaotic mixing using both inert particle trajectories and animations of fluid velocity vector fields.

40. Spanton, Shantih, Matthew M. Evans, Jessica L. Hilton, Brian D. Schultz, Christopher J. Palmstrom
Interfacial Reactions and Determination of Diffusion = Coefficients and Activation Energies of Thin Film Mn on = GaAs(100)
Summer Sponsor: MRSEC
Abstract: Initial studies involved characterization of x-situ post-growth anneals of Al(50Å)/Mn(2000Å)/GaAs(100) structures at temperatures of 200-500ºC for 1-30 hours. X-ray Diffraction data for anneals above 200ºC, showed tetragonal Mn$_2$As-like and MnGa-like phases. Rutherford Backscattering spectrometry measurements indicated the formulation of a diffusion controlled Mn$_{0.6}$Ga$_{0.2}$As$_{0.2}$ reacted region. An Er marker layer between the GaAs and Mn layers, showed Mn to be the diffusive species. Once the value and nature of the diffusion coefficient was established, the activation energy of the n-Ga-As reaction was calculated. Knowledge of the activation energy, and thus diffusion rates, will allow for fabrication of Mn films on GaAs of known compositions and thicknesses at specific temperatures.
41. **Steiner, Kimberly, Alex Hiller, M.S. Lund, Chris Leighton**  
*Enhanced Coercivity in Epitaxial Fe/Cr (100) Bilayers: Caused by Cr SDW*  
Summer Sponsor: UROP  
Abstract: Fe/Cr multilayer systems have been studied extensively for GMR, however the system has not been examined for exchange bias. Fe/Cr bilayers have been fabricated using magnetron sputtering and characterized using X-Ray diffraction. The exchange bias and coercivity have been measured using SQUID magnetometry. The enhanced coercivity is thought to be caused by the Neil temperature and the Cr spin reorientation.

42. **Stokes, Jimmy, Karen Switek, Marc Hillmyer**  
*Formation of a High Density Polyethylene-Polycylcooctene Block Copolymer*  
Summer Sponsor: MRSEC  
Abstract: Many current biotechnological applications require mechanically anisotropic materials. That is, the material should be flexible in one direction, yet rigid in the other. However, these properties are rarely found in a single material. One possible path to anisotropic behavior in a single material is to form a block copolymer of polycyclohexylethylene (PCHE) and high density polyethylene (HDPE). Using ring opening metathesis polymerization (ROMP), a polycylooctene (PCOE) block can be inserted at the end of a double bond-functionalized polystyrene (PS) chain in the presence of the second generation Grubbs catalyst to form a diblock. After hydrogenation of PS and PCOE, the block copolymer consists of PCHE and HDPE.

43. **Stone, Doug, Pete Eames, Dave Dahl, E. Dan Dahlberg**  
*Magnetic Reversal In Nanoscopic Ellipsoidal Permalloy Dots*  
Summer Sponsor: MRSEC  
Abstract: The direction of magnetization of nanoscopic ellipsoidal permalloy dots can theoretically be reversed using a combination of a DC magnetic fields lightly smaller than the coercive field and a magnetic pulsed field along the hard axis of the particle. I have examined the properties of the magnetic pulse necessary to cause magnetic reversal through simulations using LLG Micromagnetics Simulator software. I have also studied magnetic reversal experimentally using arrays of permalloy dots created using Electron Beam Lithography. Preliminary experimental results are inconclusive but suggest that magnetic reversal depends on the duration of the magnetic pulse. Understanding how to control the direction of magnetization of these particles could be applied to the development of MRAM.

44. **Stotts, Corey, John A. Bumpus, Christopher J. Cramer**  
*Determination of Oxidation-Reduction Potentials of DDT Metabolites: A Computational Approach*  
Summer Sponsor: NSF RSEC Program and the Roy J. Carver Charitable Trust  
Abstract: The thermodynamic properties of DDT metabolites were studied via computational methods. The oxidation-reduction potentials of DDD(1,1-dichloro-2,2-(4'-chlorophenyl)ethane) and DDMS(1-chloro-2,2-(4'-chlorophenyl)ethane) were calculated, as was the pK\textsubscript{a} of dicofol (1,1,1-trichloro-2,2-(4'-chlorophenyl)ethanol). Geometries and frequencies were obtained at the B3LYP/6-31G(d) level of theory, energies at the B3LYP/6-311+G(d) level and standard-state aqueous free energies at the
BPW91/6-31G* level using the SM5.42R solvation model. The one and twoelectron oxidation-reduction potentials of DDD were calculated as 0.24 V and 0.071 V respectively. The corresponding values for DDMS were calculated as 0.61 V and 0.025 V. These values agree with observed accumulations in the environment.

45. Tung, Kai-Hao, Kimberly Kurtz, Richard Hsung
Ynamide “survivability”: Studies toward the synthesis and reactivity of functional groups with ynamides
Summer Sponsor: Chemistry - Heisig
Abstract: Chiral ynamides are a useful functional group in organic synthesis. They are capable of undergoing regio- and stereoselective transformations. In addition, they are stable and easily handled. While the Hsung group and others have established the utility of chiral ynamides in organic synthesis, to date, no one has tested the durability or “survivability” of these functional groups. This is the goal of my research project. So far, completed work includes the four-step synthesis of a chiral auxiliary. In addition, I have successfully synthesized an ynamide substrate bearing a protected alcohol. Future work includes deprotection of the alcohol, oxidation of the hydroxyl group, and Wittig olefination as a few examples of reactions that may be carried out in the presence of the ynamides.

46. Turgeon, Ryan, Justin Lytle, Hongwei Yan, Andreas Stein
Syntheses and Characterization of Three-Dimensionally Ordered Macroporous (3DOM) Materials
Summer Sponsor: Chemistry – Lando
Abstract: The fabrication of porous nanomaterials is an important field of materials chemistry with interesting potential applications as gas sensors, catalysts, and electrodes. Honeycomb-like three-dimensionally ordered macroporous (3DOM) nanocrystalline metals and metal oxides and amorphous silicas have been made with interconnected spherical voids. Monodisperse poly(methyl methacrylate) spheres of about 350 nm in diameter were made by a surfactant-free emulsion polymerization and packed via centrifugation into a face-centered cubic array. 3DOM SiO2 and WO3 were fabricated by infiltrating sol-gel precursors into the PMMA template followed by heating to remove the polymer and form solid walls. These products were characterized by SEM and XRD.

47. Vable, Anusha, Dr. Wayland E. Noland
A Synthesis of Indole Dimer Derivatives As Potential Antitubercular Drugs
Summer Sponsor: Chemistry – Lando
Abstract: The purpose of this work is to synthesize compounds having activity against tuberculosis. To make molecules hoped to be active, indole (1) was dimerized (to 2) and two acid groups were attached to the indoline nitrogen to form acyl derivatives 3 and 4. The compounds will be offered to the Southern Research Institute (contractor for NIH) for testing against tuberculosis.
48. van Lengerich, Henrik, Wayland E Noland

*The Synthesis of 2-Nitrosobenzaldehyde and the Structure of the Intermediate Agnotobenzaldehyde*

**Abstract:** The goal of this work is to synthesize crystalline 2-nitrosobenzaldehyde 4 in order to determine if a ring forms between the nitroso and aldehyde groups. The starting material of 2-nitrobenzaldehyde 1 reacts via the intermediates agnotobenzaldehyde 2 and N-acetyl-o-hydroxylaminobenzaldehyde 3 before the product can be formed. Agnotobenzaldehyde 2 was named so by E. Bamberger due to its unknown molecular structure, the secondary objective of this work has become the identification of this structure.

49. Vaubel, Rachel, Dr. Steven Kass

*Synthesis of 1-t-Butyl-2-phenyl-3-(trimethylsilyl)-3-cyanocyclopropene*

**Abstract:** Synthesis of enantiomerically pure 1-t-butyl-2-phenyl-3-(trimethylsilyl)-3-cyanocyclopropene was attempted. Aracemic mixture of 1-t-butyl-2-phenyl-3-
(trimethylsilyl)-3-cyclopropyl-3-carbanol was prepared in five steps starting from ethyl diazoacetate and phenylacetylene. This alcohol was then reacted with several chiral acids to generate diastereomers that could be separated by crystallization or MPLC.

50. **Vera, Eymi, Nadiya Sydorenko, Richard Hsung**  
*Chiral &A,&B-unsaturated iminium approach to stereoselective formal [3+3]cycloaddition reaction synthesis*  
Summer Sponsor: Chemistry - Heisig  
Abstract: Over the past few years the Hsung group has been developing a formal [3+3]cycloaddition strategy, which involves reaction of an a,b-unsaturated iminium ions with 1,3-dicarbonyl equivalents resulting in the formation of complex oxygen and nitrogen heterocycles. However, this protocol was not successful in the formation of single ring systems. The recent use of latent acyclic vinylogous amides (i.e. tetronimides) in a formal [3+3]cycloaddition reaction has provided precursors for the preparation of monocyclic dihydropyridines that could serve as useful templates for synthesis of natural piperidine alkaloids and azasugars. Obtaining proper stereoselectivity of these precursors has become of great importance. This led to examination of an asymmetric variant of this particular formal [3+3]cycloaddition reaction using chiral a,b-unsaturated iminium salts to control the stereochemistry of a newly formed chiral center. We report a highly stereoselective chiral enal approach towards synthesis of latent poly-functionalized piperidines.

51. **Vereen, Danny, Sara Isley, Dr. Lee Penn**  
*Investigation of TiO2 Nanoparticles and their Monodispersity*  
Summer Sponsor: IGERT  
Abstract: The purpose of this study is to develop a synthesis that produces monodisperse TiO₂ particles similar in both size and shape. Monodispersity, a size distribution were the variation is less than 5% rms of the average diameter, is key due to the particles’ ability to form in different sizes and shapes. Once accomplished, the particles impurity level and phase will be examined through the use of X-ray diffraction (XRD). XRD will be used to identify and quantify the phase and crystallite size of the synthesized TiO₂ particles. In addition, TEM will be used to determine particle sizes, growth mechanisms, atomic structure, particle morphologies, crystallography, and defect types and locations.

52. **Verma, Prateek, Victor Sussmann, Bill Brenessel, John Ellis**  
*New Developments in Low-valent Tantalum Chemistry*  
Summer Sponsor: Chemistry – Heisig  
Abstract: Using tris(naphthalene)tantalate(-1) as a precursor, tris(1,3,5,7-cyclooctatetraene)tantalate(-1) has been synthesized via a high yield route. Three different types of reactions of this compound are under examination 1. Reactions with electrophiles. 2. Reactions with oxidants. 3. Reactions with dienophiles. Oxidation of tris(1,3,5,7-cyclooctatetraene)tantalate(-1) with elemental iodine resulted in the formation of the previously unknown neutral bis(1,3,5,7-cyclooctatetraene)iodotantalum. X-ray crystallography studies have shown that the two cyclooctatetraene rings are bound differently to tantalum. Nuclear magnetic resonance studies indicate that this structure is also likely to persist in solution. Reaction of maleic anhydride with tris(1,3,5,7-
cyclooctatetraene)tantalate(-1) resulted in a mixture whose main component is an orange red solid, which crystallized on itself in the reaction flask. This solid has yet to be purified and characterized.

53. **Webber, Carrie, Lian Luo, Marian Stankovich**

*Kinetic resolution of ethyl 2-fluoroctanoate and its application to mechanistic studies of medium-chain acyl-CoA dehydrogenase*

Summer Sponsor: Chemistry – Lando

Abstract: Enantiomerically pure (2S)-2-fluoroctanoyl-CoA and (2R)-2-fluoroctanoyl-CoA, the fluorinated substrate analogs of medium-chain acyl-CoA dehydrogenase (MCAD), are prepared from a racemic mixture of ethyl 2-fluoroctanoate. Enantiomeric purity of ethyl 2-fluoroctanoate is achieved via lipase-catalyzed hydrolysis and checked using chiral HPLC. The isomers are converted to their CoA derivatives and used to probe the mechanism of MCAD through proton exchange experiments in the presence of enzyme. The extractability of an a-proton is measured by $^{19}$F NMR techniques. It was found that the rate constant for the exchange of the a-proton of (2S)-2-fluoroctanoyl-CoA is $2.4 \times 10^{-2}$ s$^{-1}$, while that for (2R)-2-Fluoroctanoyl-CoA is ca. 10 times slower because its a-proton is not properly oriented to be removed by the enzyme.

54. **Weyer, Lynn, Bethany Buck, Gianluigi Veglia**

*Analysis of stannin mutants with organotins by circular dichroism spectroscopy*

Summer Sponsor: Chemistry – Lando

Abstract: Organotin compounds have been used extensively in industry and agriculture and are extremely toxic to mammals, including humans. Stannin (SNN), an 88 amino acid membrane protein, interacts with organotins, subsequently causing neuronal cell apoptosis. Cysteine and histidine residues, especially di-thiols, have been implicated as the primary binding ligands for organotins. SNN contains a di-thiol defined by a CXC motif (C32 and C34), which is the proposed organotin binding site. To test this hypothesis, the cysteine residues of SNN were selectively mutated to alanine residues using site-directed mutagenesis. The SNN cysteine mutants were titrated with various organotins, analyzed by circular dichroism (CD) spectroscopy, and compared with the data for wild type SNN.

55. **Williams, Richard, R. Mukherjee, T. Renault, J. Hafiz, X. Wang, S.L. Girshick**

*Substrate Temperature Automation and Control for the Hypersonic Plasma Particle Deposition Process*

Summer Sponsor: IGERT

Abstract: The Hypersonic Plasma Particle Deposition experimental apparatus currently has a manual temperature control for the high rate film deposition substrate. To control the temperature of the first substrate the experimental apparatus operator must vary the flow rates of the Helium and the Argon gases on the backside of the substrate. The objective is to automate this temperature control process using LabVIEW. This will enable the user to input a desired temperature into the LabVIEW virtual instrument. The LabVIEW virtual instrument will use the American Reliance PD 8-7 power supply and the Luxtron Accufiber Model 10 Thermometer to control the release of the Helium and the Argon gases on the backside of the substrate.
56. Wruck, Amanda, Dwight Stoll, Peter Carr

**Thermo-Mechanical Stability of HPLC columns**

Summer Sponsor: Chemistry - Lando

Abstract: Liquid chromatography is a very useful analytical tool, but sometimes it is extremely difficult, or impossible to fully resolve all the components in a complex mixture. That is why the use of two-dimensional chromatography is becoming important especially in bioanalytical and environmental chemistry. In order for 2D-LC to become more widely adopted the run times must be reduced from hours and days to minutes. HPLC can be speed up markedly by using higher temperatures. However, creating a thermo-mechanical stability is not easy. In this work, the column packing parameters were explored; namely sonication, solvents, wetting, and the use of polymers, in an attempt to provide further knowledge about gaining thermal stability among known stationary phases.

57. Zito, Abbigail, Jan-Uwe Rohde, Lawrence Que Jr.

**C-H and O-H bond activation by biomimetic oxoiron(IV) complexes**

Summer Sponsor: Chemistry – Lando

Abstract: A mononuclear nonheme complex with a terminal Fe\textsuperscript{IV}=O unit, [Fe\textsuperscript{IV}O(TMC)(NCMe)]\textsuperscript{2+}, was spectroscopically and structurally characterized recently. Such high-valent species are often proposed as key oxidants in the catalytic cycles of nonheme monoiron enzymes. The oxygen transfer capability of this synthetic intermediate was demonstrated in reactions with triphenylphosphine and thioanisole. We have now found by UV/VIS reactivity studies and subsequent product analysis by GC and GC-MS, that the intermediate can perform H-abstraction from both O-H (di- and tri-tert-butylphenols) and C-H bonds (dihydraanthracene), [Fe\textsuperscript{IV}(O)(TMC)(NCMe)]\textsuperscript{2+} can be converted with one equivalent of NBu\textsubscript{4}Cl to [Fe\textsuperscript{IV}(O)(TMC)(Cl)]\textsuperscript{+}. The decay of this species in the absence of substrates and presence of dihydroanthracene is greatly increased compared to [Fe\textsuperscript{IV}(O)(TMC)(NCMe)]\textsuperscript{2+} with comparable yields.